CONTRIBUTION TO THE HEAT INTEGRATION OF BATCH PROCESSES (WITH OR WITHOUT HEAT STORAGE)

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May this work, in some way, contribute to the design and operation of more sustainable and actually useful batch processes - this is my earnest wish and reward !

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ABSTRACT

This work addresses the indirect heat integration (i.e. resorting to intermediate heat storage) and the direct heat integration (i.e. heat exchanges between coexisting process streams) of batch processes. Tools and methods for the targeting of these two limiting cases of heat integration are proposed, and completed by the development and the application of an automatic design & optimization methodology using the *Struggle* genetic algorithm (*GA*). A brewery process is used to demonstrate the feasibility and the practical relevance of the proposed indirect heat integration models. The fluctuations of the process schedule and their effects on the optimal solutions are not modelled (the indirect heat integration is known to feature an inherently low sensitivity). The rescheduling opportunities are not searched for.

For the indirect heat integration, fixed temperature/variable mass inventory heat storage units (*HSUs*) are applied. Two models of indirect heat recovery schemes (*IHRSs*) are proposed : one based on a closed heat storage system, another built around an open storage system suitable e.g. for food and beverages industries. The inequality constraints of the *IHRS* models are automatically met owing to an appropriate definition of the decision variables managed by the *GA*. A rough pre-adjustment of the mass balance equality constraints on *HSUs* is achieved by a preliminary stage of heat recovery (*HR*) maximization before actually minimizing the total batch costs (*TBCs*). Optimization runs and theoretical considerations on the generation & replacement strategy of *Struggle* demonstrate that the structural and the parametric variables cannot be efficiently optimized within a single level, resulting in a two-levels optimization scheme. The automatically designed closed storage *IHRS* solutions for the brewing process are as good as the solutions obtained by another author using a combinatorial method followed by a post-optimization stage. The open storage *IHRS* is 13 % cheaper while the *HR* increases by 12 %. Optimizing the *IHRS* on a one-week period (including the non-periodic start-up & shut-down phases) results in an even more realistic solution, featuring a significantly different trade-off between energy, *HSU* capacities and *HEX* areas.

A *GA* based, two-levels optimization scheme is proposed for the design of direct batch heat exchanger networks (*HENs*). The *HEN* structures, managed by the upper-level *GA*, do not include stream splitting. The re-use of *HEX* units across time slices is a key issue and a methodology to specify the actually possible structural changes by repipe or resequence is proposed, accounting for the thermo-physical compatibility, chemical compatibility, and process schedule constraints. The optimum operation of an existing *HEN* during each time slice has been analysed and a sound solution procedure is proposed.

RÉSUMÉ

Ce travail porte sur l'intégration énergétique indirecte (par stockage intermédiaire de chaleur) et directe (par échanges de chaleur entre flux coexistant dans le temps) de procédés discontinus. Des outils et des méthodes sont proposés pour le *targeting* de ces deux cas limites d'intégration énergétique, et sont complétés par le développement et l'application d'une méthodologie de conception automatique et d'optimisation utilisant l'algorithme génétique (*AG*) *Struggle*. Un procédé de brasserie est utilisé pour démontrer la faisabilité et la pertinence pratique des modèles d'intégration indirecte proposés. Les fluctuations du *schedule* des flux et leurs effets sur les solutions optimales ne sont pas explicitement modélisés (l'intégration indirecte y est naturellement peu sensible). Le *rescheduling* du procédé n'est pas considéré.

Pour l'intégration indirecte, des stockages de chaleur travaillant à température fixe et masse variable sont utilisés. Deux modèles de réseaux d'intégration énergétique indirecte (*RIEI*) sont proposés : l'un basé sur un système de stockage fermé, l'autre construit autour d'un système de stockage ouvert adéquat par ex. pour les industries agro-alimentaires et des boissons. Les contraintes inégalités des modèles *RIEI* sont automatiquement satisfaites grâce à une définition judicieuse des variables de décision gérées par l'*AG*. Un ajustement grossier des contraintes égalité des bilans massiques des stockages est obtenu par une étape préliminaire de maximisation de la récupération de chaleur (*RC*), avant la minimisation des coûts totaux par batch (*CTBs*). Les optimisations et des réflexions théoriques sur la stratégie de génération et de remplacement de *Struggle* démontrent que les variables de structure et les variables continues ne peuvent pas être efficacement optimisées sur un seul niveau, nécessitant une optimisation sur deux niveaux. Les *RIEI* à stockage fermé du procédé de brassage conçus et optimisés par *AG* sont quasi-identiques à ceux développés par un autre auteur à l'aide d'une méthode combinatoire suivie d'une optimisation paramétrique. Le *RIEI* à stockage ouvert est 13 % meilleur marché pour une *RC* accrue de 12 %. L'optimisation sur une semaine (incluant les phases apériodiques initiale et finale) conduit à un *RIEI* encore plus réaliste, résultant d'un compromis assez différent entre énergie, volume de stockage et surface d'échange.

Un schéma détaillé d'optimisation sur deux niveaux par *AG* est proposé pour l'intégration directe. Les structures de réseaux sont gérées au niveau supérieur (sans dédoublement de flux). Le partage d'échangeurs est un problème-clé et une méthodologie pour spécifier les modifications structurelles possibles par *resequence* ou *repipe* est proposée. Le fonctionnement optimal, durant chaque tranche de temps, d'un réseau existant a été analysé et une méthode adéquate est proposée.

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NOMENCLATURE

III.1 Roman Symbols

In the table below, symbols representing variables are written in *italic* style, while abbreviations are written in regular style.

Symbol	Units	Meaning	Reference
a	[1/year] [-]	• annualization factor (annual amortization factor or capital costs pay-off factor) • activity factor of a stream during a time slice (active if a =1, otherwise a =0)	Sub-section 3.3.1 Sub-section 3.4.4 Sub-section 5.4.3
a_B	[1/batch]	pay-off factor per batch	Sub-section 3.3.1
A	[m^2]	heat exchange area	
AG		*algorithme génétique*	
A_{MAX}	[m^2]	maximum heat exchange area to be installed (in a MBC targeting context)	Appendix G
A_{MIN}	[m^2]	• smallest heat exchange area which cost has to be correctly modelized • minimum heat exchange area to be installed (in a MBC targeting context)	Sub-section 5.2.7 Appendix G
A_r	[m^2]	reference heat exchange area (in a HEX cost function)	Appendix A
BC		batch cycle	

Table III-1 List of roman symbols.

Symbol	Units	Meaning	Reference
BCC		batch cascade curve	Sub-section 2.2.8
BDV		binary decision variable	
BUC		batch utility curve	Sub-section 2.2.8
c	[ecu/batch]	• unit costs • reduced costs (costs per batch)	
c_P	[kJ/kg°C]	specific heat	
C	[ecu]	costs	
CA		cascade analysis	Sub-section 2.2.2
CC	[ecu/batch]	cleaning costs	Sub-section 8.6.3
CF		cost function	Sub-section 8.6.3
CHF		swiss franc	
$CMBB$	[kg]	cumulated mass before balance	Sub-section 5.3.5
$CMBUB$	[kg]	cumulated mass before utility balance	Sub-section 5.3.5
CN		cold process stream nb. N (short name)	
CoT		cut-off temperature	Sub-section 3.4.5 Section 6.1
CP	[kW/°C]	heat capacity flowrate ($= \dot{M}c_P$)	Sub-section 3.2.1
CPS		cold process stream	
CPU		central processing unit	
CS		consistent set	Section 8.4
CTBs		*coûts totaux par batch*	
CU		cold utility	
CUN		cold utility number N (short name)	
C_0	[ecu]	fixed capital cost	Appendix A
C_v	[ecu]	capital cost of a valve	Sub-section 8.6.3

Table III-1 List of roman symbols.

Symbol	Units	Meaning	Reference
$D(X_a, X_b)$		distance function (between individuals X_a and X_b)	Sub-section 5.2.8
DF		distance function	Section 6.1
DKK		danish crowns	
DOF		degree of freedom	
ecu		monetary unit (may be CHF, DKK, etc.)	
EI		enthalpy interval	Section 7.4
EIN		enthalpy interval nb. N (short name)	Section 7.4
EP-N		example process number N	Appendix A
FTVM		fixed temperature / variable mass (operating mode of heat storage units)	Sub-section 3.4.2
GA		genetic algorithm	Section 3.7
GCC	[kJ/batch]	grand composite curve	Sub-section 5.3.5
$GCCWP$	[kJ/batch]	grand composite curve without pockets	Sub-section 5.3.5
h	[W/m^2°C]	heat transfer film coefficient	
HEN		heat exchanger network	
HENS		heat exchanger network synthesis	
HEX		heat exchanger	
HN		hot process stream nb. N (short name)	
HR	[kWh/batch]	heat recovery	Sub-section 3.3.2
HPS		hot process stream	
HSU		heat storage unit	Section 3.4
HSUN		heat storage unit number N (short name)	
HU		hot utility	
HUN		hot utility number N (short name)	
I	[-]	number of hot process streams	

Table III-1 List of roman symbols.

Symbol	Units	Meaning	Reference
IHRS		indirect heat recovery scheme	
IR	[-]	interest rate	Sub-section 3.3.1
DV		decision variables	
J	[-]	number of cold process streams	
k_{max}		largest HSU index ensuring feasible heat exchange with given hot process stream	Sub-section 5.2.6
k_{min}		lowest HSU index ensuring feasible heat exchange with given cold process stream	Sub-section 5.2.6
K	[-]	number of heat storage units	Section 5.2
L	[-]	number of time slices in a batch cycle	
LP		linear programming	
LSTP		limiting supply temperature profile	
m	[-]	cost exponent factor	
M	[kg] [-]	• mass • number of matches • number of hot utilities	 Chapter 8 Chapter 7
$\dot{M}$	[kg/s]	mass flowrate	
Max		maximum function	
MBB	[kg]	mass before balance (before mixing)	Sub-section 5.3.5
MBC		multiple base case	Sub-section 2.2.6
$MBUB$	[kg]	mass before utility balance (after mixing)	Sub-section 5.3.5
Mdl		model	Section 6.1
MER		maximum energy recovery	
MHX		maximum heat exchange	
MILP		mixed-integer linear programming	
Min		minimum function	
MINLP		mixed-integer nonlinear programming	

Table III-1 List of roman symbols.

Symbol	Units	Meaning	Reference
MP		mathematical programming	
N	[-]	• number of enthalpy intervals (in a MBC design context) • number of cold utilities • number (with subscript)	Section 7.4 Chapter 7
NLP		nonlinear programming	
$NTCC$	[-]	number of temperature controlled connections	Sub-section 5.3.4
NPV	[ecu]	net present value	Sub-section 3.3.1
N_{CS}	[-]	number of consistent sets of slice-wise match structures	Section 8.4
N_{BPY}	[1/year]	number of batches per year	Sub-section 3.3.1
N_{Gen}	[-]	number of generations	Section 3.7
N_{Pop}	[-]	number of individuals in population	Section 3.7
N_{SMS}	[-]	number of possible slice-wise match structures	Section 8.4
OF		objective function	
OMS		overall match structure	Chapter 8
OPB		overall plant bottleneck	Sub-section 2.2.4
OS		optimization scheme (single or two levels)	Section 6.1
OV		Omnium Verfahren	Sub-section 2.2.7
P	[-]	number of process streams ($P = I + J$)	
PA		Pinch Analysis	
PM		Permutation Method	Sub-section 2.2.9
PO		post-optimization (in the context of the PM)	Sub-section 2.2.9
POP	[year]	pay-off period	Sub-section 3.3.1

Table III-1 List of roman symbols.

Symbol	Units	Meaning	Reference
PW		process water	Section 5.4
Q	[kWh], [kJ]	heat	
$\dot{Q}$	[kW]	heat rate (heat duty)	
RA	[m^2]	area reduction	Sub-section 7.4.4
RB	[-]	relative benefit	Appendix B
RC		*récupération de chaleur*	
RIEI		*réseau d'intégration énergétique indirecte*	
$RMFD$	[-]	relative mass flowrate deviation	Sub-section 5.3.4
SSs		storage sub-system	Sub-section 3.4.3
SSsN		storage sub-system nb. N (short name)	
Sty		strategy	Section 6.1
SMS		slice-wise match structure	Chapter 8
t	[min]	time	
t_{end}	[min]	stop time of a batch cycle	
$t_{initial}$	[min]	start time of a batch cycle	
t_l	[min]	time point (stop time of time slice l, start time of time slice $l+1$)	
t_{start}	[min]	start time of a stream	
t_{stop}	[min]	stop time of a stream	
T	[°C]	temperature	
T_{in}	[°C]	• supply temperature (of a utility) • inlet temperature in a heat exchanger	
T_{out}	[°C]	• return temperature (of a utility) • outlet temperature from a heat exchanger	
TR	[-]	temperature range	Appendix E
T_S	[°C]	supply temperature (of a process stream)	Sub-section 3.2.1

Table III-1 List of roman symbols.

Symbol	Units	Meaning	Reference
T_T	[°C]	target temperature (of a process stream)	Sub-section 3.2.1
$TACs$	[ecu/year]	total annual costs	
TAM		time average model	Sub-section 2.2.1
$TBCs$	[ecu/batch]	total batch costs (reduced costs)	Sub-section 3.3.1 Sub-section 8.6.3
TCC	[ecu]	temperature control costs	
TDF		temperature driving force	
TEM		time event model	Sub-section 2.2.5
TS		time slice	
TSN		time slice number N (short name)	
TSM		time slice model	Sub-section 2.2.3
V	[m^3] [-]	• volume (volumic capacity) • number of valves	Sub-section 3.4.4 Sub-section 8.6.3
V_r	[m^3]	reference volume (in a HSU cost function)	Appendix A
w	[-]	weight factor (in distance function)	Appendix D
x	[-]	• dimensionless continuous decision variable manipulated by GA • binary variable (in MBC context)	Sub-section 5.2.4 Appendix G
$\boldsymbol{X}$		vector of continuous decision variables of one individual	Sub-section 5.5.2
X		HEX match (pair of streams for heat exchange)	
y		binary variable to control connections to HSUs	Appendix E
$\boldsymbol{Y}$		vector of discontinuous decision variables of one individual	Sub-section 5.5.2 Section 8.6

Table III-1 List of roman symbols.

III.2 Greek Symbols

Symbol	Units	Meaning	Reference
α	[-]	scatter factor (Struggle GA context)	Sub-section 3.7.3
$\Delta\dot{H}$	[kW]	enthalpy change	
ΔM	[kg]	mass difference (variation)	
Δt	[h], [min]	time difference (duration)	
ΔT	[°C]	temperature difference	
ΔT_{Chen}	[°C]	approximation of the ΔT_{LM} according to Chen J.J.J.	Chen, 1987
ΔT_{min}	[°C]	minimum temperature difference at the pinch point	
ΔT_{LM}	[°C]	logarithmic mean temperature difference	
ρ	[kg/m^3]	density (specific mass)	

Table III-2 List of greek symbols.

III.3 Subscripts & Indices

Symbol	Meaning	Reference
AB	after balance (in a HSU mass balancing context)	
AU	additional utility	Sub-section 5.4.4
BB	before balance (in a HSU mass balancing context)	Sub-section 5.3.5 Sub-section 5.4.4
BC	batch cycle	
BU	balancing utility	Sub-section 5.4.4
cap	capital (costs)	Sub-section 3.3.1

Table III-3 List of subscripts and indices.

Symbol	Meaning	Reference
$circ$	circuit (inlet-outlet)	Appendix A
cu, CU	cold utility	
cv	conventional design (in a MBC design context)	Sub-section 7.4.4
cs	index of consistent set (cs = 1 .. N_{CS})	Section 8.4
C	cold streams	Sub-section 3.3.2
hu, HU	hot utility	
H	hot streams	Sub-section 3.3.2
HR	heat recovery (internal, process to process HEXs)	
i	• index of hot process streams (i = 1 .. I) • index of capital cost contribution (in TBCs definition)	Sub-section 3.3.1
j	• index of cold process streams (j = 1 .. J) • index of operational cost contribution (in TBCs definition)	Sub-section 3.3.1
k	• index of heat storage units (k = 1 .. K) • index of storage sub-systems (k = 1 .. $K-1$)	Chapter 5
l	index of time slices (l = 1 .. L)	
lim	limit	
ll	lower level	
lb	lower boundary	
m	• index of hot utilities (m = 1 .. M) • index of match	Chapter 8
max, MAX	largest value of a variable	
min, MIN	smallest value of a variable	
M	mixing (of heat storage fluid)	Sub-section 5.3.5 Sub-section 5.4.4
MB	mass balance (in a HSU mass balancing context)	
n	• index of cold utilities (n = 1 .. N) • index of enthalpy intervals (n = 1 .. N) (in a MBC design context)	Chapter 7

Table III-3 List of subscripts and indices.

Symbol	Meaning	Reference
neg	negative (outgoing mass flowrate)	Sub-section 5.4.4
n_{gen}	index of generation (n_{gen} = 1 .. N_{Gen})	
$oper$	operational (costs)	Sub-section 3.3.1
opt	optimal value	
O	overall (subscript in a direct batch HEN design context)	Chapter 8
p	index of process streams (p = 1 .. P)	
pc	process-cold utility (subscript of HEX match)	
ph	process-hot utility (subscript of HEX match)	
pos	positive (incoming mass flowrate)	Sub-section 5.4.4
pp	process-to-process (subscript of HEX match)	
ps	process-storage (subscript of HEX match)	
pu	process-utility (subscript of HEX match)	
Pro	process (pinch)	
PW	process water stream	Chapter 5
r	reference value (for HEX and HSU cost functions)	
rs	resequence design (in a MBC design context)	Sub-section 7.4.3
sc	storage-cold utility (subscript of HEX match)	
seg	segment (of streams)	
sh	storage-hot utility (subscript of HEX match)	
sms	index of slice-wise match structure (sms = 1 .. N_{SMS})	Section 8.4
su	storage-utility (subscript of HEX match)	
st	index of heat storage types (st = 1 .. ST)	
S	• heat storage (in a HSU cost function context) • supply temperature of a process stream (in T_S) • heat storage	 Sub-section 3.3.2
SF	storage fluid (storage medium)	

Table III-3 List of subscripts and indices.

Symbol	Meaning	Reference
Sto	storage (pinch)	
tot	total	
T	• target value (calculated by targeting) • target temperature of a process stream (in T_T)	
u	index of utilities (u = 1 .. U)	
ul	upper level	
ub	upper boundary	
xt	index of heat exchanger types (xt = 1 .. XT)	
X	heat exchanger (in a HEX cost function context)	

Table III-3 List of subscripts and indices.

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Part I

CONTEXT & PROBLEM STATEMENT

Chapter 1

INTRODUCTION

This Chapter introduces batch processing and places the related heat integration problems within the wider context of the design and operational issues of batch plants. The objectives and scope of this work are described and an outline is provided.

1.1 What is Batch Processing ?

In continuous processes, streams exist and flow continuously through the equipment units of the plant; the properties (mass flow, temperature, concentration, etc.) at any point of the plant are independent of time. Hence time may also be left out when analysing the heat integration - except for the profitability, which strongly depends on the overall operation time in a year.

In fact, the continuous assumption for most processes is actually an approximation of the reality: not only operational conditions are likely to slightly change over time, but any continuous process has to be started and shut down (for maintenance, etc.). During these phases, the process operates in a discontinuous manner, e.g. the properties evolve and streams do not exist permanently [1].

Processes also exist which are essentially discontinuous in nature. This is the case of industrial batch production processes; but discontinuous (or rather non-permanent) operation may also be found in power, combined heat and power, and district heating plants, in heating, ventilating & air conditioning (*HVAC*) in buildings, etc. Discontinuous heat integration problems may also be found in industries operating

1. With respect to the heat integration, the assumption of continuous processes obviously holds as long as the discontinuous phases are much shorter than the continuous operation phase.

several semi-continuous processes or steps (e.g. pasteurization) asynchronously throughout the day (e.g dairies and other food processing industries).

Batch processes are discontinuous processes in which heat, mass, temperature and other properties may vary (either in a discrete or a continuous manner) over time. The product of batch plants is not delivered continuously, but in discrete quantities (batches).

Batch processing can be illustrated by the single-product batch plant (*Gremouti*, 1991) corresponding to the flowsheet represented in **Figure 1-1**. The production

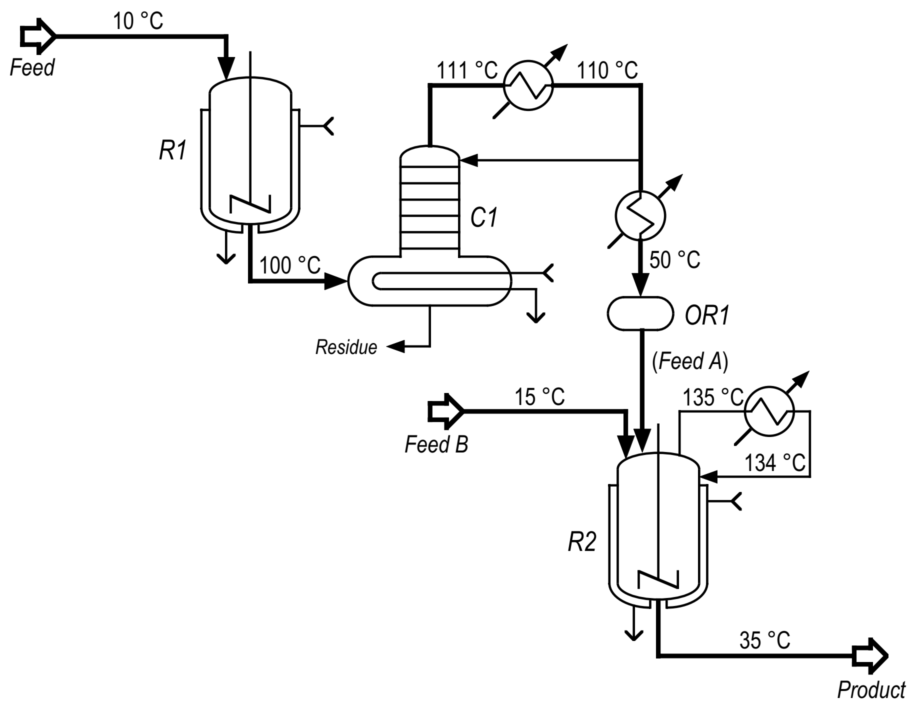

Figure 1-1 Flowsheet of a single-product batch plant (*Gremouti*, 1991).

line comprises two batch reactors and a batch distillation column. The production recipe requires the following steps. Raw materials at 10 *°C* are charged into the stirred jacketed reactor *R1* and heated to 60 *°C*, the temperature at which they react. The reaction is slightly exothermic and the temperature rises to 100 *°C*. The product from reactor *R1* is discharged hot in the batch distillation column *C1*. The column operates at 120 *°C*. The distillate is subcooled from 110 *°C* to 50 *°C* and accumulated in the overhead receiver *OR1*. The product from the receiver (*Feed A* at 50 *°C*) and other materials (*Feed B* at 15 *°C*) are charged into reactor *R2* equipped with a reflux condenser. The mixture is then heated to approximately 95 *°C* to start the highly exothermic reaction and the solvent boils-off at 135 *°C*. Once the reaction is completed, the product is cooled from 140 °*C* to 35 °*C* and discharged from the vessel to be treated in another section of the plant.

The tasks achieved by the main pieces of equipment of the plant (*R1*, *C1*, *R2*) as a function of time are represented on the *Gantt Chart* of **Figure 1-2**. The overall time

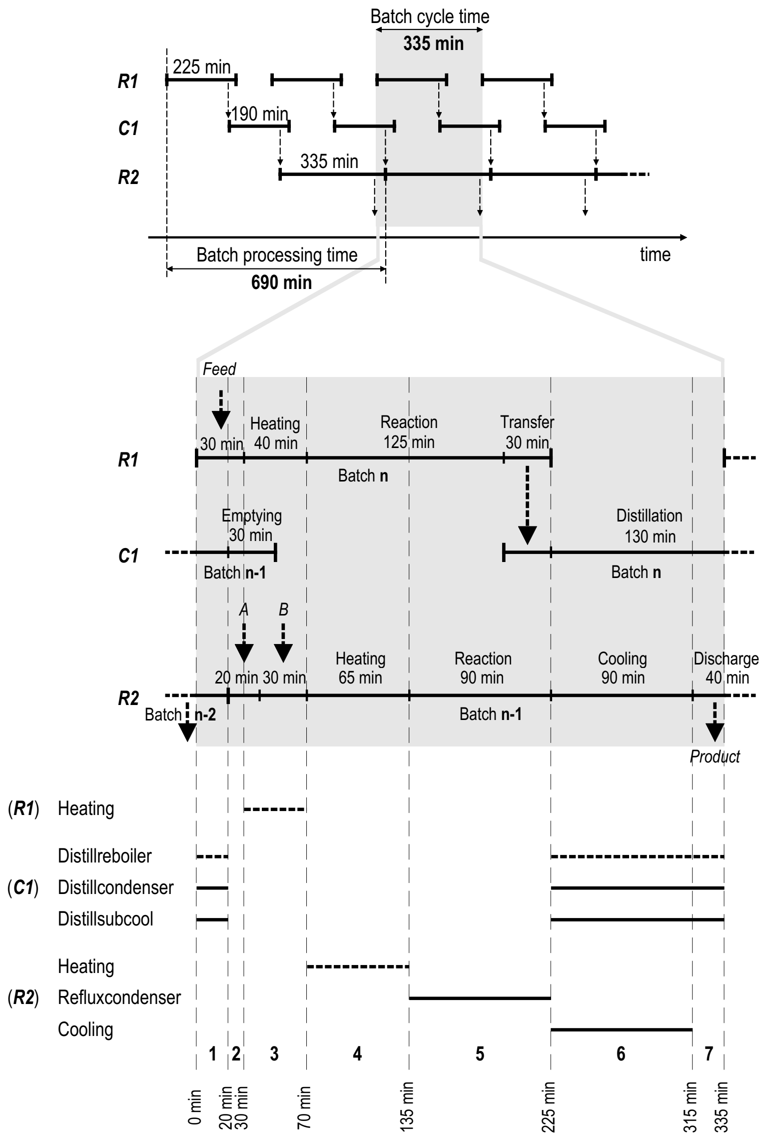

Figure 1-2 Gantt Chart corresponding to the flowsheet of Figure 1-1.

needed to process one batch of product (i.e. to achieve all the operations described above) is called the *batch processing time* and amounts in this case to 690 *min*. To maximize the production capacity of the plant, a new batch may be started before the processing of the previous batch is completed, provided that the required equipment units are available when needed. The time separating the start of two successive batches is called the *batch cycle time*. The smallest batch cycle time is determined by the processing unit featuring the longest cycle time, here *R2*. Observing that the cycle times of *R1* and *C1* are significantly shorter, *R2* is clearly the time bottleneck which limits the production capacity of the plant.

The hot and cold process streams within a batch cycle time are represented in the lower part of Figure 1-2. It can be seen that the discontinuous existences of the streams define so-called *time slices* (here 7 time slices) within which the set of streams are assumed not to change. In other terms, from a heat integration point of view, the decomposition into time slices makes a discontinuous process like a sequence of continuous sub-processes. But, unlike continuous processes, the heat transfer from hot to cold streams is significantly more tricky: heat may be available from hot streams but not simultaneously needed by cold streams, or reversely, or more generally heat supply and heat needs may be largely out of balance in given time slices. Time is therefore an essential dimension of the problem which restricts the feasibility of heat exchanges.

Batch production plants are roughly categorized into *single-product*, *multi-product* and *multi-purpose* plants. The batch plant described above is called a single-product plant if the equipment topology is fixed and only one product is to be produced. Dedicated plants are used in case of large production volumes needed for e.g. fermentation products (beer, etc.).

In a multi-product plant (also called *flowshop* plants), all products follow essentially the same path through the processing equipment units. The similarity of the products and hence the similarity of their processing path is high.

In a multi-purpose plant (also called *jobshop* plants), there is no common pattern for the processing route and use of equipment units. A variety of dissimilar products, each with its own distinct processing sequence is produced.

Depending on the category of batch plant being considered, the main issues may significant differ.

1.2 Why Batch Processing ?

Batch processing is used to manufacture a large variety of products: from the high volume production of beer, food, agricultural chemicals to low tonnage, high added value chemicals and biochemical products, polymers, resins and pigments, pharmaceutical products [2], etc.

Low production volumes generally preclude continuous production processes from being an economic alternative. But the production volume is not the only selection criteria and other factors favour batch processing modes. Batch plants are usually simpler and more flexible than continuous plants, so that a satisfactory product can be produced even when a certain level of processing uncertainty remains. Batch processes are easily scaled up from bench scale experiments and provide opportunities for further adjustment and improvement in production; in a rapidly changing environment, with the ever shorter or insecure lifetime of new products, batch processes allow for a shorter time to the market and an easier re-use of equipment units. Batch processing can better meet the specific customer demands, as well as the individual quality control and traceability of the product (e.g. isolation of spoiled/deficient pharma product batches). Processes requiring long residence times are difficult to achieve in continuous operation. Process with feedstock and/ or product which cannot be handled efficiently in a continuous manner such as solids and highly viscous materials are usually carried out in batch facilities. Batch production is better suited to processes requiring complex synthesis steps and closed control of the process conditions. This production method is attractive for processes involving multiple grades, variability in the feed materials, and product with unusual specifications or requiring subjective test such as the taste in the food industry.

1.3 Issues in Batch Processing

A simple batch process has been described in Section 1.1. Issues with respect to the optimal design of this plant have been overlooked, for instance : given a recipe and a likely annual production, how should the plant be designed and the equipment units be sized ? Could the recipe be more cost-effectively achieved using another set of equipment units differently assigned to the tasks (heating, mixing, react, cooling, crystallizing, hold, etc.) of the recipe, involving e.g. the use of dedicated equipment units best suited for individual tasks versus general purpose equipment units meeting the most demanding conditions of one task but wasting capital when used for less demanding tasks ? Facing an increase of production demand, how could the plant be best debottlenecked (e.g. doubling the equipment which is the time

2. The value of a single batch of product may be so high that in case of problems priority is given to saving the batch, even if the reactor equipment is lost and must be replaced ...

bottleneck to work out-of-phase, revisiting the equipment assignment to tasks to better use the available equipment units, etc.) ?

In the context of multi-product and multi-purpose plants, the above issues must be completed by additional considerations, with respect to the design as well as the operation of the plant. Note that equipment units are often standardized (i.e. available in a limited number of sizes and configurations). Additional design issues include : knowing the product recipes, the cycle time and the mass to be processed in each equipment, should several identical equipment units be installed in parallel (either working out-of-phase to remove a time bottleneck, or working in-phase to remove a capacity bottleneck) to suit the various recipes ? Should a temporary storage of intermediate products be used to adapt (decouple) the operation of equipment units featuring short cycle times to an equipment featuring a much longer cycle time ? With respect to the operation of the plant : how to schedule the production of the different products; in case of widely different cycle time of the processing units, does a simultaneous or a mixed sequence of production (mixed production campaign) provide a production capacity increase over a sequence of separated production campaigns (single product campaign) ? Consider product change over, the loss of valuable product and the cleaning issues, etc.

These questions are all about minimizing the capital costs of the plant while meeting the production requirements of the different recipes (design problem), and maximizing the utilization of the equipment units subject to the constraints of delivering the required quantities on time (operational constraints). They have been the subject of numerous contributions in the late 1980s and in the 1990s, in particular using mathematical programming solutions approaches (refer to e.g. *Reklaitis*, 1989; *Voudouris* & *Grossmann*, 1992; *Rippin*, 1993; *Shah* et al., 1993; *Kondili* et al., 1993, *Ravemark*, 1995).

In order to maximize the profit, the maximization of process yield and the product quality are of paramount importance. Since the process understanding & modelization is often limited when starting production, a significant potential for improvement and continuous adaptation/correction to varying conditions of the recipe by systematic measurements and optimization can be expected (see e.g. *Verwater-Lukszo*, 1996).

The above non-exhaustive list of issues is only given to put the heat integration issues summarized in Section 1.4 into the broader perspective of batch plant design and operation. These problems are time dependent and feature a highly combinatorial nature; a simultaneous consideration of all aspects is not possible at present and the problems are tackled according to a hierarchical decomposition. But decisions at the lower levels may affect decisions previously made at the upper levels, so that iterations are needed.

1.4 Significance of Heat Integration

In high volume, consumer products processes like brewing, the energy costs may amount to several percent of the production costs, hence to a large proportion of the profit margin. In the case of high added value products, the energy costs are actually quite small or even negligible compared to the profit margin. In the latter case, the primary objectives of operators are the process yield, the quality of product, the production on time and flexibility, while energy consumption is not seriously considered. In several chemical batch processes (e.g. pharmaceuticals, pigments), owing to the existence of large amounts of used solvents and volatile organic compounds to incinerate, there is an excess of available heat. Nevertheless, profitable energy saving measures may be realized when the capacity of the plant needs to be debottlenecked (*Gremouti*, 1991).

Owing to the above facts, the energy saving potential is large and has been estimated to be of the order of 40 %, i.e. 540 million ECU/year within the European Community (*Kleme*s et al., 1994). However, heat integration techniques to harvest this potential must not result in adverse effects on the operational flexibility of batch plants.

Considering Figure 1-2 again, it appears that heat integration may be achieved by :

1. direct heat exchanges between streams which coexist in the same time slices (*direct heat integration*) (heat exchanges are only potentially feasible during time slice 6 between product cooling and the reboiler stream);
2. indirect heat exchanges resorting to intermediate heat storage (*indirect heat integration*);
3. a mix of the two modes above (referred to as *mixed direct-indirect heat integration*).

The indirect mode implies higher capital costs, so that process *rescheduling* is often considered to avoid them by increasing the potential of direct heat exchanges. Similarly, heat integration of multi-product and multi-purpose plants is often focused on the scheduling of batch operations accounting for direct heat exchanges opportunities.

However, the indirect mode of heat integration offers the essential benefit of preserving the operational flexibility of the plant - a key criteria often encountered in practice - reason why it will take a major part of this work.

1.5 Objectives & Scope of the Work

This work aimed essentially at the development of grassroot design [3] methodologies for :

1. an automatic design & optimization method for the indirect heat integration of batch processes (i.e. resorting to intermediate heat storage);
2. an automatic design & optimization method for the direct heat integration of batch processes (i.e. by direct heat exchanges, considering the possible re-use of heat exchanger units across time slices).

The above two objectives are part of the middle term objective of addressing the more general problem of mixed direct-indirect heat integration. As stated above, this work focuses on the development of synthesis methods for indirect and for direct heat integration, and does not aim at developing guidelines for choosing the most appropriate mode of heat integration based on characteristics of the considered process [4].

One key requirement set for this work is to propose methods relevant for engineering practice. The solutions delivered by the selected optimization approach should not be obtained at the expense of severe simplifications of the problem [5]; the optimization approach has to be robust, i.e. the quality of the delivered solutions should not be dependent on particular features of the problem. With this in mind, an optimization based on genetic algorithms (*GA*) has been chosen.

Even if an automatic design & optimization can be achieved without preliminary insight and user interaction, the development of targeting tools to provide useful insight into and understanding of the above two heat integration modes has been identified as a side objective of this work. Note that in traditional *Pinch Analysis*, targeting consisted in calculating energy targets before design, based on the

3. The retrofit design problem has neither been addressed nor analysed in this work.
4. This issue is discussed in Chapter 2 and reasons to apply indirect heat integration as the *by-default* mode of heat integration are presented in Section 3.4.
5. Of course, the considered processes always result from some simplifications. Nevertheless, the solution approach should not be restricted, for instance, by the type of cost functions (e.g. defined in several ranges) or by the costs contributions actually accounted for; practical constraints should be given due consideration.

composite curves of the process and resorting to few simplifying assumptions. Then targeting has evolved to determine more targets (capital and energy costs, heat exchange area, number of units) ahead of any practical design; this is sometimes referred to as *supertargeting* (*Linnhoff*, 1994). In this work, the meaning and scope of targeting is enlarged and means additionally a preliminary stage providing insight into key high-level issues and to make decisions for the synthesis stage (e.g. regarding structural issues, refer to Section 4.3).

The proposed methods complement or improve methods developed to date by others (*Jones*, 1991; *Sadr-Kazemi* & *Polley*, 1996; *Mikkelsen*, 1998; *Uhlenbruck* et al., 2000).

Within this work, the two limiting cases of indirect and of direct heat integration are addressed assuming a fixed schedule of the processes; rescheduling opportunities (e.g. to increase the potential of direct heat integration) are not particularly searched for, but a constant preoccupation was to generate solutions featuring a low sensitivity to the likely schedule fluctuations. The tools developed in this work are in first priority suitable to address heat integration design problems of single-product batch plants (a brewery is a typical example). By extension however, the heat integration of multi-product batch plants and of any discontinuous problem may be addressed, provided that the schedule can be considered as reasonably fixed [6].

1.6 Outline

This document is made up of the following parts.

Part I introduces the problem and its context. **Chapter 2** provides an overview of the state-of-the-art contributions related to the present work. The general issues of indirect and of direct heat integration, guidelines for data extraction and process simplifications, as well as a short introduction to genetic algorithm (*GA*) based optimization are presented in **Chapter 3**.

Part II is exclusively concerned with indirect heat integration. **Chapter 4** illustrates the tools and methods based on graphical representations proposed for targeting purposes. The developed models of indirect heat recovery schemes and the *GA* based optimization strategy are described in **Chapter 5**. In **Chapter 6**, the results

6. Note that indirect heat integration solutions can inherently accommodate schedule variations, lessening the significance of the assumption of a fixed schedule.

obtained using the targeting methods of Chapter 4 and/or the *GA* based optimization approach of Chapter 5 are discussed and conclusions pertaining to indirect heat integration are drawn.

Part III addresses the direct heat integration problem. **Chapter 7** summarizes the multiple base case methodology, developed by *Jones* (1991) and adapted to the targeting & design of direct batch heat exchanger networks (*HENs*). The proposed *GA* based solution approach to the design & optimization of batch *HENs* is the subject of **Chapter 8**.

Part IV draws conclusions with respect to the contributions achieved by this work (**Chapter 9**).

Part V groups Appendices together :

- **Appendix A** provides the reference data of the case studies;
- Guidelines to reduce the number of time slices are described in **Appendix B**;
- **Appendix C** presents systematic procedures to calculate optimal mixing of heat storage fluid to achieve the mass rebalance of heat storage units;
- **Appendix D** relates to the *GA* optimization and details the difficulties encountered and the solutions developed. A mathematical model of the indirect heat recovery scheme (*IHRS*) synthesis problem is also included;
- a further extension of the *IHRS* models is proposed in **Appendix E**;
- **Appendix F** provides guidelines for setting the *GA* optimization parameters;
- **Appendix G** summarizes the derivation of constraints pertaining to the multiple base case problem considered in Chapter 7;
- **Appendix H** exemplifies and comments the methodology for the synthesis of direct batch *HENs* proposed in Chapter 8;
- **Appendix I** sketches proposals for further work.

Chapter 2

STATE-OF-THE-ART REVIEW

2.1 Introduction

This Chapter provides a literature review on the heat integration of batch processes. A classification of the contributions is complicated because of the multiple aspects and purposes of several tools and methods. Therefore, a simple categorization into tools and methods which have been given a "brand name", and unnamed approaches has been adopted. After this analysis, a short synthesis of the state-of-the-art with respect to the different modes of heat integration is provided [1].

Genetic algorithms (*GAs*) have been foreseen as being particularly suitable for the design & optimization tasks addressed by this work. Their application in the synthesis of heat exchanger networks (*HENS*) - so far exclusively for continuous processes - has also been analysed.

The origin of some of the concepts and tools is sometimes difficult to trace and in this case several contributions are cited. An extended summary of and comments on the contributions marked with a * may be found in *Krummenacher* (1999).

Whenever relevant to the present work, the meaning of several terms used below is explained later, mostly in Chapter 3.

Note also that *Furman* & *Sahinidis* (2001) propose an annotated bibliography for the heat exchanger network synthesis covering 446 publications, of which about 20 concern batch processes.

1. An overview and a classification of the most practice relevant tools & methods are provided in *Krummenacher* (1997).

2.2 Named Tools & Methods

2.2.1 Time Average Model

Early heat integration studies of batch processes were addressed with methods developed for continuous processes; the minimum energy target and hence the energy savings potential was calculated using the composites of the *Time Average Model* (*TAM*) (*Clayton*, 1986a, b). The *TAM* assumes that the streams exist simultaneously as if the process was continuous, i.e. the time schedule is ignored and the heat flows are averaged over the batch cycle time. The *TAM* composites provide a global insight into the energy integration potential, but the identified energy targets represent a lower bound which most generally cannot be achieved [2] resorting solely to direct heat integration.

2.2.2 Cascade Analysis

The *Cascade Analysis* (*Kemp* & *MacDonald*, 1987; *Kemp* & *Deakin*, 1989; *Kemp*, 1990) is a major advance in response to the limitations of the *TAM* in that it explicitly adds the schedule (time) dimension into the problem table algorithm used for the energy targeting of continuous processes. The 2-dimensional cascade analysis allows heat to be cascaded to lower temperatures (by direct heat exchanges) as well as to the following time slices (resorting to intermediate heat storage). The pinch point of continuous processes becomes a time locus of pinch points (*pinch locus*). A single ΔT_{min} is assumed for both ways of cascading heat. Energy targets for various cases such as single or repeated batches, with priority to heat cascading in temperature or in time, can be calculated using the cascade analysis (however, corresponding cost targets are not provided).

The cascade analysis provide insight into and understanding of the relations between the schedule of the process and the heat integration targets. It is used to identify rescheduling opportunities and assess them (*Kemp* & *Deakin*, 1989; *Klemes* et al., 1994). But devising rescheduling opportunities remains essentially an unstructured iterative procedure. And global insight into the cascade analysis is difficult owing to the tabular nature of the method [3]. The 3-dimensional graphical

2. Hence the energy saving potential is overestimated.
3. The table may include up to 2 x *L* x (*I*+*J*) numbers, with *L* the number of time slices, *I* and *J* the number of hot and cold process streams, respectively.

representation of the heat cascade (called *cascade plots*) is an attempt to provide more insight.

The amount of heat [4] which can be transferred between two time slices is determined graphically by plotting the two corresponding grand composite curves back-to-back.

A procedure for *HEN* design is also described. First, maximum heat exchanges (*MHX*) *HENs* are developed for each time slice using the *pinch design method* (*Linnhoff* et al., 1982). Then, the slice-wise *HENs* are merged together to form an overall *HEN*. Finally, *HEN* relaxation is achieved using loops and paths, in order to improve the cost-effectiveness. Heat storage may also be included in the heat integration scheme (generally considering fixed temperature heat storage, each dedicated to a pair of asynchronous streams).

The cascade analysis is very useful and methodologically correct for energy targeting and related purposes; economic aspects are hidden in the chosen ΔT_{min}. A procedure to calculate cost targets and determine the cost-optimum ΔT_{min} prior to design is not provided.

2.2.3 Time Slice Model

The *Time Slice Model* (*TSM*) (*Linnhoff* et al., 1988) takes the schedule of streams into account in that a discontinuous process is decomposed into a set of continuous sub-processes, a sub-process being associated to each time slice. The *TSM* energy target is obtained by summation of the (*TAM*) energy target of each time slice. Usually, a single ΔT_{min} is used for each time slice. Unlike the *TAM* target, the *TSM* target may actually be achieved by direct heat exchanges. The difference between these two energy targets gives the incentive to consider rescheduling for improving the direct heat integration.

The *TSM* is a actually a simplified cascade analysis in which heat is cascaded in temperature solely.

2.2.4 Overall Plant Bottleneck

The concept of *Overall Plant Bottleneck* (*OPB*), proposed by *Linnhoff* et al. (1988), is part of a systemic approach [5] of batch plants. It results from the observation that

4. As well as the type and operating conditions of a heat storage unit.

the overall production costs of a given product [6] are generally much more sensitive to e.g. the production capacity, the product quality, the process yield, and the labour costs than to energy costs.

The procedure starts with the identification of the *OPBs* which limit, through the main cost factors - in one way or another - the profitability of the plant (a limited capacity of a vessel may be a capacity bottleneck, a limited heat exchange area may induce a time bottleneck, the limited capacity of a boiler may be responsible for an inadequate scheduling of the processes, etc.). Then, the interrelations between the *OPBs* (and particularly energy related *OPBs*) are exploited to arrive at cost-effective solutions, in which energy savings appear as side benefits (see e.g. a debottlenecking example in *Gremouti*, 1991).

The *OPB* approach is of course mainly concerned with debottlenecking, i.e. with a retrofit situation. Although conceptually very interesting, the weak point of the proposed approach lies in the lack of guidelines or procedure to identify the *OPBs* and the interrelations between them. The screening of the possibly numerous projects is another open question.

2.2.5 Time Event Model

The *Time Event Model* (*TEM*) (*Obeng* & *Ashton*, 1988) consists in the graphical representation of the state and tasks executed by the main pieces of equipment as a function of time. Using the *TEM*, time bottlenecks and critical paths are easily identified, and proposals for rescheduling may results.

The *TEM* is conceptually similar to a *Gantt Chart* (also called *Gantt Diagram*).

2.2.6 Multiple Base Case Methodology

Jones (1991) has developed a methodology for targeting and design of flexible continuous *HENs*. The requirement for flexibility is specified using the multiple base case (*MBC*) approach. Three possible modes of re-using *HEX*s across base cases are identified : conventional, resequence and repipe. For each of these modes considered separately, the minimum *HEX* area target is stated as a *LP* problem, resorting to the assumption of vertical heat exchanges between composite curves.

5. The usual approach to debottlenecking consists in iteratively identifying the bottleneck and removing it, one after the other.
6. Not to be mixed up with the total batch costs defined in Section 3.3.

Energy, area, number of units, and total cost targets are calculated, allowing for the determination of the cost-optimum ΔT_{min} of each base case, and from which the *HEN* design may be initialized. A *MBC HEN* design strategy is also proposed [7].

Gremouti (1991), and *Krummenacher* & *Favrat* (1995, 1999) have independently drawn the parallel between the base cases and the time slices of batch processes, and applied the methodology for the targeting & design of direct batch *HENs*. The latter authors have developed a more robust *LP* based procedure to calculate the area target for the conventional mode and improved the procedure related to the consideration of utility *HEXs* [8].

2.2.7 *Omnium Verfahren* & Related Further Developments

The *Omnium Verfahren* (*OV*) (*Hellwig* & *Thöne*, 1994) is an automated calculation procedure based on the *Hungarian Algorithm* to identify the set of exclusive direct process-to-process heat exchanges which maximize the heat recovery of a given discontinuous process. Exclusive hot stream-cold stream matches mean that once a heat exchanger is placed between a hot and a cold stream, neither the hot, nor the related cold stream are allowed to further exchange heat with any other streams (be it simultaneously, for the possibly remaining unused heat, or during another time slice, while one of the stream pair does not exist). The problem is represented in a matrix form in which the hot streams are organised in columns, while the cold streams are entered in rows. Each element of the matrix (i.e. the possible match of a cold stream with a hot stream) is assigned the maximum amount of heat that may be recovered if the corresponding match is selected. The economics is accounted for by the specification of a ΔT_{min} value for heat exchanges between any hot stream-cold stream match.

Detailed comparative analysis between *OV*-designed *HENs* (*OV-HENs*) and Pinch Analysis-designed *HENs* (*PA-HENs*) have been performed by *Uhlenbruck* (*Uhlenbruck,* 1995 *; *Uhlenbruck* & *Vogel*, 1999 *; *Uhlenbruck* et al., 2000); the comparison involves both continuous and batch *HENs* and focuses on the energy targets and the number of *HEXs* units (but without any cost calculation). The batch *PA-HENs* are designed by the standard method described by *Kemp* & *Deakin* (1989), with some additional "tricks" to re-use *HEXs* units across time slices.

7. A description of the *MBC* methodology of *Jones* applied to batch processes may be found in *Krummenacher* & *Favrat* (1995), and the key methodological aspects are summarized in Chapter 7 of the present document.
8. The conventional and the resequence targeting have been implemented in the *PinchLENI* software programme.

While the *OV-HENs* are easier to design than their corresponding *PA-HENs* equivalent (especially for batch processes), they feature significantly higher utility consumptions than the *MER* targets achieved by the *PA-HENs*. Since the process pinch is not taken into account, heat is often transferred across the pinch. The number of *HEX* units is not smaller, less process *HEXs* units generally occurring at the expense of more utility *HEXs*. The relaxation of *PA-HENs* makes them evolve towards the *OV-HENs*, while heat recovery still remains significantly higher.

To remove the limitation introduced by the assumption of exclusive matches and increase the heat recovery of the *OV-HENs*, *Uhlenbruck* proposes a repeated application of the *OV*: after a first *OV* run, the remaining streams or part of streams are listed and a corresponding matrix of (remaining) maximum heat recovery is calculated. The *OV* is run to find further matches, which are then added to the matches identified during the first *OV* run. If needed or still possible, a third *OV* run can be applied on the remaining matrix after the second run, etc. It is claimed that using this procedure, the *OV HENs* move towards and actually reach the relaxed *PA HENs* [9]. Another proposal concerns the introduction of heat storage after opportunities for direct heat exchanges have been exhausted by a repeated application of the *OV*. The cost-efficiency of the resulting schemes is unfortunately not addressed.

The reduced heat recovery and the poorer economics of basic *OV-HENs* has also been observed by *Krummenacher* & *Auguste* (1997) on a set of two test cases.

2.2.8 Batch Utility Curves (or Batch Cascade Curves)

The *batch utility curves (BUCs)* [10] have been proposed by *Gremouti* (1991) and renamed into *batch cascades curves* (*BCCs*) by *Ashton* (1992), and later mentioned by *Klemes* et al. (1994). The cold batch composite curve sums up, as a function of temperature, all remaining heating needs after the possibilities for direct heat exchanges have been exhausted within each time slice. The hot batch composite curve does the same for the cooling needs. Since the heating and cooling needs are extracted from the grand composite curve (*GCC*) of each time slice, for which the direct heat exchanges occurs in priority under ΔT_{min}, the *BCCs* represent the needs at their lowest exergy level, offering the highest opportunities for further heat integration by heat storage, given by the superposition of the *BCCs*. The non-overlapped part of the *BCCs*

9. However, from a conceptual point of view, this strategy corresponds to a sequence of partial sub-optimizations, which can miss the global optimum.

10. The *BUCs* are somewhat similar to the total sites profiles, cumulating the remaining heating and cooling requirements of processes once "locally" heat integrated.

represents the utility requirements. By construction (the pockets of the grand composite curves being left out (or cut-off) during the extraction of the *BCCs*), the heat exchanges between the overlapped parts of the *BCCs* never involve streams which exist simultaneously.

The global *BCCs* representation efficiently replaces and extends the technique proposed in the frame of the cascade analysis consisting in the back-to-back representation of a pair of *GCCs* to identify the opportunities of heat storage.

The batch composite curves have been further studied by *Krummenacher* & *Favrat* (1995). They demonstrated on a simple example that building the *BCCs* without consideration of the pockets present in the *GCCs* may result in an infeasible energy target in case a pocket is placed across the global pinch (i.e. heat transfer across the pinch). When the pockets are also extracted [11], more heat storage units are required but the heat integration achieves the energy target and may be cheaper too. Their contribution also highlights the fact that the *BCCs* (and residual composites as well) are useful for energy targeting, but the economical optimum solution may significantly deviate from these purely energetic considerations. The introduction of the storage streams in the slice-wise composites significantly modifies the optimum ΔT_{min} and more heat is actually transferred through heat storage than targeted using the *BCCs*.

Note however that the *BCCs* are often used to devise rescheduling, for which the semi-quantitative information they provides is adequate.

2.2.9 Permutation Method & Related Further Developments

The *Permutation Method* (*PM*), first presented by *Stoltze* et al. (1992, 1995), has been further improved and extended (*Mikkelsen*, 1998 *; *Mikkelsen* et al., 1998).

The *PM* assumes that the heat recovery is exclusively achieved by indirect heat exchanges using a number of intermediate heat storage units (*HSUs*) specified *a priori* (of fixed temperature/variable mass type). The discrete basic set of possible operating temperatures of the *HSUs* is established considering the supply temperature of process streams to be integrated, and a reasonable minimum temperature approach. This method essentially achieves an exhaustive search of the most profitable set of process stream – *HSU* matches [12]. Heuristic rules are used to decide the pair of *HSUs* to be matched with each stream, and to achieve the mass

11. Resulting in so-called *residual composites*, to highlight the difference with the standard *batch cascade curves* which do not extract pockets.

balance of the *HSUs* (a repeated operation is assumed). In addition, depending on the shape of the *TAM* composites, separation of the streams at the pinch may be needed, and a *HSU* be located at this point. In the case of a large number of streams, decision regarding which set of streams should be checked for integration may be needed. Additional possible operating temperatures of the *HSUs* may be introduced in the basic set of temperatures to evaluate solutions featuring different temperature driving force distributions (i.e. additional samples of a structure). The *PM* actually carries out a structural optimization of indirect heat recovery schemes, and thanks to the heuristic rules the method is based on, the delivered solutions are expected to feature reasonable parametric values. A set of further improvement opportunities (i.e. additional degrees of freedom to be exploited) has been identified (*Mikkelsen*, 1998 *; *Mikkelsen* et al., 1998); the application of the proposed techniques is called post-optimization (*PO*). Hence the design methodology involves three steps: 1) determination of the pinch using *TAM* composites; 2) simplified combinatorial search (*PM*); 3) post-optimization (*PO*) of the most interesting configurations resulting from step 2.

The method delivers good solutions which are of practical relevance. However, the post-optimization is difficult to apply and time-consuming. More importantly, the structural optimization achieved by the *PM* might fail to identify the structure featuring the best potential as a result from either improper distribution of the possible *HSU* temperatures (i.e. insufficient sampling of each structure) or from the other heuristic decisions (e.g. the pair of *HSUs* to be used for the heat integration of each stream, or the decision to connect to an intermediate *HSU*). The comparison between structures is not meaningful when the structures do not feature the same degree of "optimization" while the difference of their objective function is small. This problem is confirmed by the fact that the improvement potential by the application of the *PO* might be as high as 25 %.

2.2.10 Time Pinch Analysis

Wang & *Smith* (1995) have proposed a new approach for analysing the heat integration of batch processes. The *Time Pinch Analysis* treats time as the primary constraint, while temperature driving forces are treated as secondary constraints (i.e. the respective role of temperature and time are reversed). The time pinch analysis assumes that heat is first shifted in time, at the highest temperature level, and then, if a heat surplus still exists, cascaded in temperature. The *time composite* is introduced :

12. This combinatorial approach is possible thanks to the significantly reduced number of configurations to evaluate compared to the problem of designing a direct heat exchange network.

the cold time composite is obtained by plotting ΔQ of cold process streams versus time; similarly, a hot time composite can be drawn. Unlike temperature composites, time composites can be shifted vertically, i.e. time coordinates are unchanged, while ΔQ coordinates are arbitrary. Break points on time composites are located at start and/or stop times of streams, i.e. at the limits of time slices. No temperature information is included in the time composites. This means that heat recovery from a hot composite to a cold composite by heat storage implicitly assumes that the constraint of positive temperature driving forces is satisfied. To make sure that this is the case, given a ΔT_{min} [13] constraint, the process is divided into (shifted) temperature intervals and a pair of hot / cold time composites is drawn for each temperature interval. This way, the condition of positive temperature driving forces is satisfied, at the expense of a more complicated analysis, because of the temperature interval by temperature interval analysis.

The total heat recovery potential can be targeted, while the indirect heat recovery (and the storage time) is easily identified by plotting the time grand composite. The time grand composite provides insight into the problem of selecting which stream should be rescheduled in order to decrease the requirement for heat storage.

Note however that the introduction of the temperature constraints for a real process generally leads to a large number time composites, since one pair of time composites is required for each temperature interval, a representation which is not easier to handle and understand than the (temperature) slice-wise composites. An overall assessment of the required heat storage units is not possible - combining the information from the various temperature intervals into a single comprehensive representation is hardly possible.

2.3 Unnamed approaches

Vaselenak et al. (1986) were the first to propose methods for predicting the maximum heat integration potential between a number of tanks which require heating or cooling. Co-current, counter-current and combinations of the two are considered. Heuristics and a multiperiod *MILP* formulation are applied to find the optimal matching problem. The time schedule of the process is not taken into account - it is assumed that all tanks are available for matching at the same time.

13. As for the cascade analysis, a single ΔT_{min} for all stream matches is required when accounting for the temperature constraint.

Gremouti (1991) emphasizes the importance of correct data extraction and stresses the need for the schedule of a process to be questioned: 1) is the best equipment being used for the operation ? 2) is the current schedule making the best use of time ? Observing that reactors are inefficient heat exchangers, the following rule for the process integration of batch plants is proposed : whenever possible, *preheat externally and cool externally using heat exchangers* [14], resulting in opportunities for both an increased heat integration and a debottlenecking of the plant. *Gremouti* (1991) concludes her contribution by stating that " ... heat storage may be the answer for the heat integration of batch processes. It offers the advantage of flexibility and does not impose any constraints on the schedule".

Papageorgiou et al. (1994) address the problem of optimal short term scheduling of an existing multi-purpose batch plant in order to maximize the profit while also accounting for the heat integration. The formulation uses and extends the *State-Task Network* concept developed by *Kondili* (*Kondili* et al., 1993). Heat exchangers and heat storage units are assumed to exist and their suitability for different tasks is known *a priori*. Opportunities for heat integration between operations (either by direct or by indirect heat exchanges) is known *a priori* (kind of superstructure). The schedule of heat integrated operations may be different from the schedule of the same non-integrated operations (but also known *a priori*). Cleaning cycles may be accounted. A uniform discretization of the time horizon is used (e.g. 1 hour). Accounting solely for direct heat exchanges results in a *MILP* problem. The additional consideration of the indirect heat exchanges makes it into a non-convex *MINLP* problem (the non-linearity arises from the heat and mass balance of the heat storage units). The proposed resolution scheme resorts to an approximation of the non-linear terms and uses a modified *branch* & *bound* algorithm delivering upper and lower bounds for the optimal solution. The scheduling *MILP* problem without heat integration consideration at all already involves several thousands of binary variables for practice relevant problem (the number of variables is proportional to the time step); special methods exploiting the particularities of this MILP are necessary (*Shah* et al., 1993). *A fortiori*, with consideration of heat integration, the scheduling problem is significantly more difficult to solve, and industrial applications are still out of reach. Nevertheless, the formulation is versatile (ability to account for numerous types of constraints) and the search is carried out in the "full" solution domain, in that heat integration is not considered as an afterthought but simultaneously optimized. The authors state that numerous optimal schedules meeting the production requirements often exist, while their heat integration potential may be significantly different.

14. I.e. transform non-flowing streams into semi-continuous flowing streams.

Corominas et al. (1994) propose a methodology for the maximization of the heat integration when scheduling multi-product batch plants. Heat integration is restricted to direct heat exchanges and rescheduling (by delaying streams - within the stability time limits of intermediate products) is possibly introduced in order to increase the simultaneity of streams. The assignment of tasks to equipment units is assumed to be known a priori for all products to be produced. For any given production campaign, the methodology determines the required heat exchanger network to maximize the heat integration (resorting to rescheduling). A single ΔT_{min} is assumed for all heat exchanges. Merging the required *HENs* for the different campaigns results in a global macronetwork. Considering the macronetwork, the energy savings, the capital costs, as well as the associated increase of the production campaign owing to the rescheduling, the user may decide which heat exchangers are most cost-effective. He is provided with the consequences (penalties) of the heat integration decision; he can decide whether the consequences are acceptable or not. Note that the methodology does not optimize the profit, and intermediate solutions possibly featuring a more profitable trade-off between the duration of the campaign and the energy savings are not assessed.

Ivanov et al. (1993) consider different heat integration schemes (with a common or with two storage tanks) for the heat integration of batch reactors operating in different time intervals and develop the related mathematical models.

Ivanov & *Vaklieva-Bancheva* (1994) propose a 3-steps decomposition of the heat integration of batch processing plants. First, a number of schedules suitable for heat integration are suggested. Then, a superstructure of possible matches is generated. Finally, the scheduling problems considered during the first step are solved using *branch* & *bound* techniques.

The final report of the *EUROBATCH* project (*Klemes* et al., 1994) provides additional methods and calculation procedures for heat integration related problems. These include : 1) the account of the variability of the schedule and procedures to predict, compensate and prevent related perturbations (time-sensitivity tables; 2) methods for the analysis and control of utility consumption, as well as a limitation of the peak load by the introduction of heat storage; 3) computer programme for the heat integration analysis of single-product and multi-product/ multi-purpose batch plants. Four industrial case studies are also described.

Roslyng-Jensen et al. (1995) compare three methods for designing batch *HENs*: 1) the classical approach based on the time slice model (direct heat exchanges during each time slice - see Sub-section 2.2.2); 2) the permutation method (i.e. indirect heat exchanges exclusively - refer to Sub-section 2.2.9) and 3) the sequential application of the above method 2) followed by method 1), which is called the combined procedure (*CP*). The results are related to a coincidence factor which expresses the degree of simultaneity of the streams. As expected, a large coincidence factor favours method 1), low coincidence factors favour method 2). For mean coincidence factors, method 3) does not always result in the most economic solution. The coincidence factor is not the only evaluation criteria : the available temperature driving forces are also of importance since they significantly influence the cost-effectiveness of the indirect heat integration. Proposal for improving the cost-efficiency of *HENs* designed using the combined procedure 3) are also sketched.

Krummenacher & *Favrat* (1995) also address the mixed direct indirect heat integration using the *MBC* methodology of *Jones* adapted for batch processes, and the batch cascade curves. The search for minimum total costs (largely by trial-and-error) of a simple process including two time slices and two stratified heat storage units indicates that complex trade-off effects exist and suggests that the mixed direct-indirect heat integration problem requires a simultaneous consideration of the two modes instead of the usual sequential approach.

The problem of selecting the operating temperature of heat storage units (*HSUs*) based on composite curves is addressed by *Krummenacher* & *Favrat* (1995) and *Sadr-Kazemi* & *Polley* (1996) *. The first mentioned actually consider the problem on the batch composites curves, i.e. in the frame of a mixed direct-indirect heat integration; *HSUs* are of the stratified tank type. The latter focus on the *TAM* composites representation assuming an indirect heat integration exclusively; fixed temperature/ variable mass inventory *HSUs* are applied. Drawing the parallel between the starting temperature of residual streams of each time slice and the supply temperature of streams, the proposed resulting rules are similar. Note that these rules are implicitly embedded in the Permutation Method of *Stoltze* et al. (1992, 1995) although not based on the graphical representation of composites. Further, the search procedure proposed by *Sadr-Kazemi* & *Polley* (1996) share some similarities with the Permutation Method; they also consider opportunities for rescheduling to reduce the capacity of *HSUs*. Unsteady state heat storage systems (i.e. mixing *HSUs*) are also proposed when the external preheating and cooling strategy of *Gremouti* (1991) cannot be applied. Decision criteria to operate unsteady heat storage schemes are mentioned but remain unclear.

Vaklieva-Bancheva et al. (1996) propose a *MILP* formulation for the design of heat exchanger networks of multi-purpose batch plants. The additional scheduling complications resulting from heat integration between different products of the same campaign are accounted for in the formulation.

Zhao et al. (1998, part 1) propose a *MILP* formulation based on the cascade analysis for the scheduling of batch processes with heat integration.

Zhao et al. (1998, part 2) develop a 3-steps *HEN* design method for batch/semi-continuous processes. First, initial individual *HENs* are developed using techniques of continuous processes. Then, rematching design using *MILP* considers the relationship for all times slices. The final overall design looks at the trade-off between energy and capital cots among time slices.

2.4 Synthesis & Perspectives

The variety of the proposed tools and approaches reflects the variety of issues found in batch processing. No single comprehensive approach suitable to address all issues simultaneously is available or possible; this is even more true for the existing targeting tools, which efficiently focus on one aspect at a time but ignores the others (e.g. *Time Pinch Analysis* versus *Time Slice Model*).

Present targeting tools (*Time Average Model*, *Time Slice Model*, *Cascade Analysis*, *Time Pinch Analysis*, *Batch Cascade Curves*) essentially address energy targeting and are suitable for making conceptual decisions such as incentive for rescheduling. Except the *MBC* supertargeting applied to batch processes by *Gremouti* (1991) and *Krummenacher* & *Favrat* (1995), the trade-off between energy and capital costs is not addressed at the targeting stage - economic issues are generally hidden in a single ΔT_{min} ! Nevertheless, economic optimization of grassroot or retrofit designs must be considered. Without a sound assessment of the economic performances of the various heat integration solutions, no conclusions can be drawn concerning e.g. the price to be paid to achieve a robust [15] heat integration solution (i.e. the cost for flexibility). Contributions reported in *Klemes* et al. (1994) address the problem of the variability of schedule and provide compensation methods to be applied in operation, but further work is required to address the problem at the design stage.

So far, the optimal scheduling of multi-product and multi-purposes batch plants are the privilege of mathematical programming techniques. A realistic incorporation of direct and/or indirect heat integration results however in very complex problems which require simplifying assumption and a lot of skills to be solved.

15. I.e. featuring a low sensitivity to schedule variations.

Direct heat exchanges : the methods for designing direct batch *HENs* generally apply a bottom-up strategy (first generate a feasible *HEN* for each time slice, then merge them into an overall *HEN*). Except for simple processes, designing direct batch *HENs* using the pinch design method (or the improved *MBC* method) is time consuming and requires skills. The *Omnium Verfahren* generates batch *HENs* automatically, at the expense of a reduced heat recovery and poorer profitability; the improved strategy consisting in a repeated application of the *OV* delivers better *HENs* but might still miss the global optimum owing to its sequential sub-optimization nature. The re-use of *HEX* units across time slices is often limited to the conventional mode. An automated design method considering other modes of *HEX* re-use and explicitly minimizing the total costs (i.e. not relying on an single reasonable experience value of ΔT_{min}) is desirable.

Indirect heat integration : in presence of a significant proportion of flowing streams, the *Permutational Method* followed by *Post-optimization* appear to be the most practice relevant method. Nevertheless, it remains a semi-automatic method, and the screening stage achieved by the *PM* may miss a global optimum unless the method is further developed to automate the selection of some parameters. Graphical tools providing insight into the relationship between costs, heat recovery and the number of heat storage units would be helpful. At the same time, an automated design method addressing the degrees of freedom explored during the post-optimization should be developed.

Mixed direct-indirect heat integration : few contributions actually consider the mixed mode and explore the complex costs trade-off effects between both modes. Supertargeting methods (i.e. delivering not only energy but costs targets as well) are needed to effectively restrict the search domain to be considered during design. In such an approach, the likely variations of schedule must be modelled and explicitly accounted.

Rescheduling [16]: except for simple processes for which the number of rescheduling opportunities to assess is limited, the proposed strategies, even enlightened by the cascade analysis, still include trial-and-error, except the method proposed by *Zhao* et al. (1998).

Finally, it should be remembered that direct, indirect or a mixed heat integration are not Gospel : depending on the considered process, other energy saving techniques

16. From a practical point of view, a strong reluctance of operators/plant managers has been experienced in several chemical processes, owing to the fact that the processes under consideration had already gone through a long and expensive approval (certification) process. The incentive for rescheduling may reappear in case of capacity limitations.

(e.g. mechanical vapour recompression) or different heat storage schemes (e.g. storage of hot process water) exist and should not be overlooked. Models to be developed for automatic design should allow for these cases to be accounted to ensure their practical relevance. Even more importantly, the concept of *Overall Plant Bottleneck* recalls that energy integration should be analysed in the broader perspective of the overall profitability of the plant.

2.5 Design & Optimization Using Genetic Algorithms

Few contributions make use of genetic algorithms (*GA*) for the synthesis of *HENs* (*Androulakis* & *Venkatasubramanian*, 1991 *; *Wang* et al., 1997 *; *Lewin* et al., 1998 *; *Lewin*, 1998 *). The proposed procedures differ in the optimization scope assigned to the *GA*, and hence in the way the variables managed by the *GA* are encoded. These contributions are concerned with continuous process *HENs*.

Androulakis & *Venkatasubramanian*, 1991 * propose the use of a *GA* for the structural optimization of *HENs*, while the optimization of the heat rates of the matches to achieve minimum costs (*NLP* problem) resorts to the *GRG2* non-linear (feasible path) optimizer. A *HEN* structure is coded as an ordered sequence of characters; each character represents a hot stream - cold stream match (hence I x J different characters are needed, with I and J the number of hot streams and cold streams, respectively) [17]. Stream splitting is not supported.

In the proposal of *Wang* et al., 1997 *, a general superstructure of *HEN*, organized in stages, is postulated (yet stream splitting is not supported), and the heat rates of matches are progressively optimized using a so-called *distributed continuous-formed evolutionary algorithm*. This algorithm preserves the existence of sub-populations which evolve independently; it deals with continuous variables (no binary encoding/decoding). The *HEN* synthesis is addressed exclusively by a single-level stochastic optimization. However, feasible initial solutions (obtained by other methods, e.g. by the block-based decomposition of *Zhu* et al., 1995) may be needed to speed-up convergence.

Lewin et al., 1998 * consider the synthesis of maximum energy recovery (*MER*) *HENs* (given a minimum temperature approach ΔT_{min}). This *MILP* problem is solved by a cascaded algorithm consisting of an upper level based on *GA* dealing with the optimization of match structures, and a lower level parametric optimization

17. Compare this compact description with the I x J binary variables needed in a mathematical programming approach to describe the *HEX* matches.

of the heat rate (*LP* problem) based on the *Simplex* algorithm. The number of matches is specified *a priori* by the user; the description of the *HEN* structure uses the concept of *HEN* level. Stream splitting is not supported.

Lewin, 1998 * further develops the methodology presented in *Lewin* et al., 1998 * to address the synthesis of cost-optimal *HENs* including stream splitting (not necessarily isothermal). Streams to be split are specified *a priori*. The coding of the *HEN* structure is modified accordingly. The lower level parametric optimization (which deals with a *NLP* problem) actually involves a cascaded algorithm consisting of a non-linear optimization of the stream splits (while keeping constant the heat duties), followed by a pseudo-linear optimization (modified *simplex*) of the heat rates (while keeping constant the splits fractions), and finally the calculation of the costs. In this approach, the cost optimality of the *HEN* is actually hidden in the *MER* design of *HEN* corresponding to specified ΔT_{min}. In these two contributions, the *GA* manipulates integer values and its use is restricted to structural issues.

The fact that these *GA* based approaches deliver a population of good solutions is claimed to be an important benefit.

Chapter 3

BACKGROUND & PRACTICAL ISSUES

3.1 Overview

This Chapter introduces some important definitions such as the different types of streams (**Section 3.2**), as well as the total batch costs (*TBCs*) and heat recovery (*HR*) (**Section 3.3**).

Section 3.4 briefly reviews the techniques of heat storage and explains the choice of fixed temperature/variable mass (*FTVM*) heat storage. Further, the advantages of indirect heat integration are highlighted. The mass balance equality constraints relevant to *FTVM* heat storage units (*HSUs*) are established and provide insight into the problem of searching for optimum indirect heat recovery schemes presented afterwards. The procedure for determining the minimum capacity of *HSUs* and the minimum inventory of heat storage fluid is also described.

The issues of the direct heat integration are briefly introduced in **Section 3.5**.

Section 3.6 provides guidelines for data extraction and process simplifications.

Finally, **Section 3.7** recalls the working principle of genetic algorithms (*GAs*) and describes the main features of the *Struggle GA* used in this work.

3.2 Types of Streams

Several types of streams are considered and specific names for each type are used in this work. This Section aims at clarifying their definitions.

3.2.1 Flowing and Non-flowing Streams

Continuous processes only include flowing streams. Discontinuous processes may include both flowing and non-flowing streams :

- a *flowing stream* is characterized by its *supply temperature* T_S, its *target temperature* T_T and a *heat capacity flowrate* CP which are constant (time-independent) during the period of existence of the stream. A flowing stream is not associated to a batch unit (reactor vessel, crystallizer, dryer, batch distillation column) but is part of semi-continuous operation (e.g. cooling or heating during transfer between batch vessels, pasteurizer, etc.). **Figure 3-1** represents both a *single-segment* hot flowing stream as well as a *multi-segment* cold flowing stream (comprising e.g heating, evaporation, and super-heating).

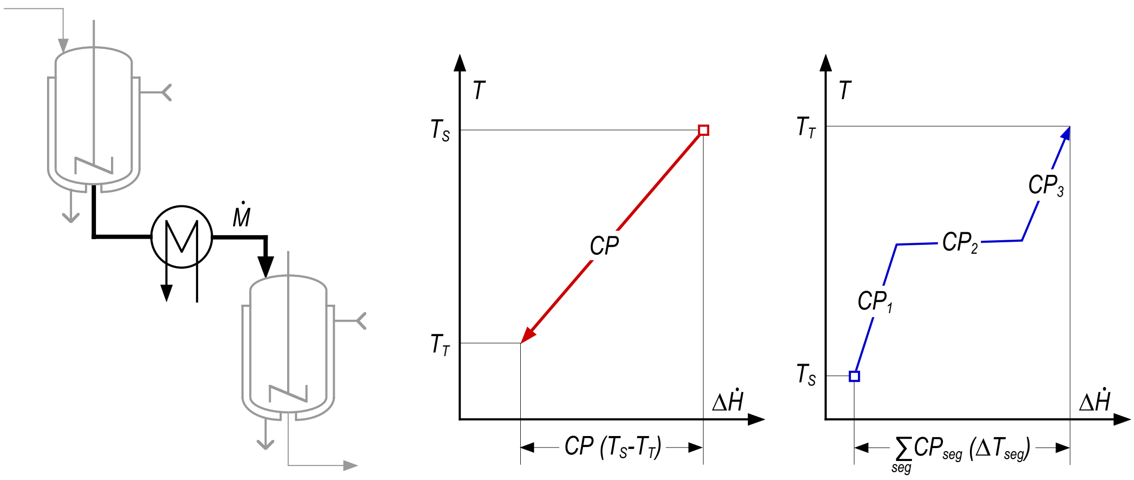

Figure 3-1 Flowing streams : a single-segment hot stream (centre) and a multi-segment cold stream (right).

- a *non-flowing stream* (refer to **Figure 3-2**)represents a heat supply to or a heat extraction from a mass in a vessel (i.e. in-vessel, or batch operation). The heat transfer occurs either through the wall of the vessel, by means of an immersed coil or by circulation through an external heat exchanger [1]. An actual non-flowing stream is characterized by a heat transfer while the mean temperature of the mass in the vessel changes as a function of time [2]. Modelling a non-flowing stream as a flowing stream may be misleading when the mean mass

1. Non-flowing streams featuring a constant mean temperature of the mass over time may be found (e.g. evaporation, cooling during exothermal reaction to hold temperature - in this latter case the transferred heat rate may not be constant) and are actually like a flowing stream.

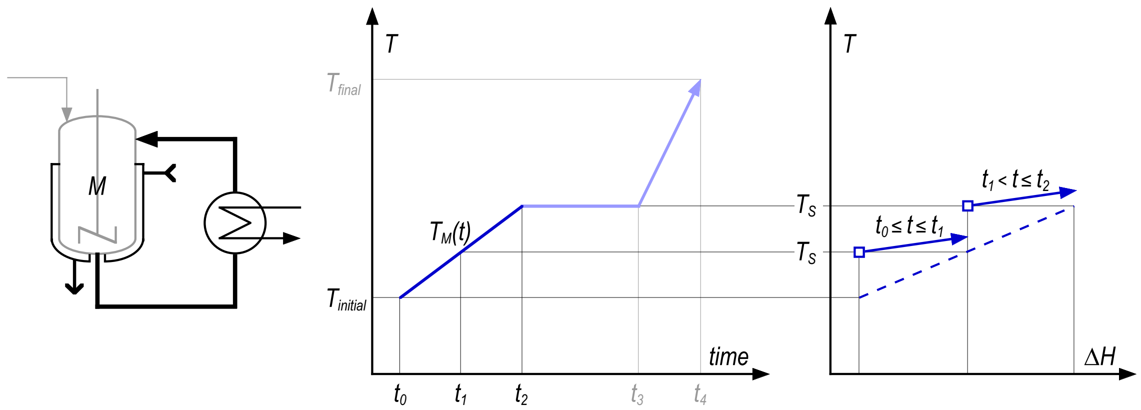

Figure 3-2 Non-flowing streams : mean temperature of the mass M *vs* time representation of a non-flowing stream (centre) and "safe-side" approximation of the first heating stage by two flowing streams for two time sub-periods (right).

temperature increase or decrease of the non-flowing stream is of the same order as the temperature driving forces of heat transfer to heat or cool the mass. A more precise modelling requires that the non-flowing stream be time-discretized into a sequence of flowing streams (see Figure 3-2 right).

3.2.2 Heat Recovery Streams

Any standard process stream has a specified target temperature which must be met. In some instances (e.g. when an intermediate product is stored before being used in another section of the plant), a fixed target temperature is not specified and the final temperature may be any value within a range of target temperatures. The target temperature is "soft" and the stream is called a *soft-temperature stream*. A heat recovery stream describes a different type of stream, which however also has a soft target temperature. Unlike a process stream, a *heat recovery stream* [3] (e.g. hot waste water, hot gas released to the environment) describes an opportunity for recovering heat - but not a necessity; the stream may also be simply ignored, unless, as might be the case of hot effluents, a preliminary cooling below a specified temperature is required before being discharged in the sewerage system. A soft-temperature stream or a heat recovery stream require the specification of a maximum and a minimum target temperature.

2. A distinction may be made with respect to the property which actually depends on the time, but it does not matter here; refer to *Kemp* & *Deakin* (1989) for a detailed classification.
3. Called a *free utility* by *Mikkelsen* (1998).

3.3 Total Batch Costs & Heat Recovery

3.3.1 Total Batch Costs

The *total batch costs* (*TBCs*) represent the costs of the energy services to produce one batch [4]:

$$TBCs = a_B \cdot \sum_i C_{cap\ i} + \sum_j C_{oper\ j} \tag{3-1}$$

where:

- a_B is the pay-off factor per batch, defined as $a_B = \frac{a}{N_{BPY}} = \frac{1}{N_{BPY}} \cdot \frac{IR}{1-(1+IR)^{-POP}}$ in which a is the annual pay-off factor, N_{BPY} is the number of batch per year, IR is the interest rate [-], and POP the pay-off period (number of years);
- $C_{cap\ i}$ is the capital cost of equipment i (heat exchangers, heat storage units, valves, piping costs [5], heat storage fluid costs, etc.);
- $C_{oper\ j}$ is the operational cost of service j (hot utility supply, cold utility supply, cleaning of heat exchangers, etc.).

The total batch costs (*TBCs*), the total annual costs (*TACs*) or the net present value of savings (*NPVs*) are equivalent concepts in that solutions (i.e. heat integration schemes) which maximize the *NPVs* minimize the *TBCs* as well.

3.3.2 Heat Recovery

The heat recovery (*HR*) achieved by a heat integration scheme is an essential parameter of indirect heat integration. Intuitively, heat recovery would be defined as the reduction of the hot utility consumption (or of the cold utility consumption) when compared to the case without heat integration. However, this definition becomes unclear when part of the hot (and/or cold) process streams are soft temperature or heat recovery streams. Consider **Figure 3-3**, sketching a simplified representation of an indirect heat integration [6]. Over a repetition period (batch cycle), the heat balance of the heat storage system must hold :

4. Relating the costs to one batch is found to be more readily understandable than considering annual costs.
5. Piping costs based on the distance between a stream and the heat storage system contribute like the fixed costs of the related *HEX* unit.

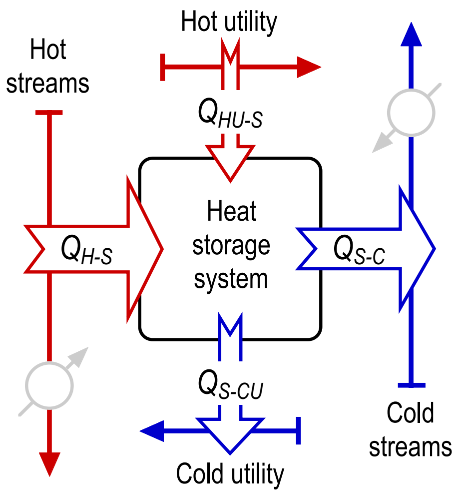

Figure 3-3 Overall heat transfers around a heat storage system (the heat losses to the environment are neglected).

$$Q_{H\text{-}S} + Q_{HU\text{-}S} - (Q_{S\text{-}C} + Q_{S\text{-}CU}) = 0 \tag{3-2}$$

where:

- $Q_{H\text{-}S}$ represents the heat supplied by the hot streams to the heat storage system over a repetition period;
- $Q_{S\text{-}C}$ is the heat extracted from the heat storage system by the cold streams over a period;
- $Q_{HU\text{-}S}$ represents the heat supplied by the hot utility to the heat storage system over a repetition period;
- $Q_{S\text{-}CU}$ is the heat extracted from the heat storage system by the cold utility over a period;

Rewriting the heat balance, the heat recovery is defined by the actually useful heat transferred from hot streams to cold streams through the storage system :

$$HR \equiv Q_{H\text{-}S} - Q_{S\text{-}CU} = Q_{S\text{-}C} - Q_{HU\text{-}S} \tag{3-3}$$

The above formulation is general and does not require a separate consideration of (compulsory) process streams and of heat recovery streams; it appears that $HR \le Q_{H\text{-}S}$ and $HR \le Q_{S\text{-}C}$ [7].

6. Note that this representation is general and holds for any type of heat storage unit (phase change, stratified, mixing, *FTVM*).
7. For instance, more heat may be supplied by hot streams than actually usable by cold streams; excess heat at a low temperature (i.e. which cannot be used by cold streams) must be removed from the heat storage system by cold utility. At the same time, it might be that cold streams extract more heat at high temperature than delivered by hot streams; to ensure the heat balance of the storage system, additional heat must be supplied by hot utility.

3.4 Indirect Heat Integration Issues

Indirect heat integration may sometimes be disregarded, as being *a priori* a costly mean of heat integration [8]. However, experience shows that the following practical difficulties may prevent the heat integration by direct batch heat exchanger networks (*HENs*) to achieve its full potential or to be accepted by plant operators :

- the schedule of process streams is generally subject to systematic (as well as accidental and unexpected) variations [9];
- the dependency links (schedule constraints, propagation paths, etc.) introduced by direct batch *HENs* reduce the flexibility of the plant and may result in adverse effects on its operability [10];
- the rescheduling of processes to achieve a profitable direct heat integration is often not possible for certified processes found in the pharma and the fine chemicals sector [11];
- to achieve the shortest-time-to-market strategy, production starts while several process parameters (in particular the schedule) are not well defined yet and are likely to evolve as result from increased process understanding and knowledge.

Considering that the schedule and the resulting decomposition into time slices are subject to variations, two main approaches may be considered :

1. develop/optimize direct batch *HENs* for the base case schedule, then analyse their sensitivity to the most likely variations of the schedule, and resort to indirect heat integration for problematic matches, if need be;
2. in order to remove the stiff schedule constraints, start by developing indirect heat recovery schemes, then remove from these schemes and integrate in direct

8. Heat storage has only been considered as a possible complement - after opportunities of direct heat integration have been exhausted - rather than a full heat integration mode. Rescheduling has often been advocated to increase the direct heat recovery potential so as to avoid resorting to heat storage.
9. For instance, due to : • the fouling of heat exchangers and reactors, leading to heating/cooling tasks of increasing duration, and requiring regular disruption of the batch cycle time for cleaning; • feeds or products of varying specifications, requiring continuous on-line adaptations of the recipe (temperature, duration, etc.); • the use of qualitative or quantitative parameters as a criteria to terminate a task, i.e. a task is not primarily defined by a fixed duration, but rather continues until the controlled parameter reaches the specified target value; • possible failures of equipment units, leading to unexpected delays and requiring the use of alternate processing routes.
10. Flexibility and operability are highly desired features of batch plants. Energy savings are not given a high priority, while production capacity and quality are often considered as key objectives. Heat integration schemes which constrain these objectives are disregarded in practice.
11. The certification procedure (developed internally or externally to the company) is lengthy and expensive.

mode only those matches which are not sensitive to schedule variations (robust direct matches).

Both approaches are complementary and a reasonable choice of the most suitable approach depends on the significance of the schedule variations and on the flexibility requirements [12]. Actually a third, more general approach would embed the two approaches by considering mixed direct-indirect heat integration simultaneously from the very beginning. However, facing the complexity involved in the development of automatic synthesis methods for the simultaneous consideration of indirect and direct heat integration, separate approaches are expected to be more manageable. Moreover, experience shows that insight and understanding gained with these two separate modes is valuable before embarking on the mixed direct-indirect heat integration.

Before describing the main issues of the indirect heat integration to be addressed in Part II, the available techniques for heat storage, as well as the heat/mass balance and the sizing of heat storage units are presented.

Heat storage may be achieved resorting to two different physical principles :

1. *latent heat storage*;
2. *sensible heat storage*.

A review of the heat storage systems may be found e.g. in *Hasnain* (1998), or *Mikkelsen* (1998). The description below focuses on the basic principles and mentions the main advantages and drawbacks of each solution from a practical point of view.

In the context of indirect heat integration, the term *heat storage unit* (*HSU*) designates a tank (or vessel) containing a mass of heat storage fluid (at a temperature uniform or not, depending on the technique of heat storage) [13].

Note that within a global heat storage system (refer to e.g. Figure 3-3), *HSUs* of different types may be combined to achieve an indirect heat integration.

12. With respect to the first approach, the various causes of schedule variations are generally non-correlated, so that numerous cases should be considered, making this approach difficult and costly. Methods for modelling the delays and their propagation / compensation throughout the schedule of a batch remain to be developed to a large extend, although this aspect has already been considered in the *EUROBATCH* Project (*Klemes* et al., 1994). Not every delay will result in a new time slice or in an infeasibility of the heat recovery network.

13. A heat storage unit has the same meaning as a *heat store* used by *Mikkelsen* (1998).

3.4.1 Latent Heat Storage

Latent heat storage uses phase change materials (e.g. hydrated salts) to store heat (generally by crystallization <=> melting). The temperature at which the phase change occurs depends on the selected material; therefore, unlike sensible heat storage, the operating temperature of latent *HSUs* has to be selected among a discrete set of values.

Latent heat storage generally results in a significantly smaller volume when compared to sensible heat storage, and is particularly recommended when large amounts of heat must be stored with small temperature differences [14].

The use of a latent *HSU* beyond its rated storing capacity results in a rapid increase/ decrease of its temperature (sensible heat of the phase change material is involved).

3.4.2 Sensible Heat Storage

Three main types of sensible heat storage systems may be distinguished [15]:

1. *mixing heat storage*;
2. *stratified heat storage*;
3. *fixed temperature / variable mass* (*FTVM*) heat storage.

For any of these three types, given a heat storage capacity, the required volume is inversely proportional to the temperature difference between the "charged state" and "empty state".

3.4.2.1 Mixing Heat Storage

In mixing heat storage, the storage of heat is achieved by an increase of the overall, mean temperature of the storage fluid in the tank; by construction or by operation, the heat storage fluid features an almost homogenous temperature in the *HSU*.

14. However, depending on the technical design of the latent *HSUs*, the actual reduction of storage volume may turn out to be smaller than expected : in some instance, the minimum volume of the *HSU* may be imposed by the peak heating/cooling rate and not by the heat to be stored, owing to a low heat transfer coefficient between the nodules containing the phase change material and the fluid circulating around them. Small temperature differences between the fluid and the phase change material (in both crystallization and melting phases) are particularly desirable when exergy losses should be minimized (e.g. in low temperature cooling).

15. A fourth solution consists in the momentary storage of a process stream in an inventory (storage tank) for later cooling or heating. This is actually a rescheduling of the process which does not involve the use of a separate heat storage fluid.

Whether jacketed, equipped with an internal coil or an external heat exchanger does not matter [16], parallel-flow heat transfer occurs in any case and heat is degraded to the mean temperature of the mass T_M of the *HSU* (mixing heat storage cannot benefit from the features of flowing streams).

If the variation range of T_M is quite limited owing to operational constraints, the required volume is large. However, the system has the advantage of self-adjusting its operating temperature as a function of the heat supply and heat sink [17]. Though not efficient for the heat integration of flowing streams [18], mixing *HSUs* are easier to operate, also because the return temperature of the storage fluid to the *HSU* does not require tight control.

3.4.2.2 Stratified Heat Storage

Stratified heat storage relies on the variation in the density [19] of the storage fluid as a function of the temperature to keep volumes of storage fluid at different temperature separated in the same tank [20]. Design (shape) and operational measures are required to avoid disturbing the layers and mixing. Nevertheless, temperature degradation by conduction and/or mixing cannot be totally avoided at the interface, even if some commercial designs of stratified *HSUs* use a moveable membrane to keep the zones separated.

With stratified *HSUs*, the storage fluid is circulated through an external heat exchanger to be heated or cooled; this allows the efficient heat integration of flowing streams since counterflow heat exchange can be achieved [21].

Unlike mixing *HSUs*, stratified *HSUs* and *a fortiori FTVM HSUs* cannot be operated beyond their rated capacity; continuous control and a safety margin must be ensured

16. Except with respect to the heat transfer coefficient, which would favour the external heat exchanger.
17. A useful feature in multi-product and multi-purpose plants for which the *a priori* definition of the optimal temperature level may be difficult and subject to changes (refer to *Krummenacher* & *Mayor*, 2000).
18. The loss in heat recovery efficiency when using a mixing *HSU* instead of stratified or *FTVM HSUs* depends to a large extent on the shape of composites and on the distribution of the supply temperature of the process streams. Tilted composites curves lying close together represent the worst case and would require significantly more mixing *HSUs* to be used to achieve the same heat recovery level.
19. Over the operating temperature range, density must be increasing or decreasing, but cannot include both (unless the two volumes at different temperatures are separated by a moveable membrane).
20. The temperature profile in the tank may be continuous (e.g. in thermal solar heat storage). In the heat integration context, a limited number a discrete temperature levels are considered: a *stratified HSU* designates a *HSU* working with two temperature levels, while a *multi-stratified HSU* involves more than 2 levels.
21. Unlike *FTVM HSUs*, the stratified *HSUs* may easily be operated under pressure, extending the applicability range of water as a storage fluid significantly beyond 100 *°C*, avoiding the need to consider glycol-water mixtures or thermal oil featuring poor heat transfer film coefficients. But pressure tanks are more expensive than atmospheric tanks.

in their operation strategy [22]. Further, the return temperature to the *HSU* after heat exchange must be controlled to match the operation temperature of the *HSU*.

3.4.2.3
FTVM Heat Storage

FTVM heat storage operates in the same way as stratified heat storage does, but prevents the temperature degradation problem by keeping the volumes featuring different temperatures in separated tanks (*HSUs*).

Figure 3-4 describes the working principle of *FTVM* heat storage : a mass of heat

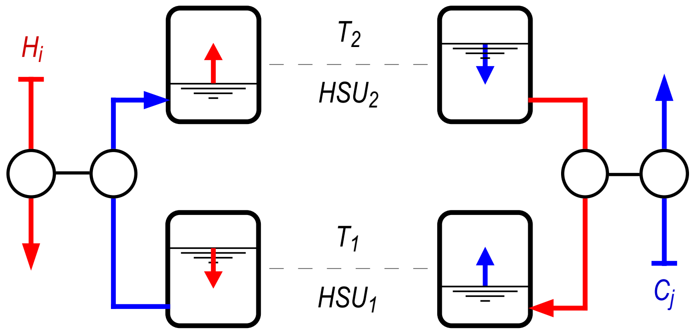

Figure 3-4 Principle of fixed temperature/variable mass heat storage (left: charging; right: discharging).

storage fluid is heated from T_1 to T_2 by heat exchange with hot stream H_i (left), while the storage fluid previously moved to HSU_2 returns, during a later time, to HSU_1 by heating cold stream C_j (right) [23]. Unlike mixing and stratified heat storage, *FTVM* heat storage working between two temperatures require two *HSUs* [24].

The suitability of *FTVM HSUs* to efficiently integrate flowing streams and the absence of the temperature degradation featured by stratified *HSUs* motivate the choice of *FTVM HSUs* for the indirect heat integration considered in Part II,

22. In the case of stratified heat storage (without physical separation by a membrane), a sudden change of the temperature occurs when the *HSU* is used beyond full charge or discharge. In the case of *FTVM*, it is even worse: no more storage fluid may flow.

23. Non-overlapping heat supply to and heat sink from the heat storage system is assumed here for demonstrating the principle. Generally, hot streams and cold streams integrated through an intermediate heat storage partly overlap in time. The effect the schedule of streams has on the minimum capacity of *HSUs* is described in Sub-section 3.4.4.

24. Because the heat storage fluid is extracted from one tank and supplied to the other tank, air or another gas must enter in the first tank and flow out of the second one, making their operation under pressure difficult and atmospheric operation recommended.Recycling the gas from the second tank to the first one requires cooling, and a buffer storage for excess volume of gas may be required. If atmospheric operation with air as gas is used, corrosion free material (e.g. stainless steel) must be used in conjunction with water as heat storage fluid.

provided that the flowing streams represent a significant proportion of the process streams, and/or the available temperature driving forces between composites are large enough. In addition, *FTVM HSUs* are suitable for *open* storage systems, which may be particularly attractive when one or several process streams involve a fluid which is at the same time a good candidate as a heat storage fluid (e.g. water) [25].

3.4.3 Mass Balance of *FTVM* Heat Storage Units

The heat balance of a heat storage system (Equation 3-2 in Sub-section 3.3.2) states that over a repetition period (batch cycle), the heat supplied to the system and heat extracted from the system must be in balance [26]. Likewise, the masses supplied to, and the masses extracted from each *FTVM HSU* over a batch cycle must be in balance (i.e. no net mass accumulation or depletion over a period) [27] [28].

The mass balance of *HSUs* are key equality constraints of any indirect heat integration scheme, and therefore must be given due consideration.

To illustrate the mass balance calculations, consider Figure 4-3 on page 59 which represents an indirect heat recovery scheme for the example process *EP-1* described in Appendix A. This scheme includes four *HSUs* : HSU_1 and HSU_4 are *terminal HSUs* (mass transfers occur with a single adjacent *HSU*), while HSU_2 and HSU_3 are *intermediate HSUs* (mass transfers occur with two adjacent *HSUs*). A *storage sub-system* (*SSs*) consists of two adjacent *HSUs* and represents an elementary *FTVM* heat storage system which must be in balance.

The mass balance equality constraints may either be written around *HSUs* (3 independent equations, e.g for HSU_1, HSU_2, HSU_3), or around *SSs* (3 independent equations for SSs_1, SSs_2, SSs_3). Writing these constraints around *HSUs* is more useful when it comes to the sizing of *HSU* capacities and is used below for consistency. First consider a terminal HSU_k (e.g. $k = 1$); the mass balance constraint over a batch cycle is written as :

25. While a standard heat storage system is *closed* (i.e. the heat storage fluid is confined in the system and therefore its mass inventory is constant), an *open* storage system is characterized by a mass inventory which varies during a batch cycle, since fluid supply to and fluid extraction from the system do not coincide - refer to Section 5.4 for more details.
26. Otherwise a cyclic operation would not be possible since the state of the system at the end of a cycle would not match the state at the beginning of this cycle.
27. Considering the mass balance constraints expressed by Equation 3-4, it can be easily demonstrated that meeting these constraints automatically results in meeting the heat balance constraints.
28. The mass balance constraints presented here apply to both closed storage systems and open storage systems.

$$\left[\sum_j M_{k,j} - \sum_i M_{k,i} - MBB_k\right] = 0 \qquad \textbf{(3-4)}$$

where:

- $M_{k,\,j}$ represents the mass of storage fluid cooled (over a batch cycle) by cold process stream j an moved from *HSU*$_{k+1}$ into *HSU*$_k$; $M_{k,j} = Q_{k,j}/(c_{pSF}(T_{k+1} - T_k))$;
- $M_{k,\,i}$ represents the mass of storage fluid heated (over a batch cycle) by hot process stream i and moved from *HSU*$_k$ into *HSU*$_{k+1}$; $M_{k,i} = Q_{i,k}/(c_{pSF}(T_{k+1} - T_k))$;
- MBB_k is the excess of mass cumulated in *HSU*$_k$ over a batch cycle when considering the contributions of process streams only (mass variation before balance, due to mass contributions of storage sub-system *SSs*$_k$ made up of *HSU*$_{k+1}$ and *HSU*$_k$); hence MBB_k is calculated as $MBB_k \equiv \sum_j M_{k,j} - \sum_i M_{k,i}$. In the case of a terminal *HSU*, the mass rebalance contribution is $-MBB_k$ and may only be applied by utility (refer to Section 5.4);
- c_{pSF} is the specific heat of the heat storage fluid; $Q_{k,j}$ is the heat contribution of *SSs*$_k$ to cold stream j; $Q_{i,k}$ is the heat contribution of hot stream i to *SSs*$_k$; T_{k+1} is the temperature of *HSU*$_{k+1}$; T_k is the temperature of *HSU*$_k$.

Considering now an intermediate *HSU*$_k$ (e.g. now with $k = 2$), the mass balance constraint includes two main terms (corresponding to mass contributions of both *SSs*$_k$ and *SSs*$_{k-1}$), each built according to Equation 3-4 :

$$\left[\sum_j M_{k,j} - \sum_i M_{k,i} - MBB_k\right] - \left[\sum_j M_{k-1,j} - \sum_i M_{k-1,i} - MBB_{k-1}\right] = 0 \qquad \textbf{(3-5)}$$

The second term of Equation 3-5 individually fulfils Equation 3-4, so that the first term is also individually equal to zero.

Note that time does not appear in the above equality constraints; these constraints are only concerned with the difference between the initial and the final states of the mass inventory of the *HSUs*, irrespective of the intermediate states.

3.4.4 Sizing of *FTVM* Heat Storage Units

The capacity of the *HSUs* must be able to cope with the mass inventory variations which occur during a batch cycle as a result from the masses supplied and masses extracted as a function of time slices. With the *HSUs* being sized for the minimum capacity, each *HSU* is empty at the time of its lowest inventory, and full at the time of largest inventory. The determination of the minimum required capacity (volume) of the *HSUs* involves the following steps :

1. calculation of the mass imbalance of each HSU_k over a batch cycle according to $MBB_k \equiv \sum_j M_{k,j} - \sum_i M_{k,i}$ (refer to Sub-section 3.4.3);
2. scheduling of the mass rebalancing contribution $-MBB_k$; generally, a constant flowrate over the whole batch cycle is assumed for simplicity and owing to the fact that $-MBB_k \to 0$ for optimal solutions (refer to Section 5.4);
3. calculation of the *assumed mass inventory* $M^*_{k,l}$ [29] at the end of each time slice, accounting for both the contributions of process streams and the mass rebalancing flowrate calculated at step 2. The time slices result from the schedule of streams (refer e.g. to Figure A-1). The mass inventory $M^*_{k,l}$ of HSU_k at the end of time slice l is given by [30] [31]:

$$M^*_{k,l} = M^*_{k,l-1} + \Delta t_l \cdot \left[\left[\sum_j a_{l,j} \cdot \dot{M}_{k,j} - \sum_i a_{l,i} \cdot \dot{M}_{k,i} - \frac{MBB_k}{\Delta t_{BC}}\right] - \left[\sum_j a_{l,j} \cdot \dot{M}_{k-1,j} - \sum_i a_{l,i} \cdot \dot{M}_{k-1,i} - \frac{MBB_{k-1}}{\Delta t_{BC}}\right]\right] \quad \textbf{(3-6)}$$

where:

- $M^*_{k,l-1}$ represents the assumed mass inventory of HSU_k at the end of time slice $l-1$ [32];
- Δt_l gives the duration of time slice l and Δt_{BC} the batch cycle time;
- $a_{l,j}$ is the presence (or activity) factor of cold stream j during time slice l : $a_{l,j} = 1$ if stream j exists during time slice l, $a_{l,j} = 0$ otherwise;
- $a_{l,i}$ is the presence (or activity) factor of hot stream i during time slice l : $a_{l,i} = 1$ if stream i exists during time slice l, $a_{l,i} = 0$ otherwise;
- $\dot{M}_{k,j}$ is the mass flowrate cooled by cold stream j from HSU_{k+1} to HSU_k; $\dot{M}_{k,j} \equiv \dot{Q}_{k,j}/(c_{pSF}(T_{k+1} - T_k))$, with $\dot{Q}_{k,j}$ the cooling heat rate;

29. The term *assumed mass inventory* $M^*_{k,l}$ is used to distinguish it from the *actual mass inventory* $M_{k,l}$: the assumed mass inventory designates the mass inventory which would result assuming an initial mass inventory $M^*_{k,0}$ (often arbitrarily set to 0).The minimum actual mass inventory can only be calculated once the assumed mass inventory has been determined for any time slice of a batch cycle: $M_{k,l} = M^*_{k,l} - Min_l[M^*_{k,l}]$ (the method is similar to the problem table algorithm which first requires an infeasible heat cascade to be calculated).
30. Equation 3-6 holds for an intermediate *HSU*, i.e. accounts for the mass flowrate contributions of both the upper and the lower storage sub-systems For a terminal *HSU*, the flowrate contributions arise from one *SSs* only.
31. A process stream - *SSs* heat transfer rate (and therefore the mass flowrate) is assumed to be constant over the period of existence of this stream and does not depend on the time slice.
32. Since the aim of the calculation is to calculate a difference of mass inventory (step 4), the initial mass inventory at the beginning of a batch cycle does not matter. Arbitrarily, the initial inventory is assumed to be zero.

- $\dot{M}_{k,i}$ is the mass flowrate heated by hot stream i from HSU_k to HSU_{k+1}; $\dot{M}_{k,i} \equiv \dot{Q}_{i,k}/(c_{pSF}(T_{k+1} - T_k))$, with $\dot{Q}_{i,k}$ the heating heat rate;
- $-MBB_k/\Delta t_{BC}$ represents the mean rebalancing mass flowrate of SSs_k over the batch cycle;
- similarly, terms with subscripts $k-1$ refer to the storage sub-system SSs_{k-1} (consisting of HSU_k and HSU_{k-1}) instead of SSs_k (made up of HSU_{k+1} and HSU_k).

4. calculation of the minimum capacity $V_{min\ k}$ of HSU_k given by :

$$V_{min\ k} = \frac{Max_l[M^*_{k,l}] - Min_l[M^*_{k,l}]}{\rho_{SF}} \tag{3-7}$$

where:

- $Max_l[M^*_{k,l}]$ and $Min_l[M^*_{k,l}]$ are the maximum and the minimum, over the time slices of a batch cycle, of the assumed mass inventory in HSU_k;
- ρ_{SF} is the density of the heat storage fluid (assumed to be constant, independent of the operating temperature).

5. calculation of the minimum total heat storage mass inventory [33]: in order for the heat storage system to operate feasibly, the mass inventory in any HSU_k must be within the range $[0,\rho_{SF}V_{min\ k}]$ at any time. Hence, the total mass inventory $M_{tot\ SF}$ is given by :

$$M_{tot\ SF} = \sum_k M^*_{k,0} - \sum_k Min_l[M^*_{k,l}] \tag{3-8}$$

where:

- $M^*_{k,0}$ represents the assumed mass inventory in HSU_k at the beginning of a batch cycle (generally set to zero for simplicity);
- $Min_l[M^*_{k,l}]$ is the minimum, over the time slices of a batch cycle, of the assumed mass inventory in HSU_k. Assuming initially $M^*_{k,0} = 0$, $-Min_l[M^*_{k,l}]$ introduces a correction only if $Min_l[M^*_{k,l}] < 0$ to remove the infeasibility, otherwise $Min_l[M^*_{k,l}] \equiv M^*_{k,0}$.

33. This calculation is particularly required when the heat storage fluid is not free, in which case its costs must be accounted in the total batch costs.

3.4.5 Main Issues

The synthesis of indirect heat integration consists in finding the most profitable scheme [34] to supply the batch process streams with the necessary heating and cooling, resorting to a combination of utility supply and internal heat recovery through intermediate heat storage (i.e. excluding any direct process-to-process heat exchange). Numerous degrees of freedom are available (see below), resulting in complex trade-offs. As previously recalled, several techniques of heat storage can be used; the best suited heat storage technique [35] depends on the shape of the *TAM* composites, the distribution of the supply temperatures of streams and their schedule, the proportion and constraining nature of non-flowing streams, and finally on constraints and costs functions associated with each type of *HSU*.

In the present work, a single type of *HSU*, namely *FTVM HSUs*, has been assumed [36]. Rescheduling of process streams is not considered, i.e. process schedule is considered as is [37].

Within this context, the indirect heat integration involves the following decisions and adjustment of parameters to be made [38]:

1. the type of *FTVM* heat storage system (closed (standard) or open);
2. the number of heat storage units (*HSUs*);
3. the re-use of *HEX* units on different process streams;
4. the streams which must not be integrated through the indirect heat recovery scheme (i.e. which are more profitably supplied by utilities);
5. the operating temperature of each *HSU*;
6. the amount of heat supplied by hot process streams to each storage sub-system, as well as the heat extracted from each *SSs* by cold process streams.

34. Owing to the large number of available degrees of freedom and considering the fact that criteria which will be applied by decision makers are often not clearly formalized *a priori* and are expected to evolve during the course of the project, the objective is rather to devise several good solutions rather than finding the "best one". This is one of the motivations to use genetic algorithms for the automatic synthesis problem (refer to Section 3.7).
35. Or more generally a combination of techniques.
36. This case has previously extensively analysed by *Stoltze* et al. (1992, 1995), *Mikkelsen*, 1998 *; *Mikkelsen* et al., 1998 as described in Sub-section 2.2.9.
37. Not ignoring the existence of schedule variations but knowing that the heat storage system inherently provides with some insensitivity margin, which can be further increased by installing spare capacity of *HSUs* (refer to *Mikkelsen*, 1998).
38. To illustrate the problem, consider e.g. the simple example process *EP-1* described in Appendix A.

The temperature of a stream after heat exchange with a storage sub-system is called *cut-off temperature* (i.e. the temperature separating the heat contributions to two adjacent *SSs*). Except the obvious inequality constraints of feasible temperature driving forces between the process streams and the *SSs* (refer to Sub-section 5.2.3), the key equality constraints linking all the parameters involved in points 5. and 6. above are the mass balance constraints expressed by Equations 3-4 and 3-5.

If the mass balance constraints are not met by the mass contributions of process streams solely, so-called *balancing utility* must be applied [39], penalizing the utility savings and the *TBCs* of the scheme.

Given a heat recovery, the minimization of the capital costs involves complex trade-offs effects between *HEX* areas/units of process streams - heat storage matches, and the capacities of *HSUs* (which are dependent on both the schedule and the amounts of the heat contributions as expressed by Equation 3-6).

3.5 Direct Heat Integration Issues

The synthesis of cost-optimal continuous *HENs* is a well known problem [40]. In the case of batch *HENs*, the following additional aspects must be taken into account :

- each time slice must be provided with a feasible *HEN*;
- the opportunities to re-use *HEX* units across time slices in various ways must be exhaustively considered (the re-use of *HEX* units allows for capital cost savings but gives rise to increased structural complexity);
- the re-used *HEX* units must generally be operated with a smaller active area in order to minimize the utility consumption during the considered time slice.

More details on these issues will be presented in Part III.

39. In some instances, mixing of heat storage fluid from the *HSUs* can reduce the required amount of balancing utility (refer to Sub-section 5.3.5). Further, if the capital costs of utility units strongly depend on their peak heat rate (such as chillers), it might be even more profitable (and secure) to size the unit for base load and operate it continuously by accumulating utility rather than sizing it for peak load and supplying it directly on process streams. This degree of freedom is also implicitly addressed.

40. Given a continuous process including both hot and cold process streams, find the process-to-process *HEX* structure and the heat rate of each *HEX* which minimize the total annual costs.

3.6 Guidelines for Data Extraction & Process Simplification

3.6.1 Motivation

Extracting data from batch processes is a critical step, since improper data extraction may severely restrict the opportunities identified during later analysis. Considering actual product recipes and their often complex schedules, a preliminary simplification step is required in order for the heat integration analysis to be manageable.

An extensive consideration of data extraction and simplification guidelines goes beyond the scope of this work; the description below is limited to :

- a short recall of basic principles;
- a simple technique to ensure correct sizing of heat exchangers while averaging the mass flowrate of batch process streams;
- a proposal for a systematic simplification of the process schedule in order to identify the most important time slices [41].

3.6.2 Basic Principles

Depending on the aims of the project and on the particularities of the process being analysed, consider the following points :

- whenever possible, prefer external heating and cooling during transfers (loading/emptying) instead of carrying out these tasks in a reactor vessel (see *Gremouti*, 1991). This guideline is particularly useful for projects aiming at a debottlenecking and rescheduling;
- beware non-isothermal mixing and cross-pinch heat transfers;
- account for the non-negligible thermal cycling and thermal inertia of batch equipment units by increasing the actual mass of process streams (the effect may be significant in case of partial batches). Consider heat losses to the

41. The number of time slices is a key issue for direct heat integration since the complexity of analysis and the required computing time increase over proportionally with the number of time slice, while the computing time for indirect heat integration is roughly proportional to this number (e.g. a simplified model of a brewing process features not less than 18 time slices, while a more realistic model would require about 25 slices, with several slices smaller than a few minutes !). There is a strong incentive to bring back this large number of slices to a more limited number of "fundamental" time slices, neglecting small or insecure time slices (i.e. slices sensitive to schedule variations).

environment (in operation and when idling) if the project aims at defining a realistic energy saving potential;

- ♦ describe the tasks carried out by equipment units on a Gantt Chart and question the actual schedule of the process with respect to the critical path and the possible existence of idling equipment units suitable for robust rescheduling of streams. This analysis should sketch potentially profitable alternative solutions which must be screened;
- ♦ search for overall plant bottlenecks after analysing the cost structure of the products (*Linnhoff*, 1988);
- ♦ register possible origins of systematic variations of the process schedule and their significance;
- ♦ take note of the existing layout of the plant and the position of processing equipment units, since piping costs may be significant. Foresee opportunities for grouping and/or sharing *HEX* units among different streams (refer to Section 8.3);
- ♦ check for the existence of process water streams allowing for an open heat storage system (refer to Section 5.4).

3.6.3 Averaging Rate

The heat rate of non-flowing streams (in-vessel heating and cooling) often features desired variations; even the mass flowrate of flowing streams (semi-continuous operations) may be temporarily disrupted by draining steps, etc. To avoid defining an additional stream and a specific schedule each time the heat rate feature a significantly different value, it is common practice to calculate the overall enthalpy change and average it over a simplified period of existence of the stream.

In doing so, the average mass flowrate $\dot{M}_{aver\ p}$ may be significantly smaller than the peak flowrate $\dot{M}_{peak\ p}$. To ensure proper sizing and costing of the *HEXs* on the considered stream, the calculated areas should be multiplied by the factor $\dot{M}_{peak\ p}/\dot{M}_{aver\ p}$. Another approximate technique consists in decreasing the heat transfer coefficient [42].

42. Ideally, the factor $\dot{M}_{peak\ p}/\dot{M}_{aver\ p}$ should be registered as an additional stream property and applied to the calculated area. In existing software programmes, a correction can only be introduced through a change of the heat transfer film coefficient of the stream; except in some particular cases in which the equivalent heat transfer film coefficient may be calculated in order to precisely result in the desired increase of the *HEX* area by a factor $\dot{M}_{aver\ p}/\dot{M}_{peak\ p}$, the modification of the heat transfer film coefficient cannot fit all possible match cases and only results in approximate area increases.

3.6.4 Guidelines for Reducing the Number of Time Slices

A few guidelines have been identified in order to minimize the number of time slices in the perspective of a direct heat integration. These guidelines may be organized in the following way :

1. eliminate "artificial", meaningless time slices generated by streams not relevant to the process-to-process heat integration (e.g. owing to infeasible temperature driving forces), or by soft streams;
2. identify highly schedule sensitive time slices and suppress them;
3. neglect streams of small duration and/or small heat content;
4. consider simple rescheduling opportunities allowed by existing equipment units (synchronization of streams using available storage capacities of process vessels), as long as the rescheduling is compatible with process requirements.

Examples and comments on these guidelines may be found in Appendix B. Simple quantitative criteria suitable for guideline 3. are also presented.

3.7 Principles of a *GA* Based Optimization

3.7.1 Introductory Comments

Resorting to a genetic algorithm (*GA*) to solve indirect heat integration problems (refer to Chapter 5) is definitely an important aspect of the proposed solution approach. *GAs* are basically optimization tools, and genetic, or evolutionary processes inspired algorithms tend to become commonly used. Therefore, they do not deserve an extended description here; rather, the working principles of *GAs* are briefly recalled, followed by a description of some distinctive features of the *Struggle GA* (*Grüniger* & *Wallace*, 1997). These features make *Struggle* a good candidate, but are also responsible for the observed optimization pitfalls, which have required special strategies (described in Section 5.5) to circumvent.

With respect to this last point, the aim of this work is not to compare the efficiency of various *GAs* to identify the *GA* best suited for the indirect heat integration problem ! The very first aim is to demonstrate the validity of the methodological approach, while a significant potential for efficiency improvement (e.g. *CPU*-time decrease) certainly remains to be harvested.

The *GA* and *MP* based approaches provide with valuable and often complementary tools [43]. *GA* approaches are *CPU*-time consuming and result in a large amount of calculations which are not exploited in the proposed optimization schemes. However, three reasons motivated the choice of the *GA* optimization road :

1. good experiences with *GAs* have been reported for complex non-linear optimization problems (e.g. at *LENI*: *Curti*, 1998; *Olsommer*, 1998; *Pelster*, 1998);
2. to deliver practice relevant solutions, a design & optimization framework has to account for often highly non-linear as well as discontinuous costs functions [44]; a realistic model of a system also requires *if ... then ... else* decisions to be implemented. These features are more difficult to readily account for within *MP* based approaches;
3. *GA* based approaches automatically deliver several good solutions instead of only "the best one" [45] [46].

A short review of the available optimization approaches and their comparison can e.g. be found in *Olsommer* (1998), section 2.5.

3.7.2 Working Principle of a *GA* Based Optimization

A *GA* mimics, in a computational manner, the natural evolution of living species, where the fittest individuals - i.e. the ones which are best suited to the constraints of their environment - have more chances to survive and reproduce, while other poorly adapted individuals tend to disappear. Characteristics of parents (coded in the genetic material) mix together in a stochastic manner during reproduction and are partly inheritated by the offspring(s); changes of characteristics may be stochasticaly introduced by mutation.

Numerous variants of *GAs* have been developed in the last decade to address a variety of problems. These algorithms can be classified according to criteria such as the coding of variables, the reproduction strategy (i.e. the way the parents are

43. A combination of both approaches could save computing time : the *GA* based optimizations performed in this work deliver solutions which, for instance, meet the mass balance equality constraints with a high precision. But the fine adjustment of the continuous variables (while all integer decisions are made) requires a large number of generations and *NLP* solvers would achieve it much faster.
44. For instance, heat exchangers as well as heat storage tanks are often available from manufacturers in series of different size ranges, each being characterized by its own cost function.
45. The criteria which will be applied by decision makers are often not clearly defined *a priori* and are expected to evolve during the course of the project.
46. This is actually not a particular feature of the *GA* approaches, since mathematical programming approaches may delivers several solutions of *MINLP* problems using integer cuts.

selected and their characteristics (genetical material) mixed in the offspring), the replacement strategy (i.e. the "offspring management"), the possible existence of groups evolving independently (e.g. *Wang* et al., 1997), etc. Beyond these differences, they all have the following common properties :

- they work with a population of individuals (solutions), which evolves over a number of generations;
- the evolution is influenced (at various degrees) by stochastic processes;
- unlike the *MP* based algorithms, they only need the value of the objective function to rate an individual.

In the context of optimization, an individual is characterized by a set of values of the decision variables (*DVs*) and represents a potential solution, with Y denoting the vector of integer *DVs*, and X the vector of continuous *DVs*. A generation actually refers to a number of offsprings equal to the number of individuals making up the population (N_{Pop}). A simple (one-level) optimization scheme is shown on **Figure 3-5** : after random initialization, the population of individuals evolves (by

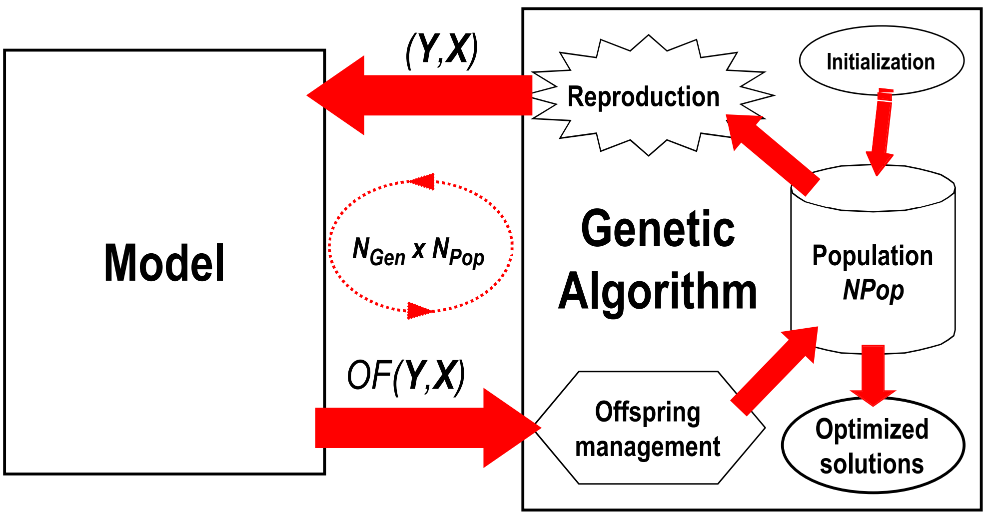

Figure 3-5 A simple (one-level) *GA* based optimization scheme.

reproduction, mutation and survival of the fittest) over a number of generations (N_{Gen}). During this evolutionary process, $N_{Gen} \times N_{Pop}$ individuals are rated, i.e. (Y, X) of each offspring is supplied to the model, which returns the corresponding value of the objective function $OF(Y, X)$.

In a basic *GA* implementation, reproduction (i.e. propagation/evolution of characteristics) is mainly controlled by the strategy of fitness proportionate reproduction which promotes the survival of the fittest, i.e. the probability for an individual to be "copied" in the next generation is proportional to the degree to which he fulfils the objective function of the problem (=fitness factor). A small mutation rate allows to randomly explore the solution space for other potential solutions (to keep the diversity of solutions), while crossover combines existing characteristics of the parents (by random mixing) with the hope that the offsprings will behave better than the parents by taking advantage of a combination of favourable features.

3.7.3 Features of the *Struggle GA*

The *GA* implementations built on the basic principles mentioned above are plagued with the problem of premature convergence: as the number of generations increases, all individuals of the population become nearly identical, i.e., in the solution space, move towards a single optimum (not necessarily the global one !) and accumulate there. Such *GAs* are unable to keep trace of the variety of local optima.

To get rid of this significant limitation, so-called niching methods (or multimodal *GAs*) have been developed (e.g. refer to *Grüniger* & *Wallace*, 1997) to preserve diversity and maintain multiple solutions in a population. They use various techniques to restrict the number of individuals in a niche (i.e. around an optimum), but feature a common foundation in that each of them applies a replacement strategy based on the concept of similarity between the offspring and individuals of the existing population. The similarity (or dissimilarity) of individuals is expressed by the distance (in the solution space) between them.

Struggle (*Grüniger* & *Wallace*, 1997) is a multimodal *GA* providing an improved niching method, demonstrated to be efficient in searching multiple optima of functions of continuous (real) variables. *Struggle* does not resort to binary coding of continuous *DVs*, which is less accurate; continuous *DVs* are treated as is, using a special crossover operator called *blend crossover*.

For any given x_i continuous *DV*, the *blend crossover* takes the value of that *DV* of both parents (x_{ia} and x_{ib}) and generates a new value with a uniform probability distribution over $[x_{ia} - \alpha(x_{ia} - x_{ib}), x_{ib} + \alpha(x_{ia} - x_{ib})]$ (uniform scatter around the mean value $(x_{ia} + x_{ib})/2$). This crossover actually includes both the exploitation of the existing characteristics of parents (values within $[x_{ia}, x_{ib}]$) and the exploration of new values (ranges $[x_{ia} - \alpha(x_{ia} - x_{ib}), x_{ia}]$ and $[x_{ib}, x_{ib} + \alpha(x_{ia} - x_{ib})]$). Exploitation and exploration are balanced for $\alpha = 0.5$, which is generally used and avoid the need for mutation in order to keep diversity.

Struggle applies the niching method sketched on **Figure 3-6**. Again, the key point for an efficient niching lies in the definition of a meaningful distance function between individuals. The distance function aims at identifying the nearest (most similar) individual to be compared with the offspring, and to be replaced only if the offspring performs better than the most comparable existing individual.

This is a sound strategy, since the comparison of *OFs* only applies to a pair of individuals which are "most similar".

3.7.4 Practical Issues for Applying *Struggle*

Defining a distance function for problems including only continuous *DVs* is not a straightforward task. This involves first the identification of the variables [47] suitable for expressing the similarity (or dissimilarity) of two individuals (called *distance variables*). Next, a weighting factor for each distance variable must be defined, owing to the fact that the distance variables feature different physical units, or more generally because a difference in one variable is not expected to result in the same dissimilarity as a difference in another variable. There is no single answer to the above two issues. Nevertheless, the optimization results are expected to show a low sensitivity to the precise definition of the distance function as long as the function is "reasonable".

Integer *DVs* add a significant complexity in the definition of a distance function. Differences in these variables, which control e.g. structural decisions, are not easily compared with differences in continuous *DVs*. *Olsommer* (1998) proposed one possible technique. In any case, insight into the problem being studied and account for the objectives of the project are required, while a significant part is ultimately left to the subjectivity of the engineer.

The second observation relates to the replacement strategy: if the decision to keep an offspring or reject it applies immediately on the basis of the *OF* comparison, the offspring is not given time to improve before a well-founded decision may be made, as is the case of a particular class of *GAs* (e.g. *Wang et al.*, 1997).

47. These variables are not necessarily the *DVs* of the individual but might be dependent or aggregated variables too.

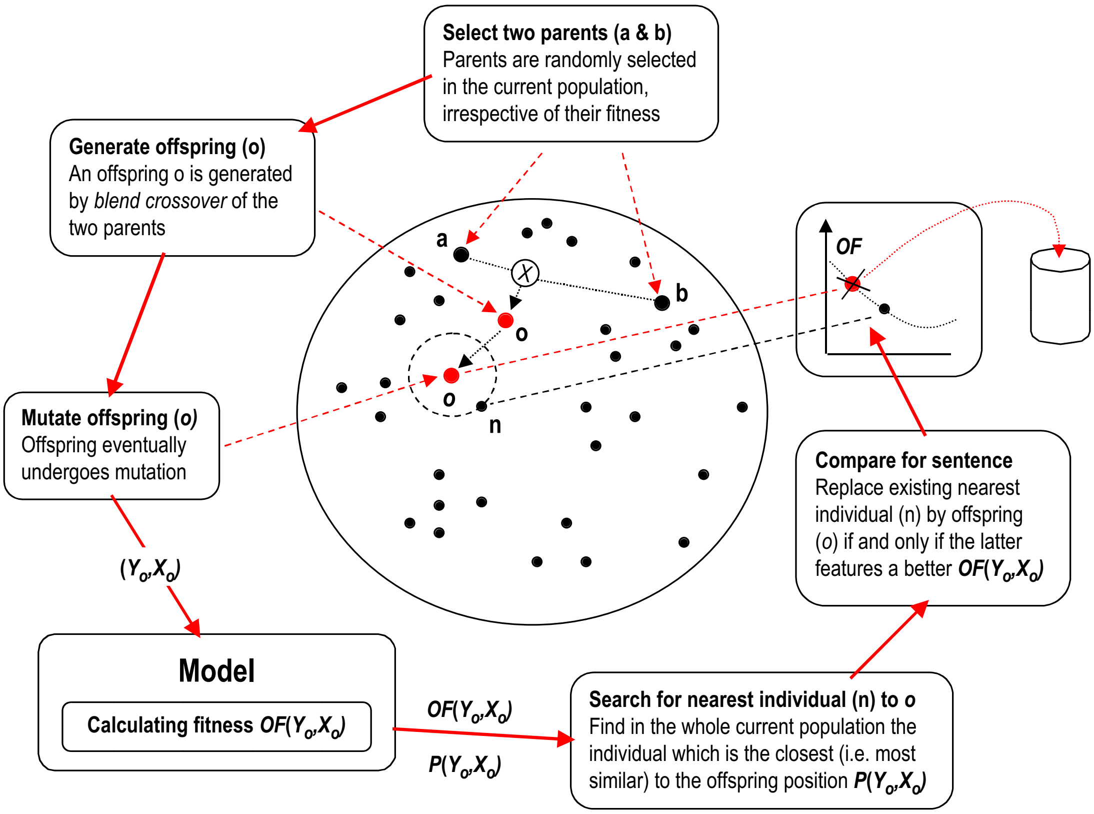

Figure 3-6 Reproduction strategy of the *Struggle GA*
(in this context, *P(..,..)* means the position of an individual in the solution space).

Since any *GA* optimization is very intensive in *OF* evaluations, which represent the largest contribution to the computing time, the following guidelines should be observed when setting up the model :

1. as far as possible, avoid the need to solve implicit equations requiring iterations;
2. whenever manageable, include the constraints in the definition of variables so as to minimize the number of infeasible solutions.

The application of these guidelines to indirect heat integration problems is explained in Sub-section 5.2.4. The insight gained into the definition of the distance function and into the side-effects of the replacement strategy, as well as the resulting improvements of the optimization strategy are summarized in Section 5.5. Typical settings of the optimization parameters and examples of results are provided in Chapter 6. Guidelines are drawn in Appendix F.

Part II

INDIRECT HEAT INTEGRATION

Chapter 4

TARGETING OF INDIRECT HEAT RECOVERY SCHEMES

4.1 Introduction

Possible causes of schedule variations frequently encountered in batch processing have been mentioned in Chapter 3. The indirect mode of heat integration can accommodate such variations and safeguard the operational flexibility of batch plants. The main issues in indirect heat integration have been highlighted and the problem has been stated in general terms. The degrees of freedom available for devising cost-optimal indirect heat recovery schemes (*IHRSs*) have also been described.

4.1.1 Motivation

The design of 100 % indirect heat recovery schemes is actually not a new idea. *Stoltze* et al. (1992, 1995) have already addressed this issue using a combinatorial approach called the *Permutation Method* (*PM*), which has been further developed by *Mikkelsen* (1998); but the proposed *Post-optimization* (*PO*) stage for fine-tuning the continuous variables of *IHRSs* remains difficult to apply in practice (refer to Sub-section 2.2.9).

From a conceptual design/targeting point of view, the rather black-box nature of the combinatorial search comes with the following drawbacks :

- although the *PM* takes the supply temperature of streams explicitly into account, the relationship between the set of integrated streams and the achievable heat recovery (*HR*) cannot be readily assessed. In other terms, graphical insight into the effect of selecting a stream, or modifying its supply temperature, is lacking;

- a technique to calculate the minimum number of heat storage units (*HSUs*) to achieve a given heat recovery level is desirable; the determination of the feasible assignment ranges of intermediate *HSUs* need to be addressed.

The more Pinch Analysis (*PA*) oriented methods proposed so far (e.g. *Krummenacher* & *Favrat*, 1995; *Sadr-Kazemi* & *Polley*, 1996; and *Krummenacher* & *Auguste*, 1997) have provided guidelines for the assignment of *HSUs* but have not explicitly considered the heat recovery dimension of the problem.

4.1.2 Overview

The proposed heuristic "targeting" methodology results from the application and the further development of the above mentioned *PA*-oriented contributions. Backed with suitable graphical tools, this method completes (but does not replace) the *PM* by providing the designer with more insight into and understanding of the *HR* – number of *HSUs* issues.

Section 4.2 introduces the simple ideas and assumptions behind the proposed tools and methods.

The graphical procedure to define the minimum number of *HSUs* and their assignment ranges according to the vertical model assumption is explained in **Section 4.3**. The storage pinch is also described.

Section 4.4 presents opportunities to relax the relationship between the minimum number of *HSUs* and the *HR* by removing small constraining streams or by considering the schedule of streams.

The proposed procedure is briefly demonstrated on the *EP-1* example process in **Section 4.5**.

Finally, **Section 4.6** summarizes the benefits and the limitations of the procedure.

4.2 Solution Approach & Assumptions

How many *HSUs* must be used to achieve a given level of heat recovery ? How to select their operating temperature ? What about the effect of selecting or leaving out a process stream on the constraints imposed to *HSUs* ?

To answer such questions and be suitable for conceptual design / targeting purposes, the method has to be backed with suitable graphical representations. The time average model (*TAM*) composite curves (in energy) are the obvious starting point for the assignment of the *HSUs*; they should be completed to account for the discrete effect of the supply temperature of streams.

Unlike continuous processes, for which the process pinch is selected as the main parameter to explore the energy-capital trade-off, the representative parameter to explore the energy-capital trade-off of *IHRSs* is the heat recovery, i.e. the heat actually transferred from the hot process streams to the cold process streams through the heat storage system (refer to Section 3.3). The heat recovery is the driving force for energy cost savings.

The mass balance of *HSUs* is a difficult issue to be addressed by a targeting method, unless the heat supplied by hot process streams to any storage sub-system (*SSs*) is automatically equal to the heat delivered by the *SSs* to the cold process streams. This condition is met if the heat recovery assigned to each *SSs* is vertically defined on the *TAM* composites. This vertical definition of the heat recovery range of each *SSs* is called the *vertical model* assumption.

At this point, consider the simple example process *EP-1* [1] which will be used throughout this Chapter to illustrate the proposed methods. The process streams are listed in **Table 4-1**, and their schedule is represented on **Figure 4-1**. The vertical

Stream Name	T supply [°C]	T target [°C]	CP [kW/°C]	Heat Rate [kW]	Heat [kWh/bat.]	t start [min]	t stop [min]	h [W/m^2°C]
C1	25	100	1	-75	-127.5	0	102	1000
C2	130	180	3	-150	-180	48	120	1000
C3	80	105	5	-125	-168.75	39	120	1000
H1	135	15	1.1	132	204.6	9	102	1000
H2	100	95	20	100	90	48	102	1000
H3	165	125	3.5	140	21	39	48	1000
H4	165	125	3.5	140	42	102	120	1000

Table 4-1 Process streams of the example process *EP-1*.

definition of the heat recovery ranges is exemplified on **Figure 4-2**, given the location of the four *HSUs* on the *EP-1 TAM* composites. The cut-off temperatures of the streams (refer to Sub-section 3.4.5) are defined by the intersection of the vertical lines passing through the location of *HSUs* making up each *SSs*. The corresponding *IHRS* is represented on **Figure 4-3** [2].

1. Detailed process and economic data are provided in Appendix A.

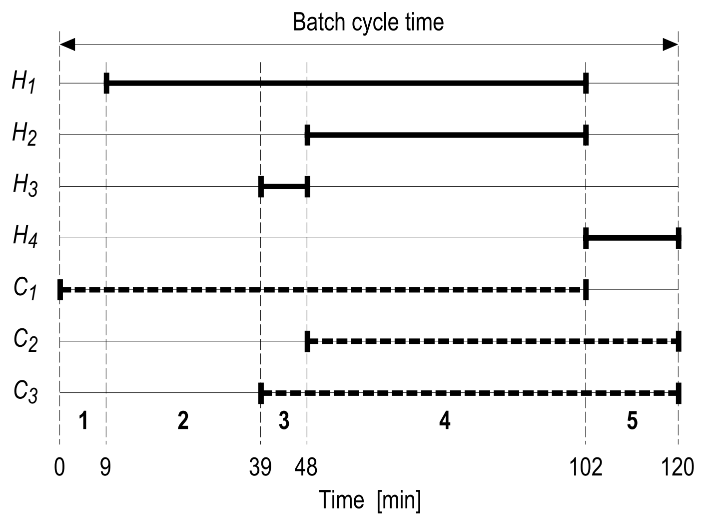

Figure 4-1 Schedule of the *EP-1* process streams and corresponding time slices (one batch cycle time).

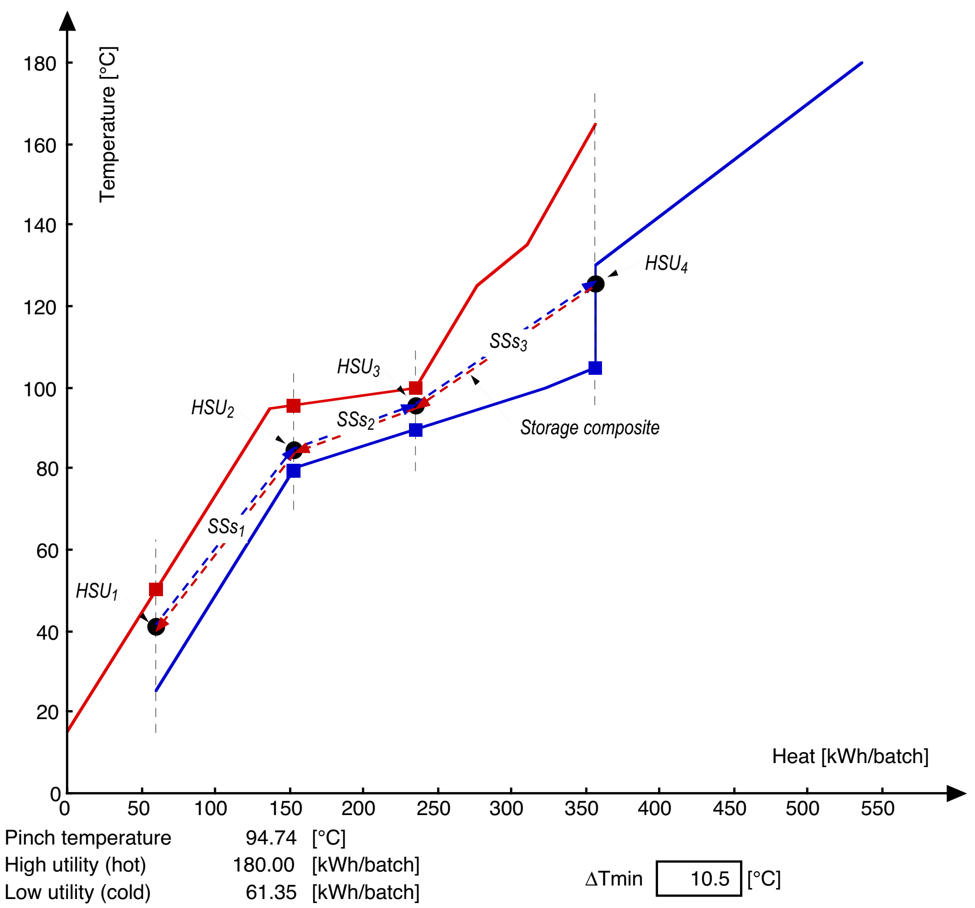

Figure 4-2 Vertical model of a heat recovery system for *EP-1* including 4 *HSUs*.

2. The calculation of the minimum capacity of *HSUs* is described in Sub-section 3.4.4.

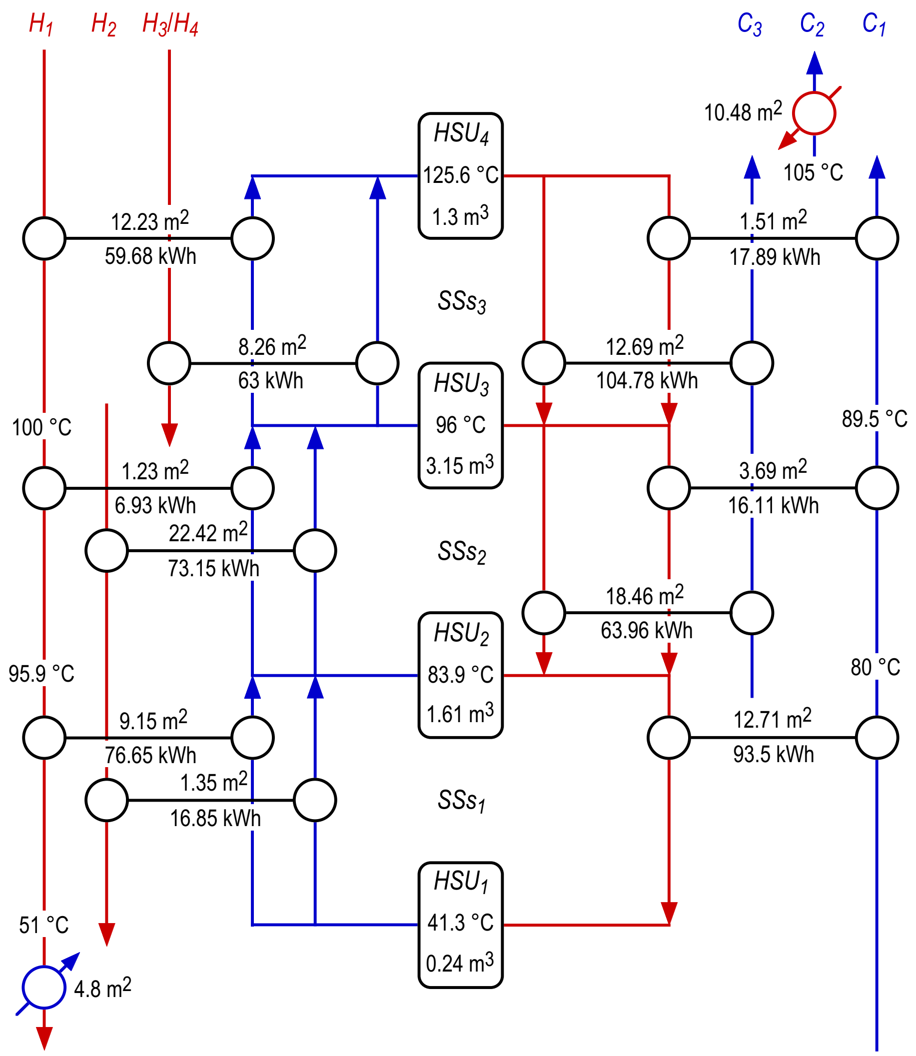

Figure 4-3 An indirect heat recovery scheme for process *EP-1* obtained using the vertical model assumption (achieves heat transfers depicted on Figure 4-2).

The vertical model corresponds to giving a high priority to the minimization of the heat transfer area [3] and not taking advantage of the sequence of heat supply and heat sink to minimize the heat storage capacity, i.e. the *HEX* area - *HSU* capacity trade-offs are not addressed. Nevertheless, the vertical model does not necessarily mean that the heat contributions of process streams are transferred vertically to/from the *SSs*, as will be seen in Sub-section 4.3.1.

The procedure to define the minimum number of *HSUs* and the feasible assignment of these *HSUs* needed to arrive e.g. at the *IHRS* of Figure 4-3 is introduced next.

3. Owing to different heat transfer film coefficients and different durations of the time slices (the *TAM* composites represent energy or mean heat rate over the batch, and give no indication of the actual heat rate), the "vertical heat transfer" between *TAM* composites does not necessarily lead to the minimum heat exchange area.

4.3 Heat Storage Unit Assignment

4.3.1 Storage Pinch

Before describing the proposed systematic method for the identification of the minimum number of *HSUs* to reach a given level of heat recovery, the concept of *storage pinch* (ΔT_{minSto}) has to be introduced. The storage pinch ΔT_{minSto} is basically a temperature pinch, like the well-known process pinch (ΔT_{minPro}), in that heat can only be transferred from a hot process stream to a storage stream (or from a storage stream to a cold process stream) if a positive temperature driving force exists.

Compared to the process pinch, a storage pinch features the distinctive property of not being apparent on the energy composites extended to include the storage composite. Storage pinches are at the root of the definition of the minimum number of *HSUs*.

Figure 4-4 highlights a storage pinch with cold streams and the way the actual temperature driving forces can be represented [4]. The operating temperatures of *HSUs* (T_2 = 99 °C, T_3 = 130.6 °C), as well as their range of possible variation, called the *temperature margin* (ΔT_2 = 1 °C; ΔT_3 = 5 °C), are imposed by adjacent storage sub-systems.

The lower part of Figure 4-4 represents a portion of the energy composites, to be heat integrated through the heat storage sub-system SSs_2 (i.e. made of HSU_2 and HSU_3). The cold composite includes three streams (C_1, C_3 and $C_{3\ rem.}$, defining the *cold limiting supply temperature profile* - a representation introduced in the next Sub-section), while the streams actually included in the hot composite do not matter for the discussion here. The lowest temperature of HSU_2 is imposed by the supply temperature of $C_{3\ rem.}$. The temperature driving forces (*TDF*) when transferring heat from SSs_2 to $C_{3\ rem.}$, tends towards zero; in other words a storage pinch appears.

The upper diagram decomposes the storage and cold composites to represent the actual match-wise temperature profiles between the split stream associated to SSs_2 and C_1, C_3 and $C_{3\ rem}$, respectively. The storage pinch (ΔT_{minSto} = 0 °C) is present at the cold end of the match SSs_2 -$C_{3\ rem.}$. Test cases indicate that economical

4. This case is part of the cost-optimal solution to a mixed direct-indirect heat integration of example process *EP-1*, which must not be compared to the (only) indirect heat integration represented in Figures 4-2 and 4-3. Although this is not the subject here, it has been chosen because it exemplifies the problem particularly well.

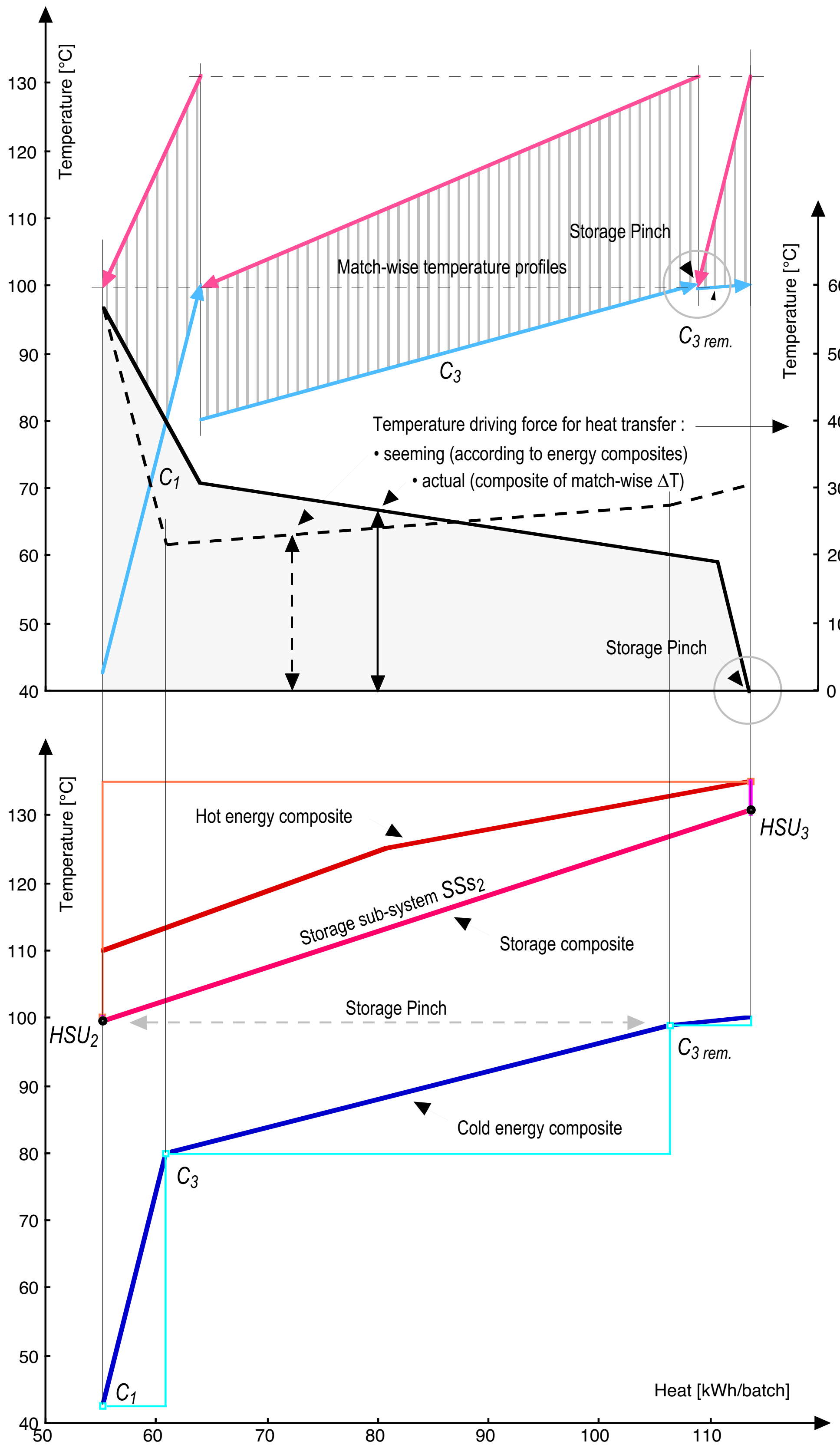

Figure 4-4 Storage pinch and related temperature driving forces representation (refer to comments in the text).

storage pinches can be in the order of 1 *°C* or even less, which are quite seldom found in continuous processes. These surprising small ΔT_{minSto} values actually result from the fact that they are related to a very local effect, i.e. pinched heat transfer applies only to a small amount of heat [5].

The match-wise temperature profiles can be composed together by sorting them in decreasing order of magnitude so as to represent the actual *TDF* from SS_2 to the cold streams; the storage pinch and its very local effect is clearly identified on the right. The dotted line represents the seeming *TDF*, as derived from the energy composites represented on the lower diagram. Note that it does not matter whether the match-wise temperature profiles are composed in increasing or decreasing order of magnitude. In order to assess the actual effect of the storage pinch in terms of heat transfer area and related capital costs, one should weight the match-wise temperature profiles by the relative duration of the related streams.

If the storage composite would include as many *HSUs* as the number of process streams, i.e. where a *HSU* would be assigned to each supply temperature of either the hot or the cold energy composites, there would not be any storage pinch effect and the actual *TDF* would be equal to the *TDF* available between the energy composites and the storage composite. The limitation to heat recovery would arise from the process pinch itself [6].

4.3.2 Defining the Minimum Number of *HSUs*

Consider Figure 4-2. Before describing the procedure for determining the minimum number of intermediate *HSUs*, notice the following points :

- to totally recover heat from the vertically defined heat recovery regions, the first and last *HSUs* have to be located at the cold end and the hot end of the overall heat recovery region, respectively. The problem is actually the number and the location (temperatures, heat recovery range) of the intermediate *HSUs*;
- the rule proposed by *Sadr-Kazemi* & *Polley* (1996) can be formulated as follows : ***the operating temperature of any HSU has to be higher than the highest supply temperature of cold***

5. They are also found because of complicated direct-indirect heat integration trade-off effects.
6. But a design featuring a large number of rather small *HSUs* (i.e. a number of *HSUs* significantly in excess of the minimum number of *HSUs*) would not be economical. Not only are *HSUs* of small capacity a poor design (from an energy and economics point of view), but they would require a large number of small *HEXs* too. Unlike continuous processes, it appears that for most batch processes (depending on both the schedule and the discrepancy of the supply temperatures of the streams), the process pinch has a small effect on the optimal heat recovery, while the storage pinches (hence the number of *HSUs*) are deciding the optimal trade-off between heat recovery and capital costs (before any process pinch comes into play).

streams included in the storage sub-system on the right (for which the considered HSU is the cold storage of the sub-system), while it also has to be lower than the lowest supply temperature of hot streams included in the storage sub-system on the left (for which the considered HSU is the hot storage of the sub-system). Hence the operating temperature of a *HSU* is constrained upwards by hot streams, while it is constrained downwards by cold streams. The proposed systematic procedure is an application of this formulation;

- the above formulation actually contains several cases : an intermediate *HSU* can be imposed (i.e. the heat recovery range of the *SSs* be limited) by cold streams only, by hot streams only or by both;
- to minimize the number of *HSUs*, the heat recovery range of a *SSs* has obviously to be maximized. The starting point can be either the hot end or the cold end of the heat recovery region, providing two limiting cases (see below).

4.3.2.1 Limiting Supply Temperature Profiles

Given the *TAM* energy composites, first draw the *limiting supply temperature profiles* (*LSTPs*), staircase temperature profiles which define the actually most constraining cold (hot) stream supply temperature as a function of the vertically corresponding position on the cold (hot) composite [7].

The cold *LSTP* is drawn according to the following rules (refer to **Figure 4-5**) :

- start at the lowest supply temperature and move horizontally to the right, until a new supply temperature is vertically crossed;
- at this point, move vertically to this temperature on the cold composite;
- again, move horizontally until the next vertically aligned supply temperature;
- continue until the last supply temperature;
- move vertically to the hot end of the cold composite when vertically aligned with this point.

In this way, the cold staircase temperature profile begins at the cold end of the cold composite and ends up at the hot end of the same composite.

7. If utilities are to be stored too (instead of being directly applied at the target temperature side of the process streams), the procedures described in this Chapter should be applied to the balanced *TAM* composite curves, i.e. including the utility streams.

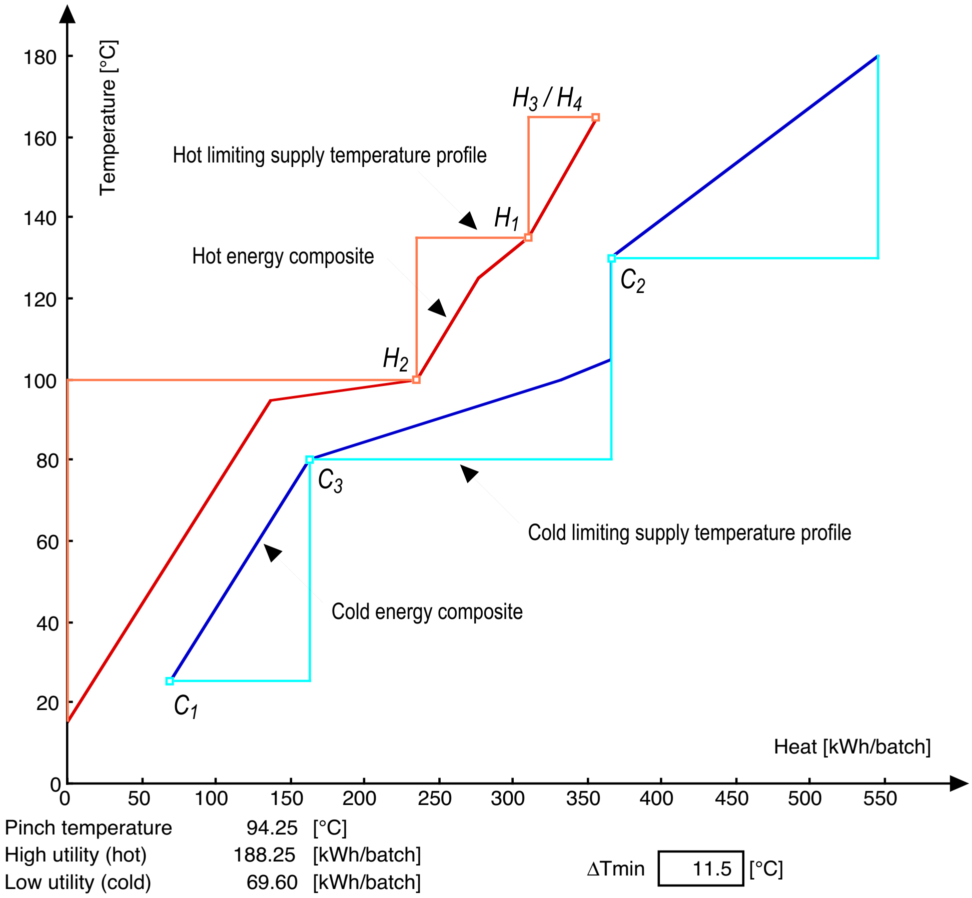

Figure 4-5 Limiting supply temperature profiles of example process *EP-1* (refer to comments in the text).

The hot *LSTP* is drawn in a similar manner, except that it starts from the hot end of the hot composite and proceeds to the left towards the cold end, as indicated on Figure 4-5.

4.3.2.2
Defining the Intermediate HSUs

Once the *LSTPs* have been drawn, the minimum number of *HSUs* can be determined with respect to the cold composite (refer to **Figure 4-6**), i.e. starting from the cold end of the cold composite (which is also the cold end of the heat recovery region).

Then, the minimum number of *HSUs* with respect to the hot composite (i.e starting from the hot end of the hot composite and progressing downwards, refer to **Figure 4-7**) is determined. Of course, the minimum number of *HSUs* does not actually depend on the search direction (temperature upwards or downwards), but the boundary position (in term of energy coordinate) of *HSUs* are different in general

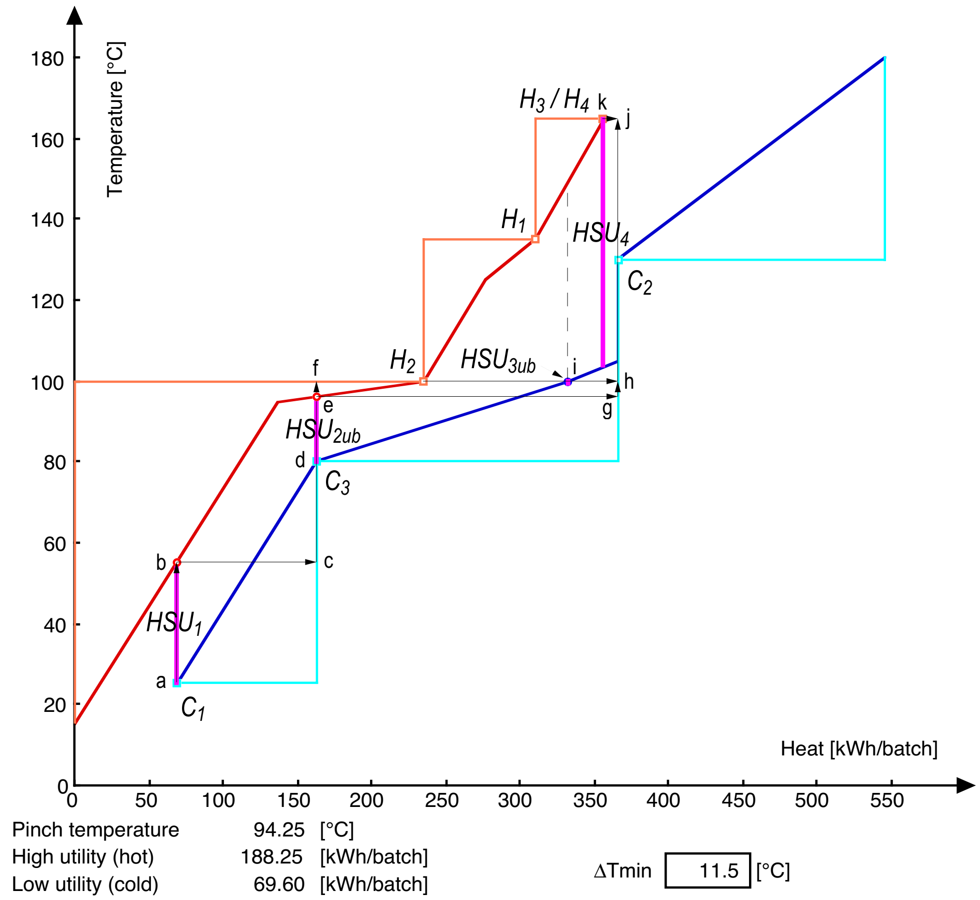

Figure 4-6 Defining the upper boundary position and the minimum number of *HSUs* with respect to the cold energy composite - example process *EP-1* (refer to comments in the text).

(e.g. compare the upper bound position HSU_{2ub} on Figure 4-6, with the lower bound position HSU_{2lb} on Figure 4-7).

The minimum number of *HSUs* with respect to the cold composite is determined according to the following rules (refer to Figure 4-6) :

1. the first heat storage unit (HSU_1) is of course assigned to the cold end of the heat recovery region (point a);
2. move vertically to the hot composite, defining the highest possible supply temperature of cold streams to be included in the storage sub-system (point b). Point b is not constrained by hot streams (actually it is never constrained, since it is the cold end of the heat recovery) and hence represents the absolute maximum operating temperature of HSU_1. Therefore moving horizontally to the vertical segment of the cold *LSTP* (point c) defines all cold streams (if any) which supply temperature is compatible with the storage sub-system SSs_1 and identify which cold stream requires the introduction of a new heat storage unit (in this case cold stream C_3);
3. the cold *LSTP* segment can be extended to a vertical line, which intersects the cold (point d) and hot (point e) composites. This defines the location of HSU_2 with respect to the supply temperature

of the cold streams. It remains yet to be verified whether the supply temperature of the hot streams are not more constraining than that of the cold streams (a case that would be encountered e.g. with a process including only one cold stream but several hot streams). This is checked by searching for the intersection of the vertical line passing through point c and the horizontal line passing through the first supply temperature encountered starting from point b (here hot stream H_2);

4. if the intersection (point f) is above point e (i.e. above the hot composite), hot streams are not constraining at all, i.e. no hot stream starts in the identified SSs_1. If the intersection is located between point e and d (i.e. in the inter-composite region), the hot streams constrain the operating temperature of HSU_2, but not its location (heat recovery range). If the intersection is located below point d (more generally below the cold composite), the hot streams are more constraining than the cold streams, since they not only constrain the operating temperature of HSU_2, but also its location, which has to be shifted on the left (see point 7. below for the procedure relevant to this case);
5. point f actually lies above point e, hence HSU_2 can be kept as is. The operating temperature of HSU_2 is not constrained on the hot side and point e represents the maximum operating temperature of HSU_2, and hence moving horizontally to the vertical segment of the cold *LSTP* (point g) will define all streams (if any) which supply temperature is compatible with the storage sub-system SSs_2 and identify which cold stream requires the introduction of a new heat storage unit (cold stream C_2 in this case);
6. the vertical line passing through point g lies outside the heat recovery range, indicating that HSU_3 could maybe be located at the hot end of the heat recovery range and that minimum number of *HSUs* would be 3. But it remains to be verified whether the hot streams are not more constraining than the cold streams;
7. this is checked by searching for the intersection of the vertical line passing through point g and the horizontal line passing through the first (hot) supply temperature encountered starting from point e (here again hot stream H_2). The intersection (point h) is located below the cold composite, and the maximum allowable location of HSU_3 is actually point i. If HSU_3 is located at point i, its operating temperature is constrained to be lower than or equal to the supply temperature of H_2, while at the same time higher than or equal to the temperature of the cold composite at point i, i.e. the operating temperature of HSU_3 is pinched on both sides;
8. moving again horizontally from the highest possible operating temperature of HSU_3 (i.e. temperature of point i) to the cold *LSTP* defines point h again. But the intersection of the vertical line passing through h and the horizontal passing through the first (hot) supply temperature above (on the right) of HSU_3 (H_3/H_4) defines point j, which is located "between" the composites but outside the heat recovery range. Therefore HSU_4 can be located at the hot end of the heat recovery region, and point j (representing the maximum operating temperature of HSU_4) be translated to point k;
9. finally, starting at the cold end, 4 *HSUs* are required. The possibly constraining supply temperatures of cold streams are accounted for by increasing the lower boundary of the temperature margin of storages. Such a case is not found here, since the lower boundary on the operating temperature of all *HSUs* is defined by the cold composite itself.

The same procedure can now be applied starting from the hot end, reversing the role of hot streams and cold streams (refer to Figure 4-7). Note that the numbering of *HSUs* is in the reverse order of placement, for easier comparison with the case resulting from the procedure starting from the cold end of the cold composite. Note also that H_1 is constraining the maximum allowable temperature of HSU_4, a case

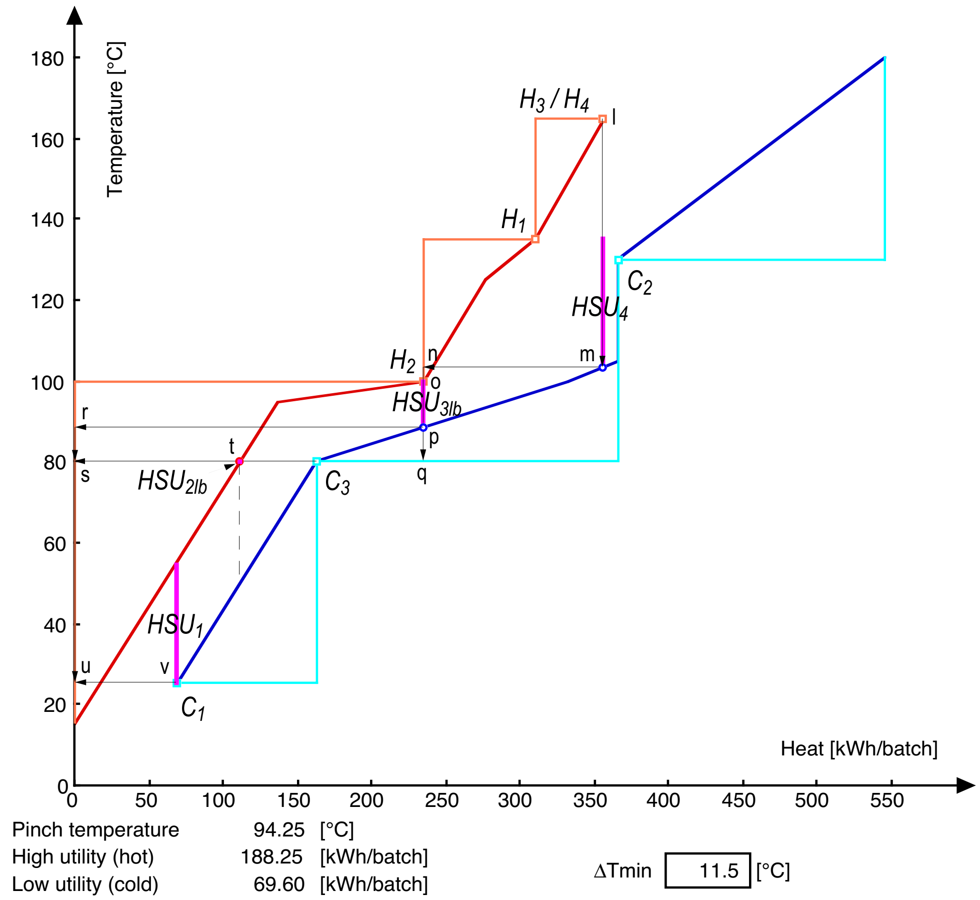

Figure 4-7 Defining the lower boundary position and the minimum number of *HSUs* with respect to the hot energy composite - example process *EP-1* (refer to comments in the text).

which was not found when defining the *HSUs* starting from the cold end of the heat recovery region (see former step 9).

4.3.2.3 Summary and Comments

Given a heat recovery value to be achieved, the minimum number of *HSUs* is independent of the starting point for their determination (cold end or hot end), as can be noticed from the above example (*EP-1*).

The results of the former steps are summarized on **Figure 4-8**, showing that at least 4 *HSUs* are required for the chosen *HR* level. With respect to energy, the positions of HSU_1 and HSU_4 are fully determined, while HSU_2 and HSU_3 can be chosen between the two boundary positions previously identified, as highlighted. Actually the operating temperature and the heat recovery ranges are linked, and the assignment of the intermediate *HSUs* can selected anywhere in the shaded regions.

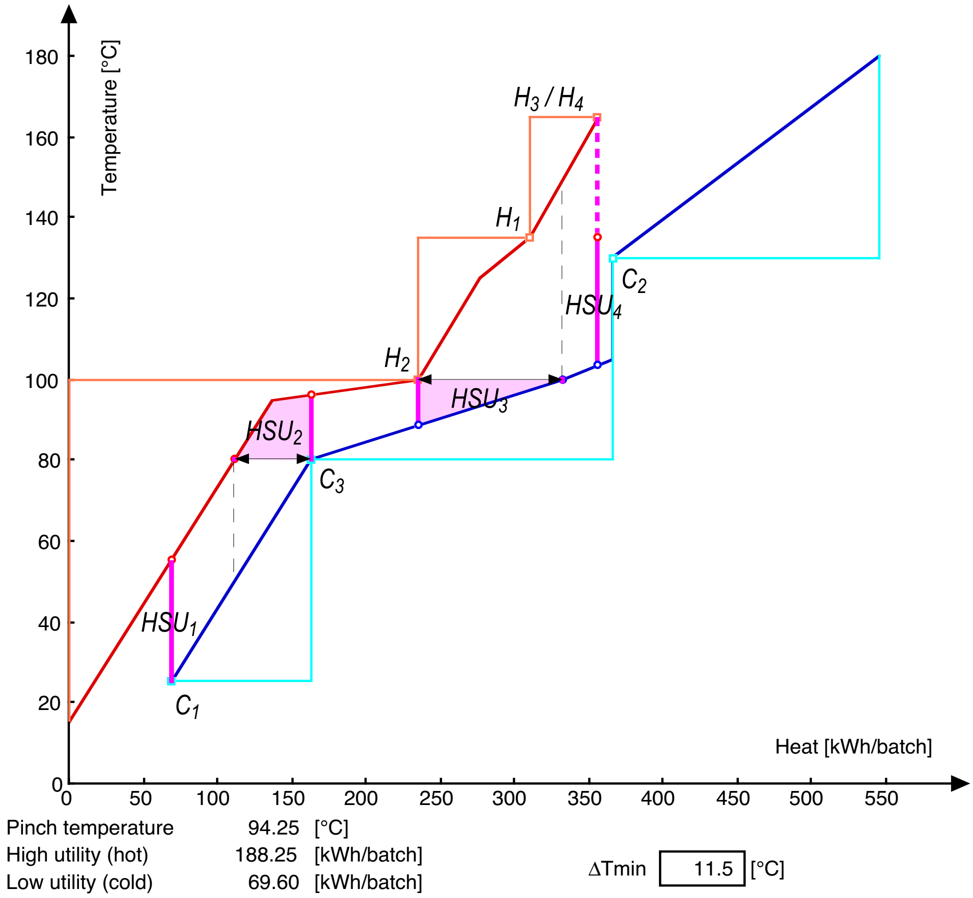

Figure 4-8 Operating temperature and heat recovery margins of the minimum number of *HSUs* - example process *EP-1* (refer to comments in the text).

This degree of freedom can be used to minimize capital costs, since e.g. HSU_2 is fully pinched at its lower boundary position, while it benefits from a full (unpinched) temperature window if at its upper boundary position.

Note that in the present case, the energy ranges of HSU_2 and HSU_3 do not overlap, but this is not a general rule, as illustrated on **Figure 4-9**, which represents a brewery process [8]. This demonstrates that the intermediate *HSUs* cannot be independently assigned any position within the identified range; in other words, once HSU_n is assigned, the assignment of HSU_{n+1} has to take the assignment of HSU_n into account (and so on for all intermediate *HSUs*). Referring to the brewery process, if HSU_2 was assigned the HSU_{2ub} position (although this would be a bad choice), HSU_3 could not be assigned the HSU_{3lb} position (or any other place on the left of HSU_2).

8. Also based on the brewery process at the *Brasserie du Cardinal*, the considered process is nevertheless somewhat different from *EP-4*, which is not an issue here for the illustration purpose.

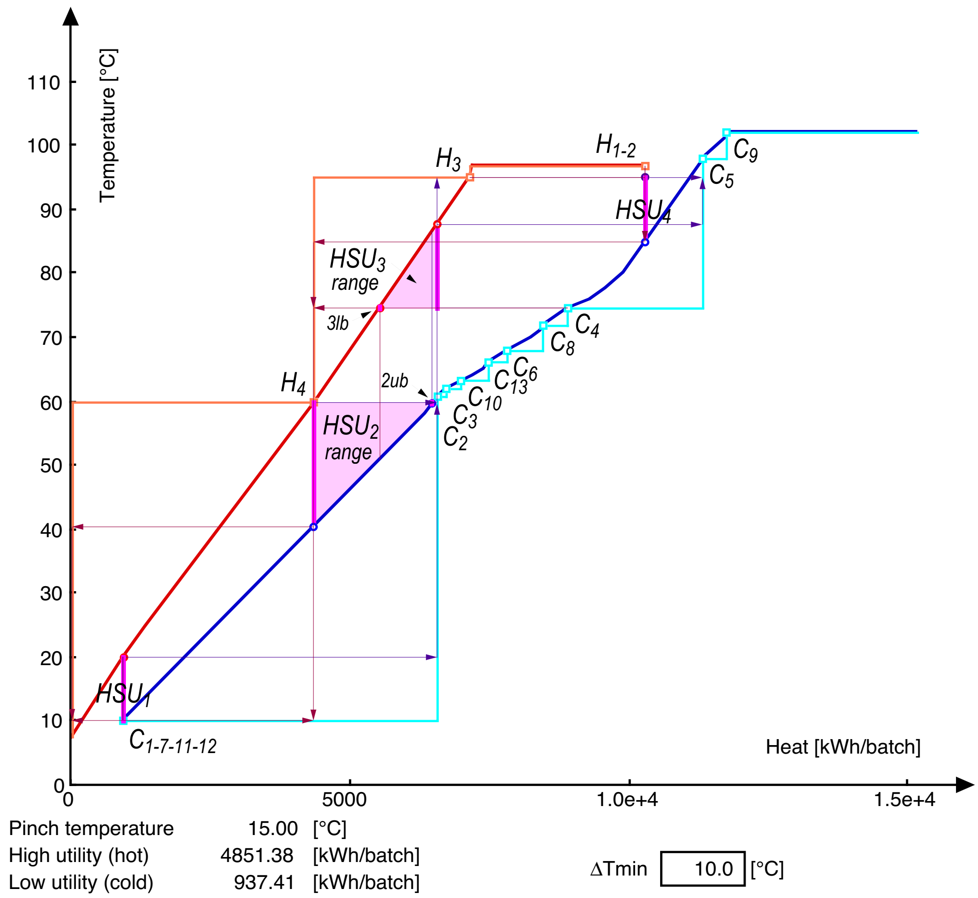

Figure 4-9 Overlapped *HSU* assignment ranges (case of a brewery process).

When selecting the position of the intermediate *HSUs*, the following aspects should also be taken into account :

1. a *HSU* should be assigned either at the end or at the start of a process stream to minimize the number of *HEX* units (i.e. avoiding the need to match a process stream with too many *SSs*) [9];
2. the heat recovery range of a *SSs* does not only influence the temperature window of intermediate *HSUs*, but also that of *HSUs* at the end of the *HR* region [10];
3. the sequence of the sub-set of streams within each storage sub-system influences the storage capacity, and the capital costs [11].

9. Assigning it at the supply temperature has the advantage of eliminating a possible constraint on the temperature margin of the *HSU*; this is recommended at least when the constraint is "hard" (i.e. significantly restrict the temperature margin of the *HSU*).
10. E.g., HSU_4 is not constrained when starting from the cold end, since hot stream H_1 is included in the storage sub-system SSs_2, while HSU_4 is constrained by H_1 when designed starting from the hot end.

Based on the preceding comments, a reasonable assignment would be : HSU_1 to C_1, HSU_2 to C_3, HSU_3 to H_2, HSU_4 to H_3/H_4. Assigning HSU_3 to H_1 to prevent H_1 from constraining HSU_4 would likely result in a sub-optimal solution, since the temperature margin of HSU_3 would still be quite small.

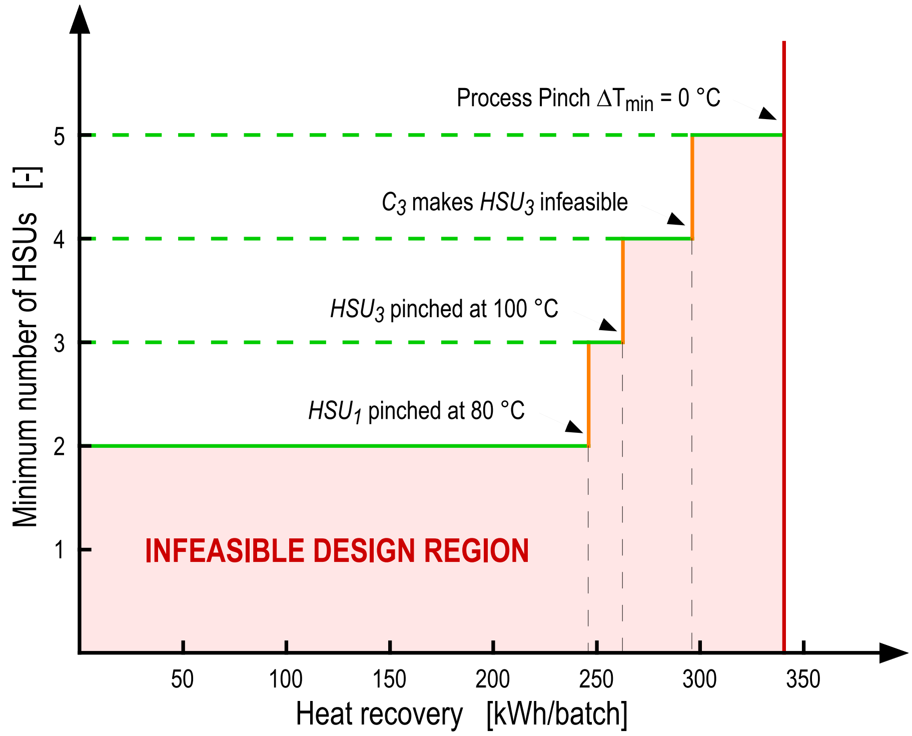

Figure 4-10 Minimum number of *HSUs vs* the amount of heat recovery (vertical model of *EP-1*).

The proposed procedure, using a graphical representation and based on the vertical model assumption, provides the designer with the necessary insight for selecting and positioning the *HSUs* :

- the "energy margin" of each *HSU* (i.e. the range of energy coordinates the *HSU* can be located at) is easily identified by systematically working from the cold end towards increasing temperatures, and from the hot end towards decreasing temperatures, respectively;
- the *LSTP* plots help in identifying critical streams with respect to the definition of the minimum number of *HSUs*;

11. But since this effect is not properly taken into account in the vertical model anyway, this is not a good selection criteria for a targeting method.

- the temperature margin as a function of the actual assignment of the *HSU* within its energy margin is highlighted, allowing for some degree of freedom to be used;
- the relationship between the number of *HSUs* and the amount of *HR* is easily calculated and allows to identify critical values of *HR* where storage pinch(es) appear and an additional *HSU* is required. This allows for the determination of the minimum number of *HSUs* as a function of the *HR* as exemplified by **Figure 4-10** for the *EP-1* example process.

The minimum number of *HSUs* is a useful information for first order calculations [12].

4.4 Improvement Opportunities

The proposed procedure for defining the minimum number of *HSUs* is based on the vertical model assumption. This is a default best guess and is the only case where a straightforward, simple application of the method is possible.

The following opportunities may be explored to reduce the number of *HSUs* below the minimum number of *HSUs* as predicted by the proposed method :

- criss-cross heat exchanges at the border between two storage sub-systems (refer to Figure 4-16) [13];
- eliminating from *HR* consideration some small streams whose supply temperature is in, but close to the end of, the *HR* region [14];
- removing from *HR* consideration some small streams fully included in the heat recovery region if these streams require an intermediate *HSU* to be introduced [15].

12. However, as will be seen, using the minimum number of *HSUs* for a given *HR* does not necessarily lead to cheaper *IHRSs*. This depends of course on the cost functions of the *HEXs* and *HSUs* (in particular of the fixed cost factor), and on the actual values of the storage pinches to achieve the considered level of heat recovery.

13. E.g. remaining heat from a hot stream normally supplied to the lower storage sub-system is supplied to the upper sub-system, while heat at the beginning of a cold stream (from the supply temperature) normally supplied by the lower sub-system is provided by the upper storage sub-system. This allows the heat recovery to be increased beyond the maximum amount of *HR* feasible with a given number of *HSUs* (according to vertical model) without requiring an additional *HSU* to be introduced. The number of *HEXs* is also reduced, while these benefits are at the expense of decreasing the temperature margin of the concerned *HSU*.

14. This prevents the operating temperature of an intermediate *HSU* to be pinched, while the temperature margin of the related *HSU* at the border of the *HR* region decreases. This is actually equivalent to trading-off the temperature margin of one *HSU* against another one.

The above opportunities actually introduce criss-cross heat exchanges, which are known to increase the necessary *HEX* area in most cases. They exploit trade-off effects between *HSU* capacities and *HEX* area. They essentially correspond to structural decisions, while parametric optimization issues are not considered.

Note also that the last two opportunities have already been mentioned independently by S*adr-Kazemy* & *Polley* (1996), and by *Stoltze* et al. (1995). However, the measures were not discussed and assessed on the basis of a graphical representation of the minimum number of *HSUs*.

4.4.1 Stream-wise or Slice-wise Supply Temperatures ?

So far, the supply temperature of all process streams have been taken into account in the limiting supply temperature profiles [16]. This is equivalent to assuming that all streams are independently scheduled and completely asynchronous with respect to any other stream.

In other terms, during a batch cycle, there is (or there might be, in the case of schedule variations likely to take place) a time period for the supply temperature of each cold stream to be the lowest temperature of all cold streams present, and a time period for the supply temperature of each hot stream to be the highest temperature of all hot streams present at that time period. All supply temperatures are deciding (this condition will be made clear below when analysing the *EP-1* example process). This is a sound assumption, since robust solutions, insensitive to schedule variations, are searched for. It leads to the most constrained limiting supply temperature profiles and the largest minimum number of *HSUs*.

However, the number of time slices is often in the order of, or smaller than, the number of process streams. Based on the rules proposed for the assignment of *HSUs* on the *batch cascade curves* (*BCCs*) (*Krummenacher* & *Favrat*, 1995), a restricted set of deciding supply temperatures can be established. This results in relaxed *LSTPs*, and in a smaller number of *HSUs*, as will be demonstrated below. But care must be taken so as to verify the feasibility of the heat exchanges.

15. In this way, the required number of *HSUs* decreases, at the expense of smaller temperature driving force, hence of increased heat transfer area. Hopefully the economics improves. Such an opportunity is seldom used in continuous processes, since the process pinch has a major effect on the capital costs, while in batch processes optimum solutions are often to be found at the transition regions between two numbers of *HSUs*, i.e. effects other than the process pinch come into play.
16. Except for the exploration of the improvement opportunities previously reviewed.

Originally, the analysis of the stream-wise versus the slice-wise approach to the number of *HSUs* was motivated by experience gained from *BCCs* (refer to *Krummenacher* & *Favrat*, 1995). In *BCCs*, the existence of process streams disappears since *BCCs* are built from the grand composite curve of each time slice. The number of time slices is deciding for the number of "supply temperatures", while in the stream-wise approach the number of streams defines the number of supply temperatures. For the problem at hand, the number of time slices (which may range from twice the number of process streams in the worst case to 1 if all streams are synchronous (hence equivalent to a continuous process) is not actually the only deciding variable.

Table 4-2 lists the "supply temperatures" of each time slice (i.e. the starting temperature of the cold and of the hot slice-wise composites) of process *EP-1*.

Time Slice	Cold Comp. T_{supply}	Hot Comp. T_{supply}
1 of 5	C1: 25 °C	–
2 of 5	C1: 25 °C	H1: 135 °C
3 of 5	C1: 25 °C	H3/H4: 165 °C
4 of 5	C1: 25 °C	H1: 135 °C
5 of 5	C3: 80 °C	H3/H4: 165 °C

Table 4-2 The cold and hot supply temperatures of each time slice (*EP-1*).

Globally, there are 2 different cold supply temperatures, and 2 different hot supply temperatures, hence 4 supply temperatures for 6 process streams (H_3/H_4 actually counts for one single stream). It is as if streams C_2 and H_2 were not deciding. Such "idle" streams are easily identified on **Figure 4-11**, redrawn from Figure 4-1, according to the following rules :

- hot streams are grouped together, and so are cold streams too;
- hot streams are listed by decreasing order of supply temperature;
- cold streams are listed by increasing order of supply temperature.

It becomes clear that whenever C_2 exists, a cold stream with a lower supply temperature (C_3) also exists. Similarly, whenever H_2 exists, a hot stream with a higher supply temperature (H_1) also exists. However, in this particular case, the

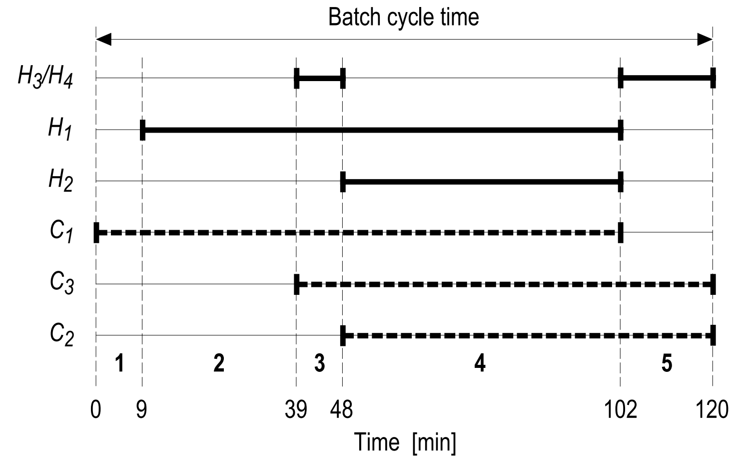

Figure 4-11 Schedule of the *EP-1* process streams, organized in order to highlight streams that are overlaid both in time and temperature.

"wiping off" effect of C_2 is sensitive to schedule variations affecting the stop time of C_3 with respect to that of C_2. The same is true for H_1 with respect to H_2, although H_4 might help overlap H_2 if the stop time of H_2 is delayed.

Hence, removing the supply temperatures of C_2 and H_2 from the list of supply temperatures to be taken into account in the *LSTPs* is not recommended, unless sufficient time margins can be guaranteed.

Compared to the case represented on Figure 4-6, if C_2 and H_2 are actually removed from the list of deciding streams, the minimum number of *HSUs* is reduced from 4 to 3, as illustrated on **Figure 4-12** when starting from the cold end, and on **Figure 4-13** when starting from the hot end. This reduction is due to the elimination of H_2, since C_2 is not included in the *HR* region anyway and therefore does not constrain the *LSTPs*.

In both Figures, the solid line joining HSU_2 to HSU_3 represents the actually highest operating temperature of HSU_3 for the given operating temperature of HSU_2. Above this line, the heat exchanges during time slice 4 are not feasible (i.e. dotted line).

Formerly, accounting for the supply temperature of each process stream (assuming single segment streams only) in the *LSTPs* guaranteed that the temperature driving forces of individual process stream - storage streams matches were feasible in practice. Such a guarantee does not exist any more if "composite process streams" [17] are to be matched with storage streams. Infeasible matches cannot be identified at a glance from the *TAM* energy composites, composing streams which do not coexist in time.

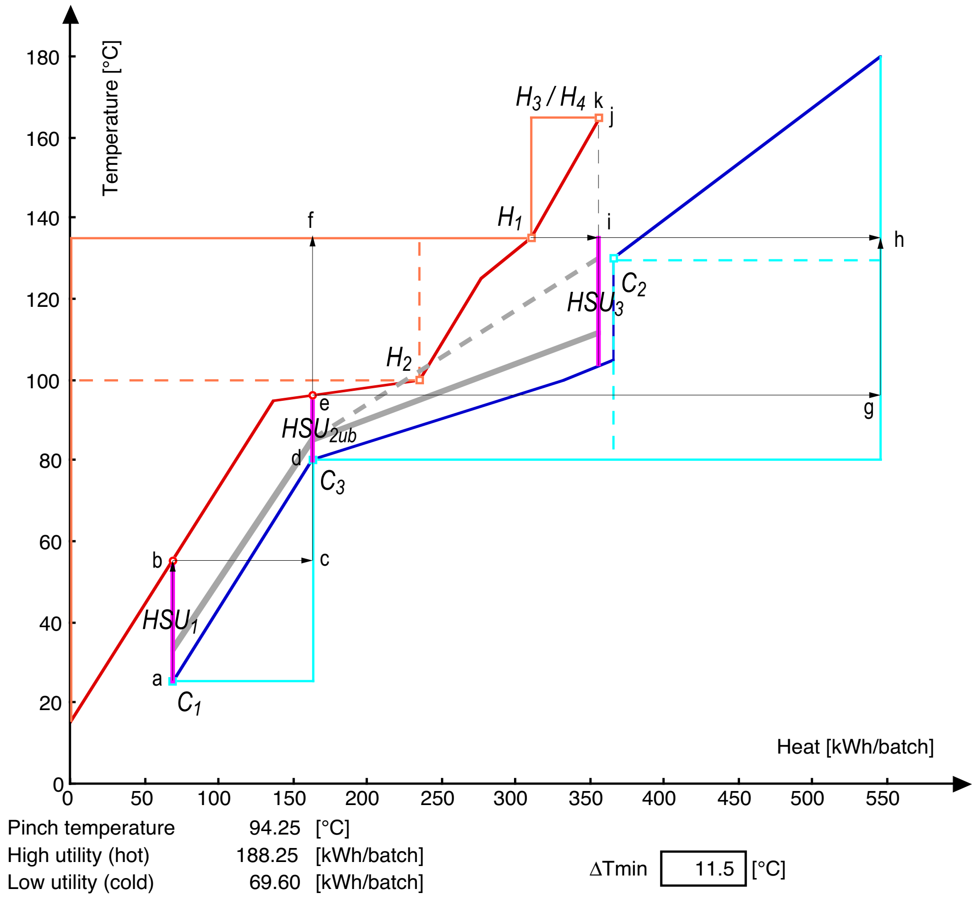

Figure 4-12 The minimum number of *HSUs* without taking the supply temperature of H_2 (and C_2) into account, starting from the cold end (same *HR* as Figure 4-6).

If the time schedule of the streams theoretically allows some "idle" streams to be removed, this can however lead to situations where intermediate *HSUs* need to be introduced so that the storage composite remains between the *TAM* composites (a storage composite has to be a straight line between two *HSUs*). This is a new situation due to "composite process streams" existing during time slices, which was not found in the basic situation of stream-wise approach to *LSTPs* [18].

Hence the *TDF* feasibility of such matches during the related time slices has to be individually checked. If an infeasibility appears, an intermediate *HSU* has to be included. A reasonable guideline for introducing an additional *HSU* would be :

17. That is having a composite temperature profile which has not a constant $\dot{M}c_p$ any more, resulting from some streams being "wiped off" from the list of deciding streams.

18. In which case all convex points of the process composite - these are problematic with respect to the feasibility of "composite process streams" - are associated to supply temperatures of process streams and reflected in the *LSTPs*.

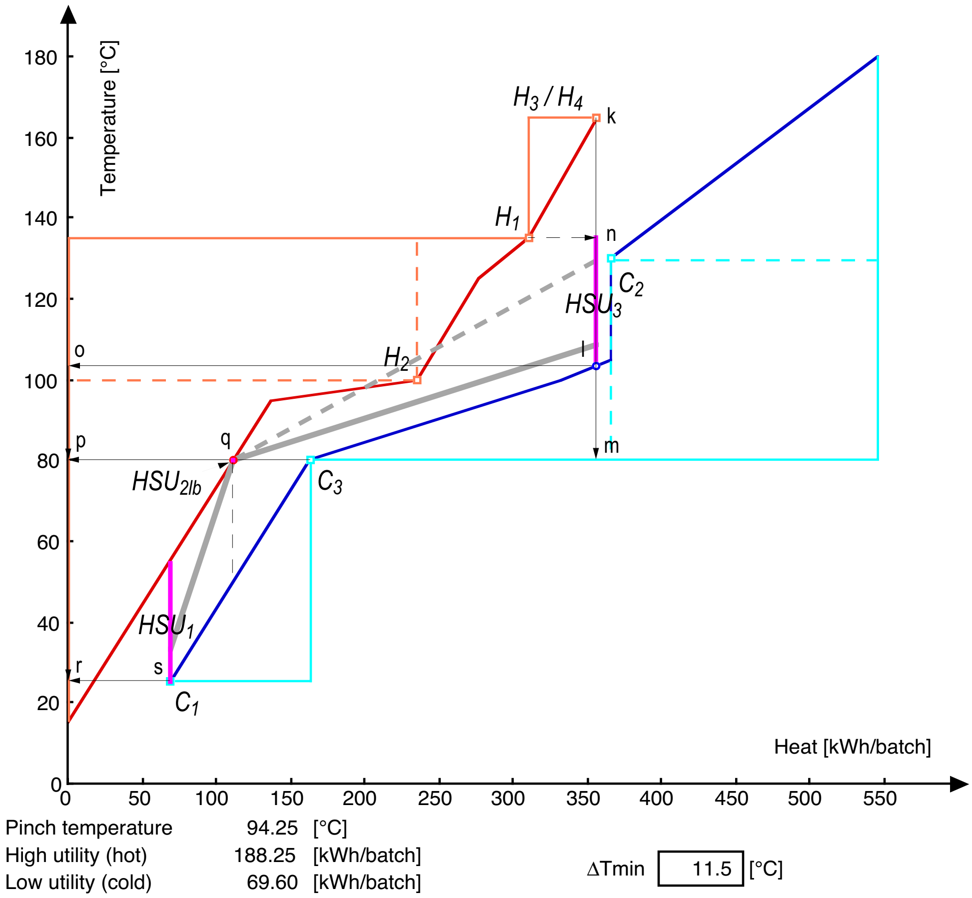

Figure 4-13 The minimum number of *HSUs* without taking the supply temperature of H_2 (and C_2) into account, starting from the hot end (same *HR* as Figure 4-7).

1. check the feasibility for all concerned streams; 2. list infeasible matches; 3. decide where additional *HSUs* are best introduced.

Summarizing the discussion on stream-wise versus slice-wise supply temperatures :

- provided that the schedule of process streams is ordered according to the above simple rules, this representation allows for an easy visual check of any "undeciding", "idle" streams. A reasonable strategy consists in first taking all streams into account to draw the *LSTPs* and defines the minimum number of *HSUs*. Then identify constraining streams (i.e. streams whose supply temperatures constrain the temperatures of *HSUs*) and check on the ordered time event model (like Figure 4-11) whether their supply temperature could be removed from the *LSTPs*, while sufficient time margin is guaranteed;

- the feasibility of matches including "composite process streams" has to be individually verified, and the design of the *HEN* has to be time slice oriented (at least for the "idle" streams);
- the elimination of some "idle" streams based on the time slice approach can lead to more cost-effective designs, at the expense of more complex *HENs*, since serial, or serial / parallel *HEN* configurations are required to avoid intermediate *HSUs*, which is not the case of the stream-wise *HSU* assignment, where only single, one-to-one matches are present.

4.5 Example

Once the number of *HSUs* and their assignment ranges are identified as a function of the *HR* using the previously described graphical procedure, the systematic calculation of *IHRSs* at various levels of heat recovery can been performed in order to get :

- a first order approximation of the optimal level of heat recovery and the required number of *HSUs*;
- an upper bound on minimum total batch costs;
- insight into the main trade-off effects around the optimum.

The *TBCs* have been systematically calculated [19] for example process *EP-1*, assuming 2, 3 and 4 *HSUs*, while the amount of heat recovery was varied [20] [21]. All supply temperatures of process streams have been taken into account. The operating temperatures of the *HSUs* have been optimized using the *Solver Tool* of *Microsoft Excel*.

Figure 4-14 represents the results obtained with the vertical model assumption. The utility costs (per batch) are drawn to provide a baseline reference. Comments related to 2, 3 and 4 *HSUs* are given below [22].

19. The calculations have been performed using an *Excel Worksheet*. But the procedure could be implemented to run automatically, while providing the user with control on the main decision parameters.
20. The initial costs of both the *HEXs* and the *HSUs* are ignored (i.e. have a zero value - refer to Section A.1). If an initial cost factor for *HSUs* was introduced, this would simply move the *TBCs* points upwards accordingly, and penalize heat integration solutions with an increasing number of *HSUs*.
21. The area contributions of heat recovery matches on a same process stream are added before applying the cost function, which is a sound assumption in case of plate&frame *HEXs*.
22. Plotting the *TAM* composites curves on a separate sheet of paper is recommended since it greatly facilitates the understanding of the comments.

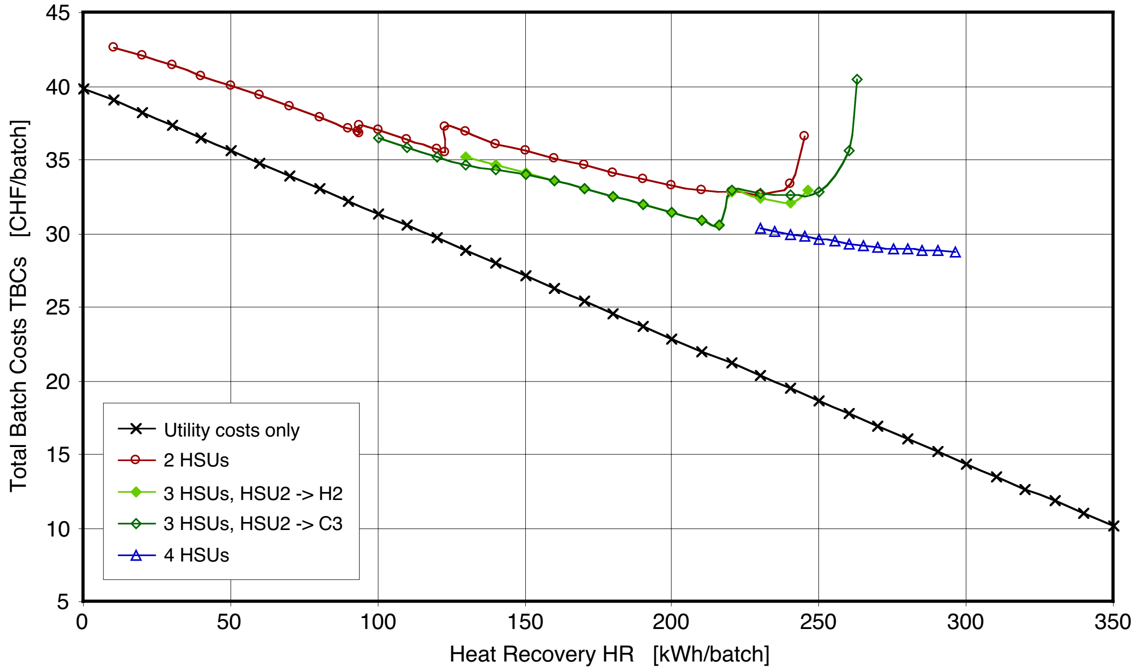

Figure 4-14 Total batch costs of *IHRSs* - example process *EP-1* with 2, 3 and 4 *HSUs* in vertical model (refer to text for further comments).

4.5.1 Two Heat Storage Units

The assignment of the two *HSUs* is straightforward. The first step change of the *TBCs* taking place at HR = 93.5 *kWh*/batch is produced by the introduction of C_3 in the heat recovery region, which heavily constrains the temperature of HSU_1 (before C_3 is introduced, the optimum temperature of HSU_1 is much below 80 °*C*).

This new constraint results in increased *HEX* and *HSU* costs. Note that the introduction of H_1 in the heat recovery region does not produce a step change, since the operating temperature of HSU_2 is already at 135 °*C* before H_1 is introduced. The step change at HR = 122.7 *kWh*/batch is due to the introduction H_2, which constraints the temperature of HSU_2 to suddenly change from 125 to 95 °*C*.

Then the *TBCs* continue to decrease smoothly, encounter a minimum, until the absolute maximum limit at HR = 246.75 *kWh*/batch is reached. At this point, the margin on the operating temperature of HSU_1 falls to zero, because the cut-off temperature of the heat recovery region on the hot composite decreases below 80 °*C* if the HR is increased (the lower limit of 80 °*C* is required by C_3). Even if the HR could be increased beyond this value, HSU_2 would soon be pinched (actually for $HR = 262.5$ kWh/batch) because the cut-off temperature of the heat recovery region on the cold composite increases above 100 $°C$ if the HR is increased (the upper 100 $°C$ limit on HSU_2 is required by H_2).

4.5.2 Three Heat Storage Units

With 3 *HSUs*, the intermediate *HSU* (now HSU_2) has to be assigned. From the case with 2 *HSUs*, it is clear that H_2 and C_3 are two constraining streams within the *HR* region (the *LSTP* plots outlined in 4.3.2.2 would make this obvious). From a *HR* point of view, C_3 is more constraining than H_2, since with 2 *HSUs*, the bottleneck is first encountered on HSU_1, whose lower temperature limit is defined by C_3, while the pinch on HSU_2, linked to H_2, would only become active for a higher *HR*.

But the *HR* point of view is not necessarily in line with the minimum *TBCs*, so that both cases - intermediate HSU_2 assigned to C_3 or HSU_2 assigned to H_2 - have to be assessed [23]. Once the decision concerning the assignment of HSU_2 has been made, the *TBCs* are calculated for various *HR* values [24]. With HSU_2 attached to C_3, a step change appears at $HR = 216.175$ kWh/batch. Below this *HR* value, the supply temperature of H_2 is on the left with respect to the one of C_3 (i.e. heat from H_2 is entirely recovered in the storage sub-system SSs_1), while above this *HR* value, part of H_2 is also integrated with SSs_2, which requires the upper bound on the temperature of HSU_3 to suddenly change from 135 $°C$ to 100 $°C$ (the optimized operating temperature changes from 126.2 $°C$ to 99.8 $°C$).

The absolute upper bound to *HR* with HSU_2 attached to C_3 is HR=262.5 kWh/batch (defined by HSU_3 being fully pinched at 100 $°C$). A similar behaviour is observed for HSU_2 attached to H_2, with a sudden change of the lower bound on HSU_1 at $HR = 216.175$ kWh/batch, changing from 25 $°C$ to 80 $°C$ (the actual, optimized operating temperature changes from 40.9 $°C$ to 80.2 $°C$). But since HSU_2 is assigned to H_2 and not to C_3, which is responsible for HSU_1 being fully pinched first in the case of 2 *HSUs*, the absolute upper bound to *HR* is unchanged at $HR = 246.75$ kWh/batch. Despite the fact that the maximum *HR* is not significantly increased, the temperature margin of one of the two *HSUs* being pinched around the minimum *TBCs* is relaxed, allowing the minimum *TBCs* to be

23. Assigning an intermediate *HSU* to the start of a stream, i.e. to a supply temperature (rather than at any other position) is the most reasonable choice, since the primary aim of introducing an intermediate *HSU* is to avoid a supply temperature from producing a bottleneck. This rule holds at least for the vertical model.
24. As a rule, the *TBCs* calculations should restart from a *HR* value which makes the introduction of the new intermediate *HSU* feasible, and not only for *HR* values larger than the limit reached with one less *HSU*.

reduced by 6.6 %. Note that assigning HSU_2 to C_3 or H_2 leads to very similar *TBCs*, but this effect is particular to this process.

4.5.3 Four Heat Storage Units

Introducing a fourth *HSU* should allow to further increase the *HR* and hopefully decrease the *TBCs*. From the former discussion for the case of 3 *HSUs*, the obvious decision is to assign the intermediate HSU_2 to C_3, and the second intermediate *HSU* (i.e. HSU_3) to H_2.

The *TBCs* slightly decrease as the *HR* increases, until an absolute maximum limit of *HR* = 296.25 *kWh*/batch. Before this point, none of the 4 *HSUs* is going to be pinched, and the *TBCs* continue to decrease slightly. But for *HR* > 296.25 *kWh*/ batch, the introduction of C_2 in SSs_3 makes HSU_3 suddenly infeasible (a fifth *HSU* should be used [25]), resulting in a vertical asymptote. The heat integration including 4 *HSUs* features a further improvement of the *TBCs* (compared to the 3 *HSUs* case) of 6.3 %, with a simultaneous increase of the *HR* of 27 %.

4.5.4 Assessing Improvement Opportunities

The consideration of the cut-off temperatures as additional improvement opportunities leads to the following results, presented on **Figure 4-15** :

- with 2 *HSUs*, opportunities are readily identified as being related to the two step changes previously mentioned. First, H_2 and C_3 are removed from heat integration, allowing the *HR* to be increased up to 127.5 *kWh*/batch (the heat content of C_1) and the *TBCs* to be decreased by 7.7 % compared to the same *HR* according to the vertical model [26]. The second opportunity is the exclusion of H_2 only (since the second step change is produced by H_2, constraining HSU_2) [27];
- with 3 *HSUs*, a step change appears when H_2 and C_3 are vertically aligned, and H_2 starts constraining HSU_3 (if HSU_2 is assigned to C_3), or C_3 starts constraining HSU_1 (if HSU_2 is assigned to H_2). To allow for a further increase

25. A case which has not been studied, because likely not optimal.
26. But since this solution integrates a limited set of process streams, it only provides an improvement of limited scope.
27. Again, this results in a local improvement of too limited scope to compete with the optimum *HR* (minimum *TBCs*) found with vertical, 2-*HSUs* heat integration solutions. This demonstrates that although H_2 is constraining the temperature of HSU_2, it provides nevertheless a large opportunity for heat recovery within a low temperature difference, which is beneficial for heat integration.

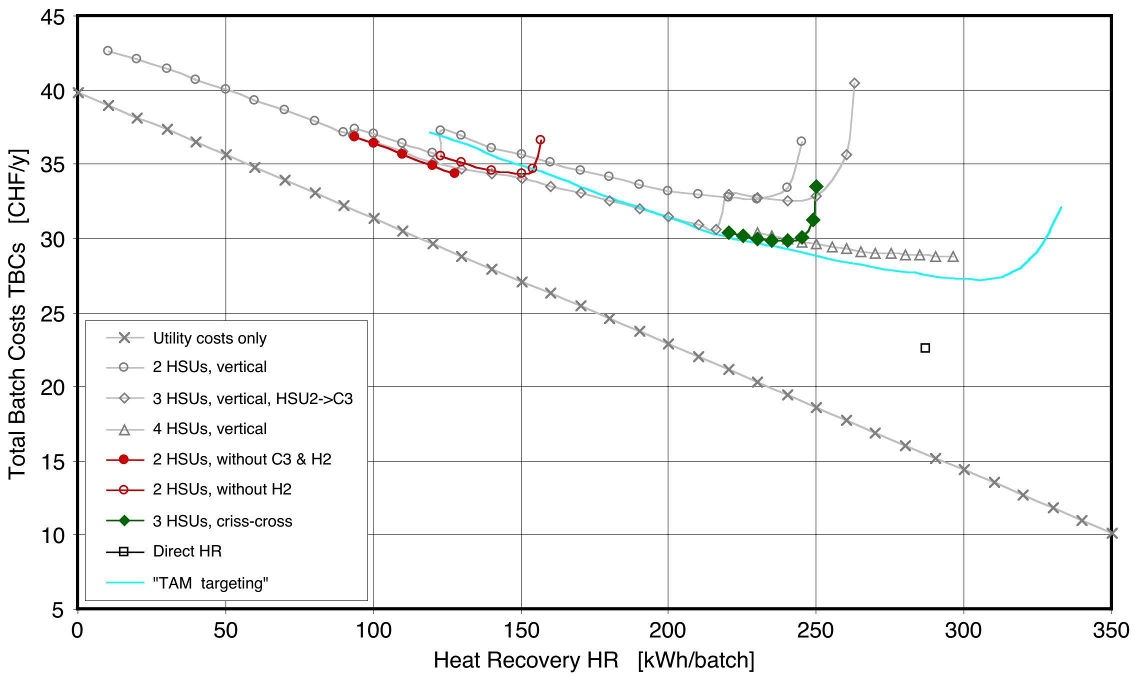

Figure 4-15 Improvement allowed by simple deviations from the vertical model (*EP-1*, refer to text for further comments).

of the *HR* without such a constraint (i.e. increase *HR* beyond the step change), criss-cross heat exchanges can be used, as shown on **Figure 4-16** [28];

- with 4 *HSUs*, around the identified optimum, opportunities for criss-crossing do not exist [29];
- for comparison, the minimum *TBCs* obtained by direct heat integration (refer to Chapter 7, Sub-section 7.6.1) are also represented on Figure 4-15, corresponding to a 21 % improvement over the minimum *TBCs* in indirect heat integration, for a similar degree of *HR* [30];
- the *TBCs* calculated using a crude targeting method are also reported on Figure 4-15. This targeting method assumes vertical heat transfer between *TAM*

28. The heat contribution from H_2 which should normally be supplied to SSs_2 is fed into SSs_1, and replaced by an equivalent amount of heat from H_1 which would normally be supplied to SSs_1. Similarly, heat for C_2 is fully supplied by SSs_2, although part of it should come from SSs_1 according to the vertical model; this is compensated by heat needed for C_1 above 80 °C which is now taken from SSs_1. This strategy prevents both C_3 from constraining HSU_1, and H_2 from constraining HSU_3. However, the temperature margin of HSU_2 decreases as the *HR* is increased, until an upper limit of *HR* = 250.2 *kWh*/batch, for which HSU_2 is fully pinched (as represented on Figure 4-16). Compared to 3 *HSUs* in vertical mode, this allows the *HR* to be significantly increased while keeping the *TBCs* at a level slightly below their minimum in vertical mode, until the pinch effect on the costs of the *HEXs* on H_1 and C_1 becomes prominent.
29. This is so because the limitation to a further increase of the *HR* results from the sudden temperature constraint introduced by C_2 (the only remaining cold stream); none of the four *HSUs* is pinched before this point. H_1 is the only stream which could be criss-crossed (with H_3/H_4). But it does not make sense because H_1 is not constraining.

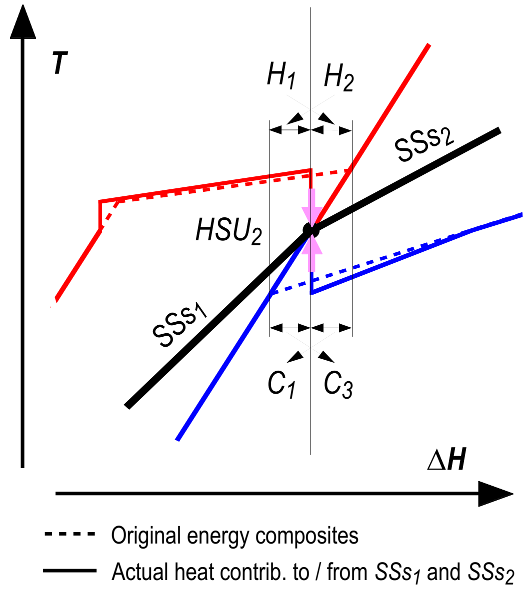

Figure 4-16 Detail of criss-cross heat transfer "around" HSU_2 to keep H_2 in SSs_1 and C_3 in SSs_2. The temperature of HSU_2 is pinched between H_1 and C_1 temperature profiles (*EP-1 TAM* composites, *HR* = 250.2 *kWh*/batch).

composites, and the assessment of capital costs is limited to *HEXs* (i.e. excludes *HSU* costs). However, to account for the need of heat transfer to (and from) intermediate storage streams, the heat transfer film coefficient of the process streams is divided by a factor four, and further multiplied by a "duty ratio" factor equal to the duration of the stream over the batch cycle time [31].

4.6 Summary

A graphical method has been proposed to determine the minimum number of heat storage units (*HSUs*) [32] and their assignment ranges as a function of the amount of

30. Facing this apparently disappointing result for the indirect heat integration, one should recall the intrinsic high sensitivity of direct *HENs* to schedule variations (a suitable method to account for the likely energy and costs penalties resulting from these variations is still lacking). In addition, the cold streams and the hot streams of *EP-1* feature a relatively high degree of simultaneity (consider Figure 4-11), which is beneficial for direct heat exchanges but not commonplace in batch processes.
31. Although the calculation method is very crude, it provides in this case results of acceptable precision for the conceptual design stage. It intrinsically fails to provide structural information such as the required number of *HSUs*. The prominence, for *EP-1*, of *HEX* costs (10.2 *CHF*/batch) compared to *HSU* costs (3.9 *CHF*/batch) partly explains the encouraging results of this crude targeting method.
32. Note however that resorting to the minimum number of *HSUs* for a given *HR* does not necessarily result in the lowest costs *IHRS*. Other effects come into play.

heat recovery (*HR*). It combines the *TAM* (time average model) energy composites and the discrete effects of the supply temperature of process streams.

The main benefit of the method is to provide insight into important issues relevant for the targeting stage: 1. which process streams should be included in the heat integration; 2. which stream requires an additional *HSU* to be introduced; 3. which process change could be envisaged to improve the heat recovery; 4. opportunities for reducing the number of *HSUs* by a heat recovery on a serial arrangement of process streams (slice-wise instead of stream-wise consideration of the supply temperatures).

The simplifying assumption of the so-called vertical model allows for the straightforward definition of the heat recovery range of each storage sub-system (and hence the cut-off temperatures of streams). In this way, the mass balances of the *HSUs* are automatically met, and feasible (yet sub-optimal) *IHRS* solutions are easily calculated. The systematic analysis of the constraints introduced by the supply temperature of streams on *HSUs*, combined with the representation of the solutions in the *TBCs* vs *HR* [33] diagram, provide understanding of the issues and therefore help deciding which way to go for searching more cost-effective designs (if an interactive design procedure is used). A systematic combinatorial search might be considered.

However, the vertical model may not properly explore the *HSU* capacity – *HEX* area trade-off.

The Permutation Method and the proposed graphical tools & procedures to address different targeting tasks are complementary.

33. Total batch costs versus heat recovery.

Chapter 5

DESIGN & OPTIMIZATION OF INDIRECT HEAT RECOVERY SCHEMES

5.1 Motivation & Overview

The heuristic targeting method described in Chapter 4 provides insight into issues such as the minimum number of heat storage units (*HSUs*) as a function of the amount of heat recovery (*HR*), and produces feasible indirect heat recovery schemes (*IHRSs*) of acceptable quality. But owing to the vertical model assumption, it fails to efficiently address the following degrees of freedom (*DOFs*) :

- the cut-off temperatures of process streams [1];
- the optimal heat contribution of heat recovery streams.

In order to design improved *IHRSs* accounting for the above *DOFs*, *IHRS* models suitable for use with a genetic algorithm (*GA*) have been developed and successfully applied. This Chapter focuses on the methodological aspects of these models, while the numerous features primarily aiming at improving the user-friendliness of the related software programme can be found in *Krummenacher* (2001). Application results are reported and discussed in Chapter 6.

The basic principles of a *GA* based optimization, as well as the main features of the *Struggle GA* used in the frame of this work, may be found in Section 3.7. It helps understanding the choices made when setting up the models and also introduces the optimization related issues and solutions described in Section 5.5.

1. I.e. the heat contribution of each process stream to each storage sub-system (*SSs*)), which generally significantly deviate from that of the vertical model. This deviation is due to complex trade-off effects between *HSU* capacities and *HEX* areas, which depend on the schedule of streams.

Section 5.2 describes the basic *IHRS* model suitable for a *GA* based optimization.

Section 5.3 introduces improvements of the basic model with focus on the underlying methodological aspects. These extensions are needed to tackle real-life industrial processes.

Derived from the improved *IHRS* model, an open storage *IHRS* model is described in **Section 5.4**.

Section 5.5 provides insight into the observed pitfalls of the *GA* based optimization of the proposed models, and presents the implemented modifications of the optimization strategy to alleviate such effects.

Finally, the main features of the models, their scope of potential application as well as their inherent limitations are summarized in **Section 5.6**.

Proposals for an extended *IHRS* model are sketched in **Appendix E**.

As already pointed out (refer to Chapter 2), *Stoltze*, *Dalsgard*, *Mikkelsen*, *Lorentzen*, *Petersen* and *Qvale* (refer e.g. to *Stoltze* et al., 1995; *Mikkelsen* et al., 1998; *Mikkelsen*, 1998) - all at the *Technical University of Denmark* - have significantly contributed to the field of indirect heat integration by means of thermal energy storage, and partly inspired the proposed models. However, it is worth noting that a great deal of ideas relevant to this field were also developed independently ... based on a common background of heat integration experience in breweries (*Krummenacher*, 1992, 1995).

5.2 Simple *IHRS* Model

The simple *IHRS* model has primarily been set up to validate the *GA* based approach, before embarking on more difficult issues; for example, convergence difficulties related to the proposed selection of *DVs* were expected (refer to Subsection 5.2.4). The description of this simple model aims at providing an easier understanding of the fundamental features which pertain to the improved *IHRS* model as well.

5.2.1 Proposed *IHRS* Superstructure

The simple *IHRS* model is based on a superstructure as exemplified on **Figure 5-1** for 3 hot and 3 cold process streams. This Figure also introduces the following nomenclature [2]:

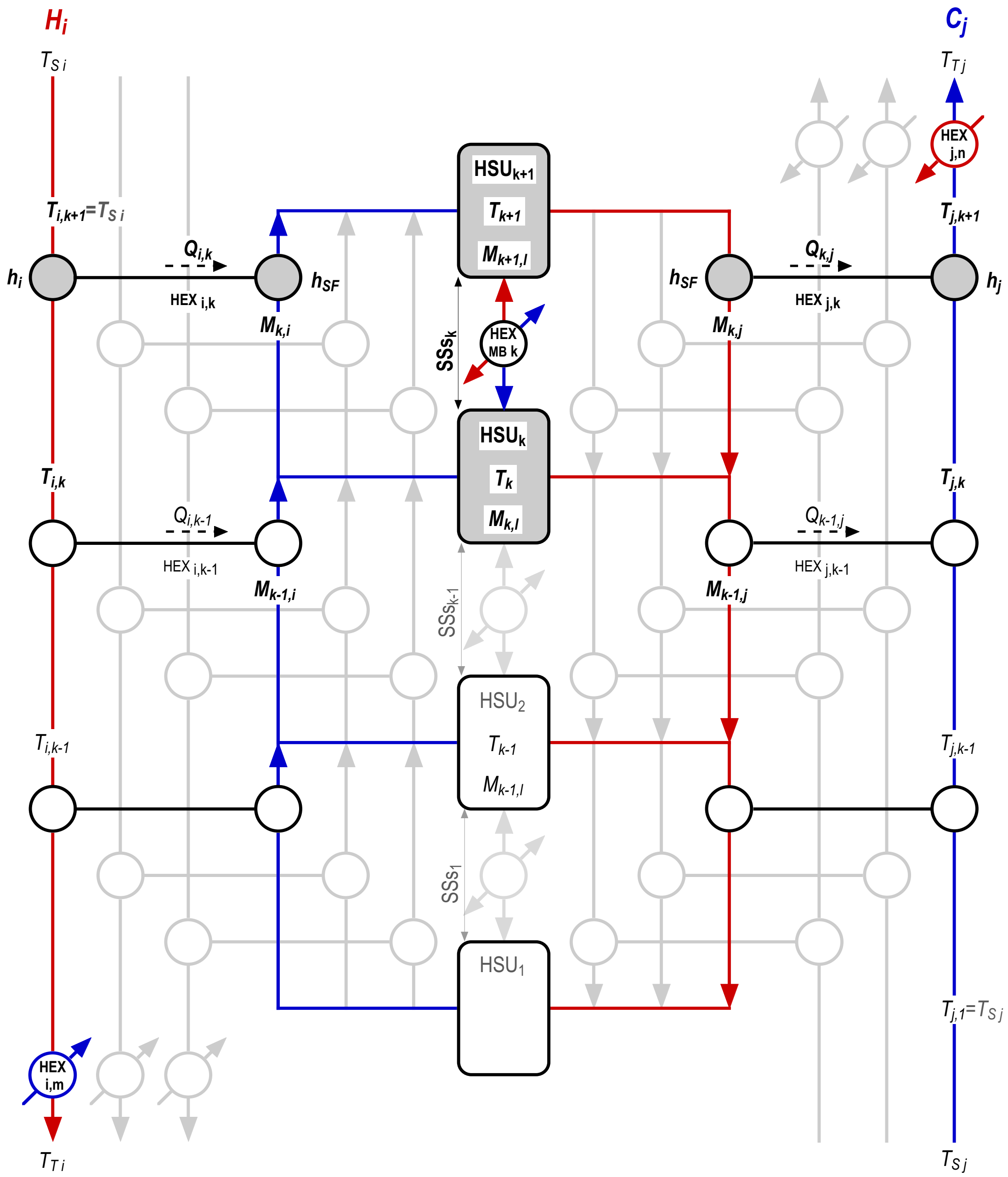

Figure 5-1 Superstructure used for the simple *IHRS* model.

- subscript i refers to hot process streams ($i : 1 \,..\, I$);
- subscript j refers to cold process streams ($j : 1 \,..\, J$);
- subscript k originally refers to *HSUs* ($k : 1 \,..\, K$); by extension, k also refers to *SSs* (in which case $k : 1 \,..\, K-1$) so that SSs_k represents the storage sub-system made up of HSU_k and HSU_{k+1};

2. Note that the time dimension (e.g. the time slices) does not explicitly appear on Figure 5-1. In fact, process streams and related heat exchanges and mass transfers are only active during their respective periods of existence (see e.g. the schedule of example process *EP-1* illustrated on Figure 4-1). The *HSU* mass inventories are continuously changing as a function of time (refer to Section 3.4.4).

- T_k is the operating temperature of HSU_k (time independent);
- $T_{i,k}$ is the temperature of hot process stream i (H_i) after heat exchange with SSs_k (also referred to as cut-off temperature), while $T_{S\,i}$ denotes its supply temperature and $T_{T\,i}$ its target temperature; $T_{i,k}$ is time independent whenever stream i exists;
- $T_{j,k+1}$ is the temperature of cold process stream j (C_j) after heat exchange with SSs_k (also referred to as cut-off temperature), while $T_{S\,j}$ denotes its supply temperature and $T_{T\,j}$ its target temperature; $T_{j,k+1}$ is time independent whenever stream j exists;
- $Q_{i,k}$ represents the heat delivered (over a batch cycle) by hot process stream i to SSs_k (i.e. storage stream coming out from HSU_k into HSU_{k+1});
- $Q_{k,j}$ represents the heat supplied (over a batch cycle) to the cold process stream j by SSs_k (i.e. storage stream coming out from HSU_{k+1} into HSU_k);
- $M_{k,i}$ represents the mass of storage fluid heated (over a batch cycle) by hot process stream i and moved from HSU_k into HSU_{k+1};
- $M_{k,j}$ represents the mass of storage fluid cooled (over a batch cycle) by cold process stream j and moved from HSU_{k+1} into HSU_k);
- $M_{k,l}$ is the mass inventory in HSU_k at time t_l (the end of time slice l, with l : 1 .. L)
- h_i, h_j, h_{SF} are the film heat transfer coefficients of hot process stream i, cold process stream j, and storage fluid, respectively.

The superstructure is based on the following assumptions :

a) the process streams feature constant heat capacity flowrate CP [3];

b) each process stream can potentially exchange with each *SSs*, subject to the constraints of feasible temperature driving forces [4];

c) after heat exchanges with the *SSs*, the temperature of process streams ($T_{i,1}$, $T_{j,K}$) is not allowed to "exceed" their target temperature; the heat balance of process streams is ensured by external utilities which can only be applied at the target temperature side;

d) the *HEX* units are not re-used across time slices on different process streams;

3. The process streams are flowing single-segment streams with the specific heat c_p constant and independent of temperature, and the mass flowrate $\dot{M}$ is constant over their period(s) of existence. This assumption avoids checking for any internal pinch point when defining the feasibility of heat exchanges with the heat storage fluid; it significantly simplifies the *HEX* area calculations. This limiting assumption is removed in the improved *IHRS* model (refer to Section 5.3).

4. This assumption leads to heat recovery schemes including more *HEX* units (or more specifically, area units) compared to the ones obtained by *Mikkelsen* (1998). However, this choice does not result in significant cost penalties, at least in cases of gasketed plate & frame *HEXs*. It also provides additional degrees of freedom to adjust the mass balance of *HSUs* which could be beneficial for further reducing their capacities. If the increased *IHRS* complexity should be experienced as a significant drawback, a further extension of the model could explicitly control connections to intermediate *HSUs* (refer to Appendix E). Since the mass flowrate of heat storage fluid can be adjusted independently for each match, there is no need for splitting process streams, allowing for this simple and flexible superstructure.

e) the number of *HSUs* (of *FTVM* type solely, refer to Section 3.4) is specified *a priori* by the user (i.e. it is fixed during an optimization run) [5];

f) the *HSU* mass balance constraints over a batch cycle (refer to Sub-section 3.4.3) are restored by utilities supposed to operate at a constant heat rate [6];

g) the heat losses of the *HSUs* to the environment are neglected [7].

Despite its inherent limitations and the above assumptions, the proposed superstructure is able to represent good *IHRS* solutions. It includes several key *GA* related optimization difficulties that have been explored during a preliminary test of the approach [8].

5.2.2 Problem Statement

Considering Figure 5-1 again, the performances (heat recovery and utility consumptions, *HEX* areas & costs, *HSU* capacities & costs, etc.) of any *IHRS* can be calculated once the operating temperature T_k of *HSUs* and, e.g. the temperatures $T_{i,k}$ and $T_{j,k+1}$ after each heat exchange match, are provided. $Q_{i,k}$ and $Q_{k,j}$ could be specified instead of $T_{i,k}$ and $T_{j,k+1}$, but this does not matter since these variables are linearly related to each other.

The problem of optimal *IHRS* synthesis may be stated as follows [9].

Given :

- a batch process, operated in a cyclic manner [10];
- a number of *HSUs* specified by the user;

5. This assumption is motivated by the fact that a variable number of *HSUs* during the optimization would increase the structural complexity and the dimension of the solution space. More importantly, leaving the number of *HSUs* up to the user's choice provides her/him with increased control over the complexity of the *IHRS* and relates to a targeting step (refer to Chapter 4).
6. Opportunities to reduce the mass rebalancing utility needs by mixing of storage fluid are not considered. This assumption is removed in the improved IHRS model proposed in Section 5.3.
7. This assumption is not essential and could easily be removed.
8. Note that any superstructure may be viewed as the resulting compromise of two opposite considerations : 1) the desire to include every practice relevant, feasible and potentially beneficial configuration; 2) the ability to represent the solutions with a minimum number of variables which can be efficiently managed by the optimization algorithm.
9. Compared to the indirect heat integration synthesis problem introduced in Sub-section 3.4.5, the problem addressed using the simple *IHRS* model is restricted to the optimization of continuous variables only. The original *Struggle* is not readily provided with the possibility to use integer or binary variables and an efficient use of discontinuous variables is known to be non-trivial.
10. Defined by a list of hot process streams to be cooled and a list of cold process streams to be heated, their respective schedule, and the related economic data and costs functions.

- the superstructure of Figure 5-1 and the associated modelling assumptions;

determine :

- the operating temperature of each *HSU*;
- the heat exchanged by each process - heat storage stream match;

which minimize the specified economic criterion (related to energy services) such as the total batch costs (*TBCs*) [11].

The associated mathematical model is presented in Section D.5 of Appendix D.

5.2.3 Constraints

The model corresponding to the superstructure of Figure 5-1 is subject to the following set of constraints [12]:

1. monotonically increasing temperatures of *HSUs* :

$$T_k > T_{k-1} \qquad (k : 2 \;..\; K) \tag{5-1}$$

$$\text{while} \quad T_{HSUmin} \le T_k \le T_{HSUmax} \qquad (k : 1 \;..\; K)$$

where:

- T_{HSUmin} is the lower bound on the operating temperature of *HSUs*;
- T_{HSUmax} is the upper bound on the operating temperature of *HSUs* [13].

2. decreasing (increasing) cut-off temperatures of hot (cold) process streams :

$$T_{i,k} \le T_{i,k+1} \qquad (k : 1 \;..\; K-1) \tag{5-2}$$

$$\text{while} \quad T_{T\,i} \le T_{i,k} \le T_{S\,i} \qquad (k : 1 \;..\; K-1)$$

$$T_{j,k+1} \ge T_{j,k} \qquad (k : 1 \;..\; K-1) \tag{5-3}$$

$$\text{while} \quad T_{T\,j} \le T_{j,k} \le T_{S\,j} \qquad (k : 2 \;..\; K)$$

11. Refer to Section 3.3.
12. Although some of them are discussed later in this Section (refer to Sub-sections 5.2.5 & 5.2.6), the constraints are worth a mention here because of their decisive role in selecting the decision variables to be managed by the *Struggle GA.*
13. The upper and lower bounds on the operating temperatures of *HSUs* result from the combined consideration of the safe working temperature range of the selected heat storage fluid and the hottest supply temperature of the hot process streams and the coldest temperature of the cold process streams.

3. feasibility of match between hot process stream i (cold process stream j) and SSs_k :

$$T_{i,\,k+1} > T_{k+1} \quad \text{and} \quad T_{i,\,k} > T_k \qquad (k\ :\ 1\ ..\ K-1) \qquad \textbf{(5-4)}$$

$$T_{j,\,k+1} < T_{k+1} \quad \text{and} \quad T_{j,\,k} < T_k \qquad (k\ :\ 1\ ..\ K-1) \qquad \textbf{(5-5)}$$

4. mass balances of *HSUs* over a batch cycle :
the mass balance equality constraints have been described in Sub-section 3.4.3 for terminal HSUs (Equation 3-4) and for intermediate HSUs (Equation 3-5).

5.2.4 Definition of Decision Variables

Among the constraints listed above, the first three (Equations 5-1 to 5-5) express simple upper / lower bounds on T_k, $T_{i,\,k}$ and $T_{j,\,k+1}$. Constant bounds are easy, but most of them are actually variable bounds (e.g. T_k is the lower bound for T_{k+1}, $T_{i,\,k+1}$ is the upper bound for $T_{i,\,k}$, etc.). In addition, the third constraint also introduces a dependency on the *HSU* temperatures.

The *GA* generates all decision variables (*DVs*) of an individual at a time, so that such a propagation of the bounds cannot be accounted. The proposed solution to solve this variable bound problem consists in the use of dimensionless variables x (x_k, $x_{i,\,k}$, $x_{j,\,k}$) representing the ratio of the actual variation (of the corresponding temperature) over the maximum feasible variation (of that temperature). The *GA* deals with the x *DVs* whose bounds are fixed ($0 < x_k < 1$; $0 \le x_{i,\,k} < 1$; $0 \le x_{j,\,k} < 1$) [14], and the decoding of the x *DVs* into actual T variables is given by :

- for operating temperatures T_k of *HSUs* :

$$T_k = (1 - x_k) \cdot T_{k-1} + x_k \cdot T_{HSUmax} \qquad \textbf{(5-6)}$$

hence : $T_k \to T_{k-1}$ for $x_k \to 0$ and $T_k \to T_{HSUmax}$ for $x_k \to 1$

Equation 5-6 is applied from $k = 1$ up to $k = K$; for $k = 1$, $T_{k-1} = T_{HSUmin}$.

- for cut-off temperatures $T_{i,\,k}$ of hot process streams :

14. The meaning (corresponding variation) of the x_k in term of T_k changes as a function of the other T variables. The similar observation applies to $x_{i,\,k}$, $x_{j,\,k}$ with respect to $T_{i,k}$, $T_{j,\,k+1}$. An unavoidable side effect of the definition of x variables is that any change of an x variable causes a cascade of temperature changes downstream, even if the corresponding downstream x variables remain unchanged. The higher in the hierarchy of dependence (with x_1 for HSU_1 at the top), the larger the number of influenced downstream temperatures. Although this could be seen as a change of variables, it remains difficult to get insight into the effect of these complex dependencies, and to devise how unfavourable the latter are for the efficiency of the *GA* optimization process.

$$T_{i,k} = (1 - x_{i,k}) \cdot T_{i,k+1} + x_{i,k} \cdot T_{lim\ i,k} \tag{5-7}$$

where:

- $T_{lim\ i,k} = Max[T_k, T_{T\ i}]$

hence : $T_{i,k} = T_{i,k+1}$ for $x_{i,k} = 0$; $T_{i,k} \rightarrow T_{lim\ i,k}$ for $x_{i,k} \rightarrow 1$

Equation 5-7 is successively applied to all feasible matches [15] on stream i from the supply temperature side down to the target temperature side.

- for cut-off temperatures $T_{j,k+1}$ of cold process streams :

$$T_{j,k+1} = (1 - x_{j,k}) \cdot T_{j,k} + x_{j,k} \cdot T_{lim\ j,k+1} \tag{5-8}$$

where:

- $T_{lim\ j,k+1} = Min[T_{k+1}, T_{T\ j}]$

hence : $T_{j,k+1} = T_{j,k}$ for $x_{j,k} = 0$; $T_{j,k+1} \rightarrow T_{lim\ j,k}$ for $x_{j,k} \rightarrow 1$

Equation 5-8 is successively applied to all feasible matches [16] on stream j from the supply temperature side up to the target temperature side.

Comments on the definition of the x variables

- The definition of the x *DVs* ensures that the contraints 1. to 3. (responsible for the variable bounds) are automatically met. Any individual described by x_k, $x_{i,k}$, and $x_{j,k}$ variables within the specified bounds is a feasible individual (maybe performing bad, but feasible anyway !). This prevents the optimization from spending time generating and evaluating infeasible individuals.
- Mass balance constraints are much more difficult to account, since these equality constraints link a large number of *DVs* together. The significance of these $K-1$ constraints is described in Sub-section 5.2.5.
- The temperatures T_k of *HSUs* determine which process-storage stream matches are actually feasible (structural effect of T_k, refer to Sub-section 5.2.6). $x_{i,k}$ and $x_{j,k}$ corresponding to infeasible matches are ignored during decoding. The actual number of *DVs* to set $T_{i,k}$, $T_{j,k+1}$ of streams at the outlet of the

15. Feasible matches on hot process streams are those meeting the third feasibility constraints mentioned in Sub-section 5.2.3. $x_{i,k}$ of an infeasible match has no influence ($T_{i,k} \equiv T_{S\ i}$) and is simply ignored. Refer to Sub-section 5.2.6 for more details.
16. Feasible matches on cold process streams are those meeting the third feasibility constraints mentioned in Sub-section 5.2.3. $x_{j,k}$ of an infeasible match has no influence ($T_{j,k+1} \equiv T_{S\ j}$) and is simply ignored. Refer to Sub-section 5.2.6 for more details.

feasible matches is generally significantly smaller than $(K-1)\cdot(I+J)$. Individual-to-individual variations of the number of *DVs* is not conceptually a problem [17].

- It can be seen from Equations 5-7 and 5-8 that whenever a stream has reached its target temperature, any match downstream becomes independent of its corresponding x variable.
- Selecting $T_{i,k}$, $T_{j,k+1}$ as decision variables to define the matches requires the use of x *DVs* on the *GA* side, and results in the dependencies discussed above. Alternatively, areas $A_{i,k}$, $A_{j,k}$ of matches could be used as *DVs* to avoid the dependency problems, since setting any $A_{i,k} \geq 0$, $A_{j,k} \geq 0$ (of feasible matches) always results in a feasible *IHRS* [18].

5.2.5 Mass Balance Constraints

The $K-1$ independent mass balance constraints described by Equations 3-4 and 3-5 include a mass rebalancing term $-MBB_k$, which involves utility consumption [19]. In most cases, the consumption of utilities for rebalancing the *HSUs* represents a cost penalty which should fade out as the solutions are optimized. The question arises whether the mass balance of *HSUs* could be automatically satisfied by the mass contributions of process streams solely : assuming that p_k process streams contribute to a storage sub-system k, the contribution of the p_k th stream would be adjusted to balance the p_{k-1} other mass contributions.

Finding $K-1$ such feasible process-storage stream matches whose contributions can be set to meet the constraints is unfortunately impractical, because :

- balancing process streams featuring feasible heat contributions large enough to cope with a mass imbalance of any value are generally not provided;
- identifying streams whose contributions can be independently adjusted without back-influencing the contribution of existing process-storage stream matches is not always possible.

17. It is as if the model becomes independent of some of the $x_{i,k}$, $x_{j,k}$ variables, i.e. the related factor of dependence falls to zero). Management of extra $x_{i,k}$, $x_{j,k}$ corresponding to infeasible matches *DVs* by the *GA* is associated with a small computational burden. As explained in Sub-section 5.2.8, ignoring $x_{i,k}$, $x_{j,k}$ corresponding to infeasible matches has no detrimental effect as long as the x *DVs* are not accounted in the distance function.
18. This strategy may be acceptable for single-segment streams, for which the cut-off temperatures of the streams may be obtained by matrix inversion; but the technique cannot be applied for multi-segment streams.
19. Sub-section 5.3.5 describes a general methodology for the mass rebalancing for exploiting the opportunities of mixing before resorting to the utility contributions.

5.2.6 Feasible Process-Storage Matches

Given the supply temperature $T_{S\,i}$ of a hot stream i, the *HSU* temperatures T_k determine up to which SSs_k the matches with process stream i are feasible (refer to Figure 5-1). The feasible match condition with SSs_k requires that $T_{S\,i} > T_{k+1}$, since T_{k+1} is the temperature at which the storage fluid has to be heated to enter into the hot *HSU* of SSs_k. $k_{max\,i}$ defines the boundary $HSU_{kmax\,i}$ beyond (i.e. above) which matches with process stream i are infeasible :

$$k_{max\,i} \quad \text{is defined as the largest} \quad k \quad \text{still satisfying} \quad T_{S\,i} > T_k \tag{5-9}$$

Matches with stream i are feasible from SSs_1 up to SSs_{kmax-1}

Similar considerations can be made to define the boundary value $k_{min\,j}$ for cold process stream j :

$$k_{min\,j} \quad \text{is defined as the smallest} \quad k \quad \text{still satisfying} \quad T_{S\,i} < T_k \tag{5-10}$$

Matches with stream j are feasible from SSs_{K-1} down to SSs_{kmin}

$k_{max\,i}$ and $k_{min\,j}$ define the feasible part of the superstructure (structural effect of the set of T_k). The above feasibility conditions could beneficially be relaxed in some cases (refer to Appendix E).

5.2.7 Flowsheet of the Model

Given the set of x decision variables (*DVs*), the calculation of the total batch costs (*TBCs*) is organized as depicted on **Figure 5-2** [20]. Note the following points :

- the superstructure is controlled by continuous *DVs* exclusively. To do without binary variables while the *HEX* cost functions includes a fixed cost, a multiplying exponential function $[1 - \exp(-(A/A_{min})^2)]$ is introduced to help the algorithm to explore towards the bounds. This allows for the fixed costs to be virtually cancelled for $A < A_{min}$, i.e. for insignificant areas;
- the *HEX* units are sized using the well known sizing equation based on the logarithmic mean temperature difference ΔT_{lm} [21].

20. Initialization stages (reading problem data, checking their consistency, reporting errors, initializing variables, performing all individual-independent calculations (e.g. decomposition into time slices, etc.)) are performed once outside the *OF* calculation loop described on Figure 5-2. Refer to *Krummenacher* (2001) for implementation details of the model.

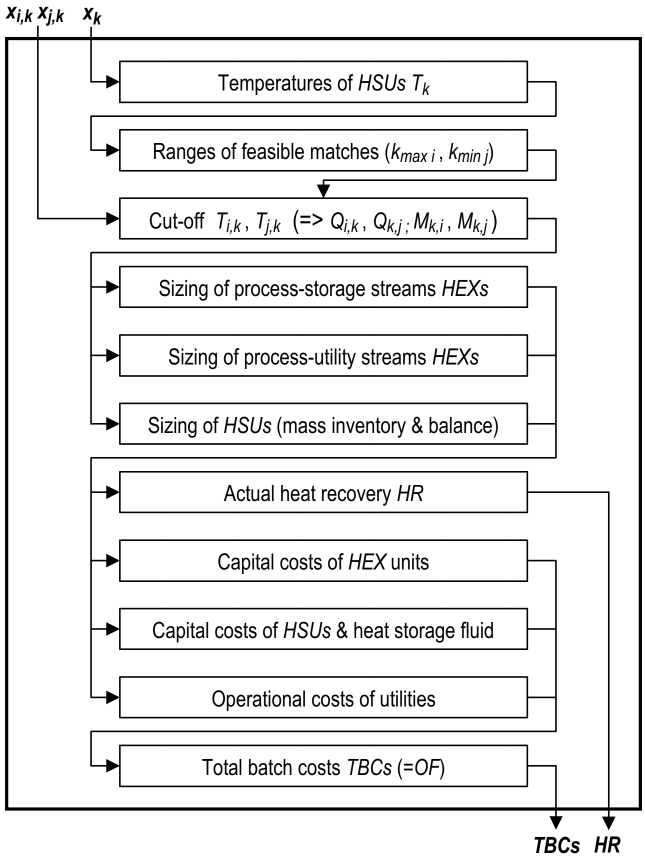

Figure 5-2 Flowsheet of the simple *IHRS* model to calculate the value *OF*(*X*).

5.2.8 Defining a Distance Function

An euclidian distance based on x variables is not recommended for at least two reasons :

1. depending on x_k variables (i.e. the *HSU* temperatures), part of the $x_{i,\,k}$, $x_{j,\,k}$ variables should simply be ignored (refer to Sub-section 5.2.6) [22];
2. the inherent dependence chain (cascade) is complex and is very much dependent on the value of the upward x variables, and invalidates the definition of fixed weights.

As far as only continuous x variables are used, the set of cut-off temperatures of process streams has been identified as a representative measurement for the

21. To avoid numerical problems with the logarithmic mean temperature difference, the approximation proposed by *Chen* (1987) has been implemented instead.
22. There is unfortunately no means to tell the *GA* to exclude these variables from the *DVs* used for the distance calculation (individual-to-individual variability of the distance function cannot be taken into account).

distance between individuals [23] [24]. This distance includes the parametric fine temperature differences (for the same structure) as well as structural differences on a common temperature basis [25].

Giving the same weight to a temperature difference on a "small" stream (from a heat contribution standpoint) as to one on a "large" stream is not reasonable. Therefore the weighting factor has been set as the relative potential heat contribution of the stream with respect to the overall heat recovery potential.

$$D(X_a, X_b) = \sqrt[2]{\sum_{i,k}[q_i(T_{i,k\,a} - T_{i,k\,b})]^2 + \sum_{j,k}[q_j(T_{j,k\,a} - T_{j,k\,b})]^2} \quad \textbf{(5-11)}$$

where:

- $D(X_a, X_b)$ represents the distance between individuals X_a and X_b;
- q_i is the ratio of the (potential) heat contribution of hot process stream i over the overall heat recovery potential;
- q_j is the ratio of the (potential) cooling contribution of cold process stream j over the overall heat recovery potential.

In optimization practice, the distance function appears to be rather a tool than a fixed concept, a tool the user can "play" with. Setting a large weight on one or several variable(s) results in an expansion along the axis of the corresponding variable(s) in the space of the distance, and produces a clustering of the individuals of the population according to the weight of variable(s). This technique is needed for *Struggle* to be able to keep the diversity of structures, but comes with additional considerations; Section 5.5 reviews this issue in more details.

5.2.9 Experience with the Simple *IHRS* Model

The simple *IHRS* model described in this Section has been tested on the *EP-1* simple process. The numerical results and comments are reported in Chapter 6.

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23. Identifying the appropriate set of model variables suitable for a similarity measurement is an open-ended problem - a sound reference does not exist. The similarity/dissimilarity measurement has not to account for the *OF*, since the *OF* is accounted for separately anyway.
24. Alternatively, the distance measurement could be based on the heat contributions of matches or on the mass contributions to the *HSUs*, which already account for the proper weighting. These definitions are even more relevant for multi-segment streams considered in the improved model described in Section 5.3. But these distance definitions have not been tried.
25. The structural influence of the *HSU* temperatures T_k is taken into account in some way through the cut-off temperature after infeasible matches which remains at $T_{S\,i}$, $T_{S\,j}$. The temperature of the *HSUs* are taken into account (not explicitly, but at least implicitly through $T_{i,k}$, $T_{j,k}$)

During early optimization runs, *Struggle* failed to explore solutions featuring high levels of heat recovery and got stuck to sub-optimal solutions (i.e. at inferior levels of heat recovery). This problem has been traced back to a mismatch of the replacement strategy of *Struggle* with the penalty induced by the *HSU* mass imbalances. A preliminary optimization stage during which the heat recovery is maximized has been developed as a remedial measure [26].

Once the remedial measure has been implemented, *Struggle* provided promising results, particularly in the light of the difficulties which were expected as a result of the complex dependencies of variables. Nevertheless, *EP-1* is rather simple to fully validate the suitability of the approach for processes of industrial relevance. In particular, the structural issues have not been addressed and binary variables to control the streams to be heat integrated have not been introduced in the model.

5.3 Improved *IHRS* Model

To deliver actual heat integration solutions to real industrial processes, the simple *IHRS* model (Section 5.2) must be significantly extended in several respects. New features include multi-segment streams, soft-temperature streams [27], multiple *HEX* and *HSU* types & cost functions, segment-wise *HEX* type specification, re-use of *HEX* units. Taking these features into account mainly results in a significantly increased coding complexity and increased *CPU*-time. Since the above mentioned features are not associated with significant methodological difficulties, they are not discussed here (refer to *Krummenacher*, 2001).

However, the additional new features associated with methodological aspects, which include the mixing of storage fluid before resorting to utilities, the introduction of binary variables to optimize the set of process streams to be integrated, and a technique to address the problem of the connections to intermediate *HSUs*, are analysed underneath. The extension to open storage systems is presented in Section 5.4.

26. Section 5.5 emphasizes the cause of the above difficulties and describes other optimization related issues.

27. A segment of stream may be compulsory (like process streams), or soft-temperature (refer to Section 3.2); in the latter case, every higher-order segment (i.e. lower temperature segments for hot streams, higher temperature segments for cold streams) has to be soft-temperature segment too. Unlike the methodology proposed by *Mikkelsen* (1998), partially or totally soft-temperature streams are not introduced as free utility after the process streams have been integrated, but are considered simultaneously like any other stream. In fact, it has been observed that depending on their schedule, the integration of soft streams may be more beneficial than that of process streams; this effect is in principle addressed by *Mikkelsen* too, although not explicitly.

5.3.1 Extended Stream Properties

From a methodological standpoint [28], the possible existence of an internal pinch point within the T-H profile of a process-storage stream match adds a third constraint to the definition of $T_{lim\ i,k}$ (corresponding to $x_{i,k} = 1$) and $T_{lim\ j,k+1}$ (corresponding to $x_{j,k} = 1$) used in Equations 5-7 and 5-8. **Figure 5-3** illustrates

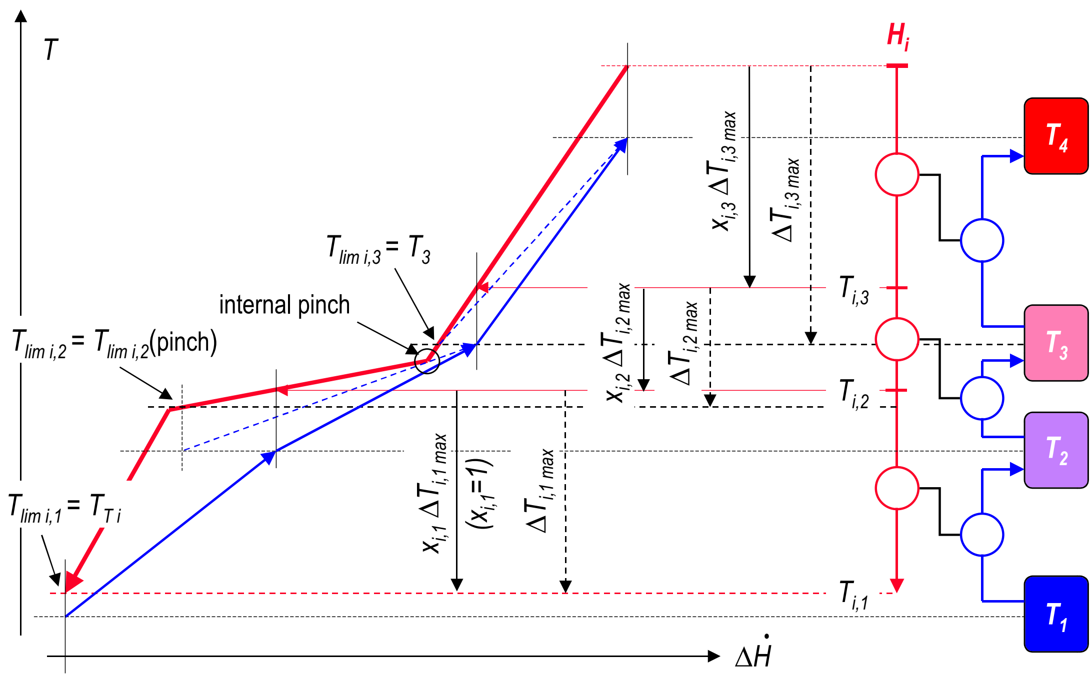

Figure 5-3 The three possible cases defining $T_{lim\ i,k}$ for $x_{i,k} = 1$.

the three possible cases when defining $T_{lim\ i,k}$:

1. $T_{lim\ i,3}$ is defined by the *HSU* temperature T_3;
2. $T_{lim\ i,2}$ results from a pinch point (concave point);
3. $T_{lim\ i,1}$ corresponds to the target temperature $T_{T\ i}$.

$$T_{lim\ i,k} = Max[T_k, T_{T\ i}, T(pinch_{i,k})] \quad \textbf{(5-12)}$$

28. Multi-segments streams introduce additional computational complexity in *HEX* area calculations, in particular when combined with match-wise (actually segment-wise) *HEX* type specifications. But these are commonly encountered in *HEN* design and are not worth a mention here (refer to *Krummenacher*, 2001, for implementation issues).

5.3.2 Match-wise *HEX* Type Specification & *HEX* Costing Issues

Realistic *HEX* capital costs can only be obtained if a specific cost function is associated with each type of *HEX* unit used. This problem is solved in the following way :

1. the list of all possible matches [29] is generated according to time overlap and temperature overlap conditions;
2. the user specifies the *HEX* type to be used for any possible match [30];
3. the definition of an *HEX* type includes as many area ranges as required or available from manufacturers, each range being characterized by its own cost function [31].

Area elements (calculated at the enthalpy interval level) are grouped together according to their type to form *HEX* units. To suit the size ranges defined for the *HEX* type considered (the ranges are supposed to fit existing ranges of an *HEX* supplier), splitting into several *HEX* units is taken into account.

Cost functions, engineering costs, installation costs, running costs, etc. are all subject for debate, depending in particular on the stage of the project - whether conceptual design, pre-design or detailed engineering stage - and on other project parameters. For a pre-design (or a later stage), it seems important to properly account for the cost implications of postulating one process-storage match with each *SSs* [32] (refer to the Sub-section 5.2.1).

Therefore, a distinction is made between *HEX* types allowing multiple area units to be grouped together onto a single *HEX* (typically plate & frame *HEX*), and types which do not allow for grouping and expansion (typically shell & tube *HEX*). This results in different cost structures :

- for *HEX* types like plate & frame, two separate fixed cost factors are considered: one associated with the frame, and one for inlet-outlet connections associated with each circuit;
- for *HEX* types like shell & tube, only one fixed cost factor in considered.

29. At the segment level, since the type of *HEX* can be dependent on the state/phase of the fluid.
30. Only if this type is different from a by-default/general type - the type is not subject to optimization for lowest cost among a list of suitable types.
31. The area ranges of different design series (for standard products) do not necessarily overlap, and cost discontinuities generally exist when changing from one serie to the next.
32. If the feasible match conditions expressed by Equations 5-9 and 5-10 are met.

The splitting of the heat transfer area on process streams into several units (one with each *SSs*) is not the only potential cost penalty induced by the postulated superstructure; each connection to an intermediate *HSU* results (in principle) in the need to individually control the return temperature of the storage fluid, requiring a control valve, a pumping unit, a control circuit, etc. The related costs are accounted and referred to as *temperature control costs*. A technique to account for and optimize the connections to intermediate *HSUs* is described in Sub-section 5.3.4.

5.3.3 *HEX* Re-use

In the present context, the re-use of *HEX* units (e.g. process-storage matches) on several process streams is specified by the user and allows to automatically account for the associated savings on *HEX* capital costs. It is not an optimization variable as it is the case in the *MBC* supertargeting methodology for direct heat integration described in Chapter 7.

HEX re-use is allowed between streams which are specified as part of the same *generalized stream*. The feasibility of re-use requires that the streams sharing the same *HEX* unit(s) do not overlap in time (this condition is checked by the programme). The re-use is *HEX* type dependent, i.e. an *HEX* unit of a given type, say type *A,* cannot be re-used on another stream or segment requiring an *HEX* unit of another type, say type *B* (refer to *Krummenacher*, 2001).

The *HEX* re-use capability is particularly useful for a realistic modelling of non-flowing streams by their discretization in time [33]; the cost of a double wall, a coil or external heat exchanger associated to a vessel is then accounted once and sized to meet the largest area requirement.

5.3.4 Control of Intermediate *HSU* Connections

The superstructure considered in this work postulates a process-storage stream match whenever feasible temperature driving forces exist. Among other motivations, this provides with additional degrees of freedom [34] to explore the trade-off effects between the capacity of *HSUs* and the area of *HEX* units, while meeting the mass balance of connected *HSUs*. But in the absence of a variable to

33. The discretization is needed in case of large temperature increases/decreases, of restricted temperature driving forces with respect to *HSUs* compared to the mean temperature increase/decrease in the vessel (refer to Sub-section 3.2.1). Each time-segmented stream of a discretized non-flowing stream has to be associated with its own x variables, since the operating temperatures change from a time-segmented stream to the next.

control the connection to any intermediate *HSU*, this method may improperly account for the actual number of *HEX* units in the trade-offs.

The present superstructure has originally not been provided with variables to control the low level structure [35]. Instead of introducing binary variables into a model poorly suited for that, a "passive" calculation technique to identify opportunities and to keep track of them is proposed.

From a mass contribution point of view, bypassing a *HSU* is equivalent to supplying a *HSU* with as much storage fluid as being extracted at the same time [36]. The so-called *relative mass flowrate deviation* ($RMFD$) is defined as :

$$RMFD_{k,\,i} = \left|\frac{\dot{M}_{k,\,i} - \dot{M}_{k-1,\,i}}{\dot{M}_{k-1,\,i}}\right| \qquad \textbf{(5-13)}$$

where:

- $\dot{M}_{k,\,i}$ is the mass flowrate of heat storage fluid coming out of HSU_k and going into HSU_{k+1} (due to heat contribution of hot process stream i);
- $\dot{M}_{k-1,\,i}$ is the mass flowrate of heat storage fluid leaving HSU_{k-1} and entering HSU_k (due to heat contribution of hot process stream i).

According to this definition, it can be said that the intermediate connection is virtually non-existent whenever $RMFD_{k,\,i} < RMFD_{min}$, where $RMFD_{min}$ represents a small relative mass flowrate deviation used as a threshold criteria (e.g. in the order of 0.01, i.e. 1%). Whenever this criteria is met for a connection to an intermediate *HSU*, this should result in a sudden decrease of one *HEX* unit. However, to prevent a possible numerical disturbance of the *GA* associated to that sudden step change, the $RMFD$ criteria is applied through an exponential smoothing function :

$$[1 - \exp(-(RMFD_{k,\,i}/RMFD_{min})^2)] \qquad \textbf{(5-14)}$$

34. One per connection to an intermediate *HSU*. In most cases, process-storage stream matches of *IHRSs* designed by *Mikkelsen's* method bypass intermediate *HSU(s)*, i.e. the storage fluid does not go into and out of intermediate *HSU(s)* (see optimization results for *EP-3* in Chapter 6). However, a connection to an intermediate *HSU* can be beneficial to accurately adjust the mass balances of *HSUs* - in particular if the associated match has to cope with small temperature driving forces. In addition, an intermediate connection is generally required if the process-storage stream match extends on both sides of the global *TAM* pinch to achieve the corresponding energy target.
35. Structural decisions are only concerned with the set of process streams to be integrated.
36. For the number of *HEX* units (and associated temperature control), this is not equivalent but this point is described later in this Sub-section.

This function not only applies to the calculation of the *number of temperature controlled connections* (*NTCC*), but also to the calculation of the equivalent number of *HEX* units as well as the size of these units. For example, if the criteria $RMFD_{k,\,i} < RMFD_{min}$ is met, the intermediate connection to HSU_k may be omitted and the *HEX* units on both side of HSU_k be grouped together in a single unit. The way the *HEX* units and their size are influenced by $RMFD$ depends on the *HEX* type(s) [37].

The developed formulas are general and apply to any number of matches, for any sequence of active (i.e. $RMFD_{k,\,i} \gg RMFD_{min}$) or virtual (i.e. $RMFD_{k,\,i} \ll RMFD_{min}$) intermediate connections. The formulas can be understood as a sum of terms weighted by their probability, with [38]:

$$[1 - \exp(-(RMFD_{k,\,i}/RMFD_{min})^2)] \tag{5-15}$$

being the probability for the intermediate connection to be active, and

$$\exp(-(RMFD_{k,\,i}/RMFD_{min})^2) \tag{5-16}$$

the probability for the intermediate connection to be virtual (refer to *Krummenacher*, 2001).

Experience so far indicates that the efficiency of this technique is limited. Optimum *IHRSs* meeting the $RMFD_{k,\,i} < RMFD_{min}$ criteria for a pair of adjacent matches are observed, but this does not allow to obtain the optimum *IHRSs* proposed by *Mikkelsen*.

The following reasons may explain the observed poor efficiency of the technique :

- due to the complex dependencies inherent in the definition of the x variables (refer to Sub-section 5.2.4), keeping track of the narrow region of *DVs* values meeting the $RMFD$ criteria for one match while searching to meet this criteria for other matches is too difficult [39];
- meeting the $RMFD$ criteria or not results from a set of *DVs* values but is not directly controlled by a variable, adding to the already difficult tracking mentioned above.

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37. More specifically whether they allow for multiple area units to be grouped together onto a single HEX or not (refer to Sub-section 5.3.2)
38. With this formulation, the number of units is a continuous function of $RMFD$, i.e. the equivalent number of units is allowed to be non-integer. In principle this is not a problem, since the technique aims at helping the *GA* to explore the possibility of either omitting or keeping an intermediate connection. These are the two possible limit cases towards which the optimized solutions should tend.
39. Including the $RMFD$ criteria in the distance function could potentially improve the tracking capability, but this remains to be applied and verified.

Although the technique has not been analysed in details [40], a more direct control over intermediate connections by means of binary variables is recommended (refer to Appendix E).

5.3.5 Mixing of Storage Fluid to Minimize Mass Rebalancing Costs

Opportunities for mixing of storage fluid prior to *HSU* mass rebalancing by utilities may exist in *IHRSs* including at least three *HSUs* [41]. The issue specifically addressed in this work is how can these opportunities be identified and be exploited in a systematic way [42] to ensure minimum mass rebalancing costs. The developed procedures include :

1. a systematic decomposition of any overall mixing mass contributions into a set of elementary and independent mixing steps [43], each of which implies only mixing of fluid from the two surrounding *HSUs*;

2. a systematic procedure to calculate the optimal mixing mass contributions which minimize mass rebalancing costs;

3. a graphical representation of the optimal mixing mass contributions inspired by the grand composite curve.

A detailed description of these procedures may be found in Appendix C. The systematic calculation of the optimal mixing mass contributions, which applies to any number of *HSUs,* is illustrated on **Figure 5-4**, and the overall graphical representation of these contributions is given on **Figure 5-5**. The optimal mixing mass contributions $M_{M\,k}$ are obtained by sequentially calculating :

1. the *mass before balance* MBB_k left out by mass contributions of process streams;
2. the *cumulated mass before balance* $CMBB_k$ starting from the highest T *HSU*;
3. the *grand composite curve* GCC_k corresponding to $CMBB_k$;
4. the *grand composite curve without pockets* $GCCWP_k$ (pockets=mixing opportunities);

40. Specific trials should be made to ascertain the possibilities and the actual limitations.

41. Whenever possible, mixing of storage fluid provides with utility savings, and could additionally prevent the need for utility *HEXs* (if not needed anyway). However, mixing is associated with exergy losses which could be used to improve the temperature driving forces of *HEX* units (*Krummenacher* & *Auguste*, 1997; *Mikkelsen*, 1998). Hence the existence of mixing in a *IHRS* solution indicates a potential for further improvement. Nevertheless, mixing may be present in optimal solutions in case of topology traps.

42. Resorting to mixing of storage fluid for mass rebalancing *HSUs* has already been proposed by *Stoltze* et al. (1992, 1995), and further developed by *Mikkelsen* (1998). However, a systematic procedure, backed with a graphical representation, has not been presented.

43. Which can be independently scheduled, if need be.

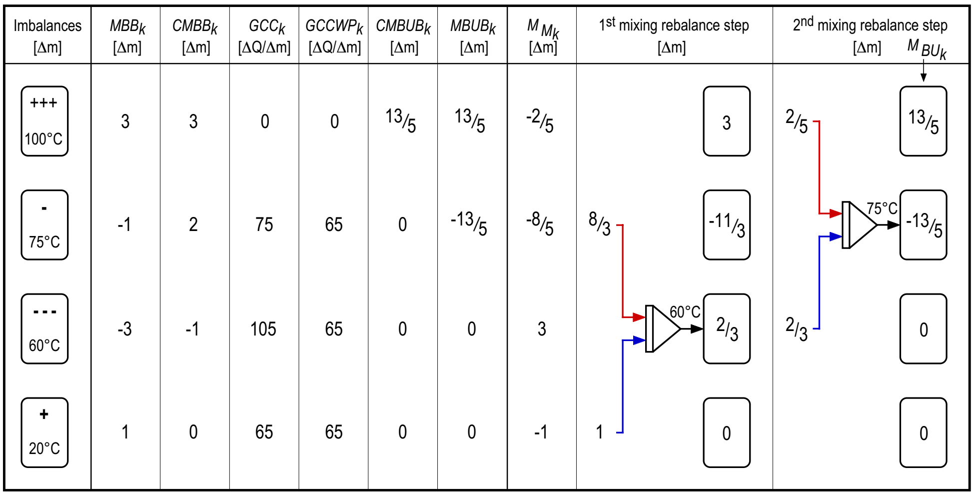

Figure 5-4 Illustration of the proposed systematic procedure to calculate the optimum mixing mass contributions in order to minimize mass rebalancing utility requirements.

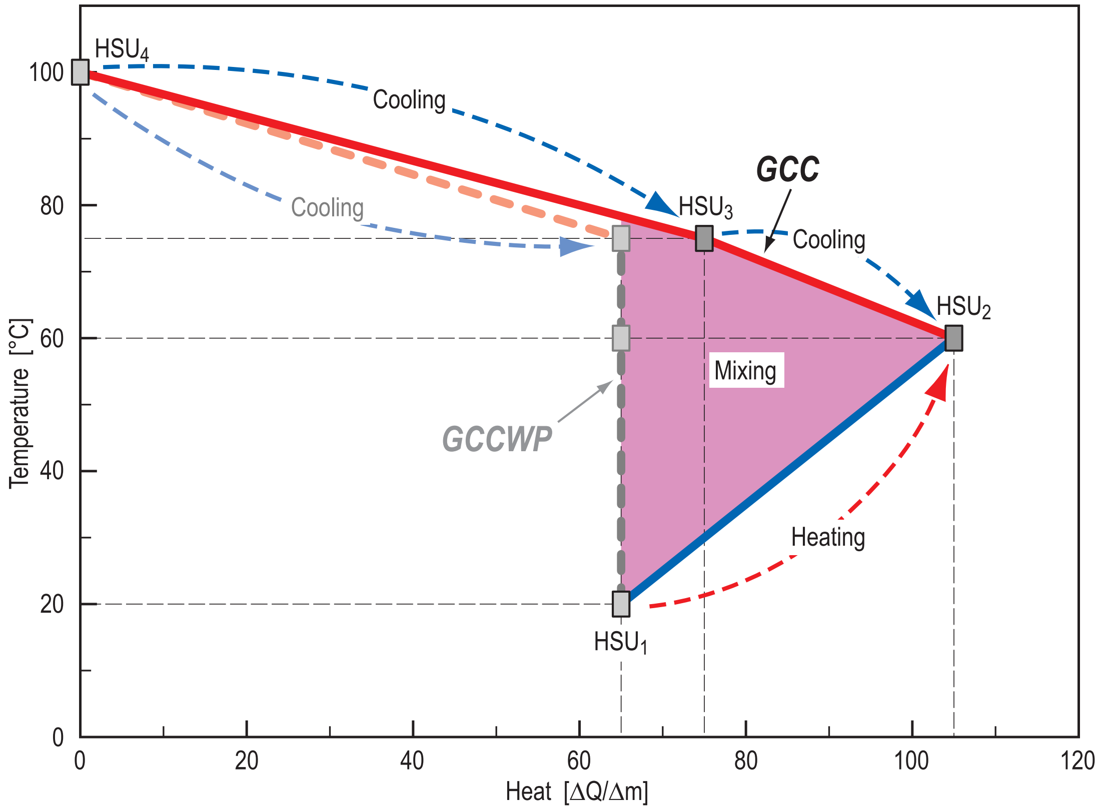

Figure 5-5 *Grand Composite Curve* representation of the mass imbalances of the system represented in Figure 5-4.

5. the *cumulated mass before utility balance* $CMBUB_k$;

6. the *mass before utility balance* $MBUB_k$;
7. and finally, $M_{M\,k} = MBUB_k - MBB_k$.

Proper scheduling of the mixing mass contributions could decrease the capacities of *HSUs*. But this issue is not addressed in this work, considering that :

- the optimization of the schedule would require $(L-1) \cdot (K-2)$ continuous *DVs* to be introduced, each representing the quantity to be mixed during each time slice for a given *HSU* [44];
- as mentioned, mixing is seldom part of the optimized solutions, and even if it would be, the mixing mass contributions are expected to be relatively small, so that the potential benefit of introducing $(L-1) \cdot (K-2)$ additional *DVs* would be very small indeed [45].

5.3.6 Binary Variables to Select Process Streams

A binary *DV* is associated to each stream to decide whether the stream should to be included in the heat integration or not [46] [47]. However, the stream related binary *DVs* do not provide a direct control over the actual *IHRS* structure, because matches on a stream may be infeasible (depending on the temperature of *HSUs*) even if the binary *DV* indicates that the stream should be included. These binary variables are unfortunately not discriminating, in that the same *IHRS* structure may be obtained by different set values of binary *DVs*. This results in increased computing time but does not induce methodological problems.

The introduction of the binary *DVs* allows to address the structural optimization, but its use has required several cascaded modifications (refer to Section 5.5 for the motivations and details) :

1. introduction of the binary *DVs* in the distance function and use of a large weight compared to the weights of cut-off temperatures;

44. A heuristic best-guess strategy is seldom possible, because of the complex dependencies of *HSUs* capacities on mass transfer.
45. Remember that the motivation to adopt the indirect heat integration is the desire to decouple the heat supply of hot process streams from the heat sink of cold process streams; the *HSUs* should include some spare capacity since the system have to cope with schedule variations anyway.
46. The targeting methodology described in Chapter 4 helps to identify small constraining streams which should preferably be excluded from heat integration. But the *GA* based approach has to be able to operate without this preliminary analysis as well.
47. This is definitely safer than including all of them and hoping that the *GA* shall, after a huge number of generations, set all continuous *DVs* of streams to be supplied by utility simultaneously to 0 !

2. development of an optimization on two levels: structural optimization addressed at the upper level, and parametric optimization, given a structure, at the lower level;
3. use of the set of $k_{max\ i}$ and $k_{min\ j}$ (describing the actual *IHRS* structure) in the distance function, instead of the "structure" given by the binary *DVs*. This prevents the loss of diversity in the *HSU* temperatures in the low-level structural optimization.

The results obtained with the simplified brewing process *EP-3* are reported and discussed in Chapter 6. They confirm the suitability of the model, subject to the limitation introduced by the connection to the intermediate *HSUs*, and to the *CPU*-time constraints imposed by the yet interpreted *Matlab* code.

5.4 Open Storage System *IHRS* Model

Food and beverage industries use large amounts of hot process water and are at the same time good candidates for cost-efficient *IHRSs*. To properly account for the potential benefits associated with process water streams in the context of indirect heat integration (e.g. *HEX* unit/area savings, potential for reducing the number of *HSUs*), a model suitable for open storage systems is required [48].

A superstructure including the process water supply network as a special *"HSU"* is first presented (**Sub-section 5.4.1**). The supply temperature of the process water (*PW*) streams is supposed to be at a single and constant temperature. Two possible mixing techniques to reach the target temperature of *PW* streams are proposed (**Sub-section 5.4.2**). The mass flowrate constraints around the *PW HSU* (**Sub-section 5.4.3**) and a systematic procedure to meet them (**Sub-section 5.4.4**) are described. To simplify the calculations and because the condition of constant c_p of a stream segment applies to *PW* streams as well, the assumption $c_{p\ PW} = const.$ holds throughout the developments below.

Selecting an open storage system or a closed (standard) storage system is a decision from the user. If need be, he has to run the optimization for both cases and compare the results.

48. Such a system exists as part of the heat recovery scheme of the brewhouse at the *Brasserie du Cardinal* (process *EP-4* described in Section A.4) and has provided inspiration for the present development.

5.4.1 The Modified Superstructure

The superstructure developed for closed storage systems is adapted by including the process water supply network as a special *HSU*, called the *PW HSU*. The process water at the supply temperature $T_{S\ PW}$ is transferred to the adjacent *HSU(s)* by process-storage stream matches, i.e. in the same way the storage fluid is transferred between the standard *HSUs*. Such a superstructure including three *HSUs* ($K = 3$) and the *PW HSU* is represented on **Figure 5-6**. The position of the *PW HSU* with respect to the other *HSUs* depends on the temperature of the *HSUs* (i.e. on the x_k *DVs*): the *PW HSU* may be located between two *HSUs* as on Figure 5-6, or be a terminal *HSU*, depending on the individual being evaluated.

However, the *PW HSU* is a special *HSU* in that it has no storage capacity, or rather, has a "single way capacity" : the supplied mass flowrate has to be $\dot{\bar{M}}_{PW\ l} \geq 0$ whatever the time slice l, i.e. it can supply (at any time) but not receive and accumulate process water. A systematic procedure to meet the L mass flowrate inequality constraints (one for each time slice) is proposed in Sub-section 5.4.3.

The *PW* mass flowrate results from the balance of flowrates around the *PW HSU* (supply network) [49].

The superstructure is provided with the same decision variables as for the standard closed storage system, except for the process water streams, for which two possibilities exist to control the mixing flowrates. This issue is described in the next Sub-section. To keep the parametric distance function unchanged (i.e. use of the cut-off temperatures), equivalent temperatures of mixing are defined.

The absence of a storage capacity at the supply temperature $T_{S\ PW}$ is open for discussion : process water often undergoes a preliminary treatment, and treated demineralized process water accumulates in a buffer tank, meaning that a storage capacity (like any other *HSU*) is available at $T_{S\ PW}$. This case would be easier to model since it is less constrained. However, the development of the open storage system aims at analysing whether a storage capacity at $T_{S\ PW}$ can be saved or not. The optimization of the brewing process *EP-3* illustrates this point (refer to Chapter 6).

49. In this respect, postulating a process-storage stream match with each *SSs* (whenever the temperature feasibility is met) might seem detrimental and one would prefer to bypass the *PW HSU* and e.g. transfer directly from HSU_1 to HSU_3. But this is in contradiction with the basic postulate of the superstructure (considerations of Sub-section 5.3.4 also apply here); the best way the process water should be transferred to/from the adjacent *HSUs* will be a result of the optimization and cannot be decided *a priori*.

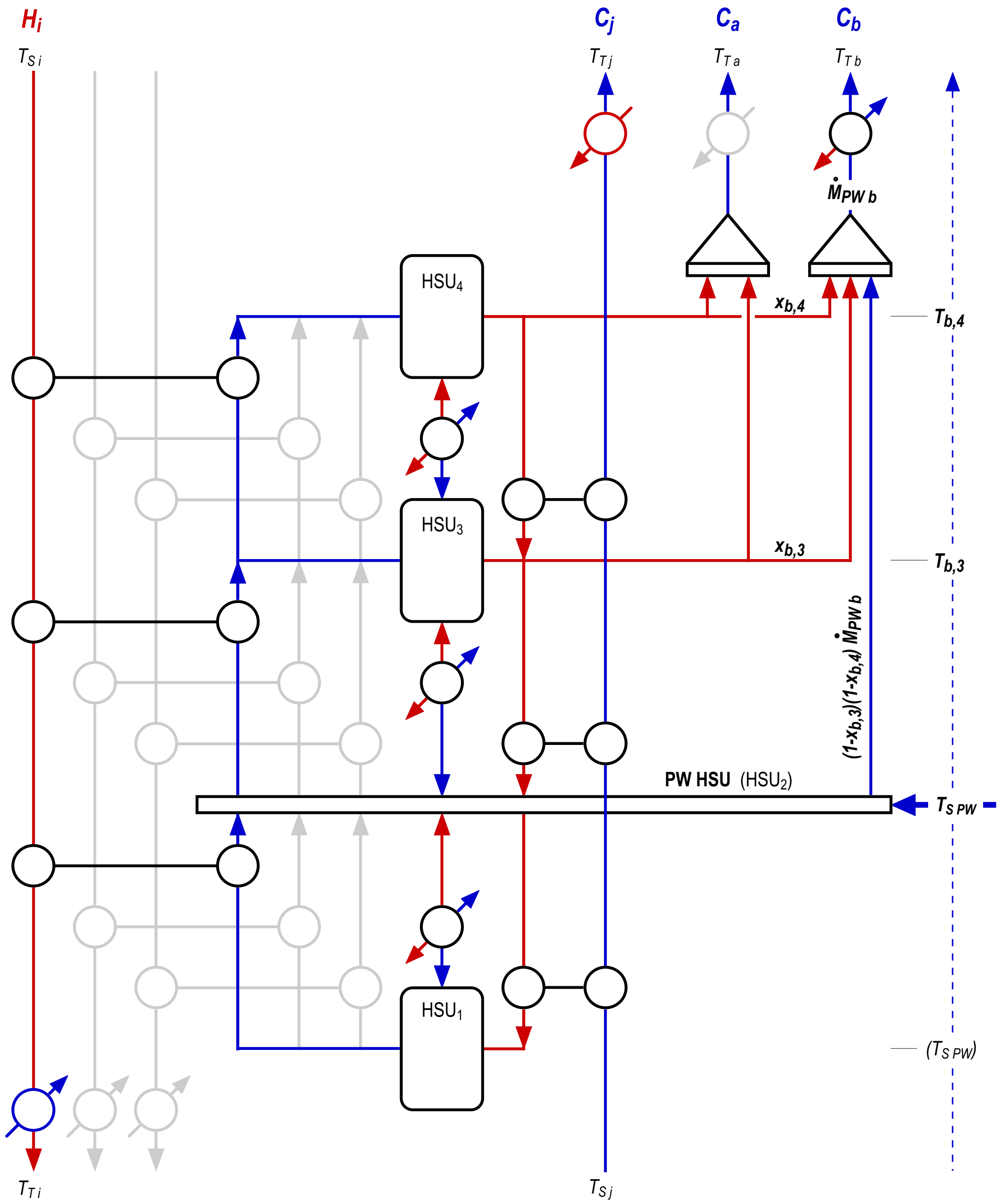

Figure 5-6 Modified *IHRS* superstructure built around an open storage system (see text for comments on the mixing strategy to prepare process water (*PW*) streams C_a and C_b).

5.4.2 Process Water Streams

To reach the target temperature $T_{T\ PW\ j}$ of each (cold) *PW* stream, two mixing techniques are proposed [50] :

1. a simple technique consists in the mixing of storage fluid (water) from the two *HSUs* whose temperatures surround the target temperature $T_{T\ PW\ j}$ of the *PW* stream (e.g. C_a on Figure 5-6). If $T_{T\ PW\ j}$ is higher than the hottest *HSU*, full mass flowrate is extracted from this *HSU*, and post-heating occurs with hot utility. This is a deterministic technique, and the $x_{j,\,k}$ *DVs* of *PW* streams using it are simply ignored.

2. a more general technique consists in the mixing of storage fluid from the *PW HSU* and all *HSUs* above it (for cold *PW* streams, e.g. C_b on Figure 5-6) [51]. In this case, the $x_{j,\,k}$ *DVs* determine the proportion of flowrate to be extracted from the corresponding *HSU*. From the hottest *HSU* down to the *HSU* just above the *PW HSU*, the mass flowrate $\dot{M}_{PW\ j,\,k}$ is calculated from $x_{j,\,k}$ as :

$$\dot{M}_{PW\ j,\,k} = x_{j,\,k} \cdot \left(\dot{M}_{PW\ j} - \sum_{n\,=\,k+1}^{K+1} \dot{M}_{PW\ j,\,n}\right) \tag{5-17}$$

The *PW HSU* supplies the remaining flowrate $\dot{M}_{PW\ j,\,k_{PW}}$ after mixing of storage fluid of all *HSUs* above the *PW HSU* (i.e from k_{PW+1} up to $K+1$) :

$$\dot{M}_{PW\ j,\,k_{PW}} = \dot{M}_{PW\ j} - \sum_{n\,=\,k_{PW}+1}^{K+1} \dot{M}_{PW\ j,\,n} \tag{5-18}$$

In this way, the mass flowrate of the stream is met in any case. The resulting mixing temperature $T_{mix\ PW\ j}$ can be lower or higher than the target temperature $T_{T\ PW\ j}$ (actually $T_{S\ PW} \le T_{mix\ PW\ j} \le T_{K+1}$); in the latter case, reverse utility (cold utility on cold stream) is applied, until the *GA* adjusts the $x_{j,\,k}$ so as to avoid this penalty.

In order for the contributions of *PW* streams to the distance function to be expressed in equivalent cut-off temperatures as for "standard" process streams, the following conversion is applied (from k_{PW+1} up to $K+1$) :

50. The selection of the mixing technique to be applied is a decision from the user !

51. Compared to the simple mixing technique, the exergetic losses are potentially larger, but this could be balanced by additional degrees of freedom to minimize the capacity of *HSUs*.

$$T_{j,k} = T_{j,k-1} + \frac{\dot{M}_{PW\ j,k}}{\dot{M}_{PW\ j}}(T_k - T_{S\ PW}) \tag{5-19}$$

$T_{j,k} - T_{j,k-1}$ is the equivalent temperature increase of the total flowrate $\dot{M}_{PW\ j}$ due to the *PW* flowrate $\dot{M}_{PW\ j,k}$ out of HSU_k. By convention, the temperatures $T_{j,k}$ up to k_{PW} remain at $T_{S\ PW}$.

5.4.3 Mass Flowrate Constraints Around the *PW HSU*

Over a batch cycle, the total mass M_{PW} supplied by the *PW HSU* is obviously equal to the sum of masses of the PW stream(s) :

$$M_{PW} = \sum_{PW_j} M_{PW\ j} = \sum_{l=1}^{L} \Delta t_l \cdot \dot{\bar{M}}_{PW\ l} \tag{5-20}$$

where:

- Δt_l is the duration of time slice l;
- $\dot{\bar{M}}_{PW\ l}$ represents the overall *PW* mass flowrate (including the contributions of process streams and any mixing and/or utility mass balancing contributions discussed in Sub-section 5.3.5) leaving the *PW HSU* during time slice l.

Considering **Figure 5-7**, the *PW* mass flowrate $\dot{\bar{M}}_{PW\ l\ BB}$ leaving the *PW HSU* during time slice l, and due exclusively to the contributions of process streams (i.e. before any mass rebalance of *HSUs*), is given by :

$$\dot{\bar{M}}_{PW\ l\ BB} = \sum_i a_{i,l}(\dot{M}_{k_{PW},i} - \dot{M}_{k_{PW}-1,i}) + \sum_{j \neq PW\ j} a_{j,l}(\dot{M}_{k_{PW}-1,j} - \dot{M}_{k_{PW},j}) + \sum_{PW\ j} a_{PW\ j,l}\dot{M}_{PW\ j,k_{PW}} \tag{5-21}$$

where:

- $a_{i,l} = 1$ if hot stream i exists during time slice l, $a_{i,l} = 0$ otherwise;
- $a_{j,l} = 1$ if cold stream j exists during time slice l, $a_{j,l} = 0$ otherwise;
- $a_{PW\ j,l} = 1$ if cold *PW* stream $PW\ j$ exists during time slice l, $a_{PW\ j,l} = 0$ otherwise;
- $\dot{M}_{k,i}$ is the *PW* mass flowrate due to match of hot stream i with SSs_k;
- $\dot{M}_{k,j}$ is the *PW* mass flowrate due to match of cold stream j with SSs_k;
- $\dot{M}_{PW\ j,k_{PW}}$ is the mixing mass flowrate contribution of *PW HSU* to *PW* stream $PW\ j$.

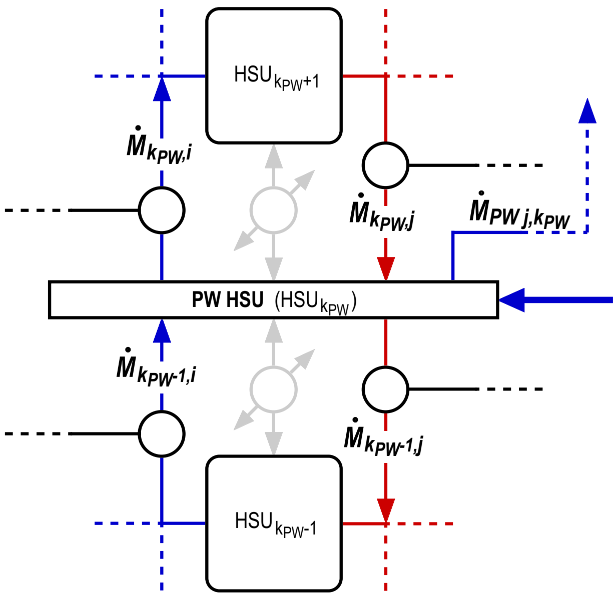

Figure 5-7 Mass flowrates around the *PW HSU* (contributions of process streams only).

The mass flowrate prior to any mass rebalance contributions $\dot{M}^{-}_{PW\ l\ BB}$ may be > 0 (i.e. a resulting flowrate leaving the *PW HSU*), be =0 , or be <0 (i.e. an incoming flowrate, $\dot{M}^{+}_{PW\ l} = -\dot{M}^{-}_{PW\ l} > 0$), depending on the time slice and on process stream contributions as set by the $x_{i,\,k}$ and $x_{j,\,k}$ *DVs*.

The *PW HSU* is actually a supply network, and hence the following L constraints have to be met in any case :

$$\dot{M}^{-}_{PW\ l} \geq 0 \qquad (l\ :\ 1\ ..\ L) \qquad \textbf{(5-22)}$$

The global mass balance of the *PW HSU* expressed by Equation 5-20 is generally not met by the process stream contributions given by Equation 5-21, defining the mass imbalance of the *PW HSU*, while the mass imbalances of the other *HSUs* are determined as for the closed storage system. The elementary mixing mass contributions and the (minimum) mass balancing utility contributions are calculated by the procedure presented in Sub-section 5.3.5. Unlike the process streams, whose schedule is fixed, the mixing mass contributions (if any) and the mass rebalancing utility contributions (if any) may be scheduled so as to minimize the deviation from the constraints expressed by Equation 5-22. A systematic procedure covering all possible cases has been developed; the scheduling of both mixing and utility contributions is not optimized by additional *DVs* (their number would be excessively large compared to the potential benefits) but results from a sound heuristic strategy summarized in the next Sub-section.

5.4.4 Scheduling of the Mixing and the Utility Mass Contributions Around *PW HSU*

This Sub-section provides insight into the problem and in the main ideas behind the scheduling procedure, while an exhaustive description can be found in *Krummenacher* (2001).

Figure 5-8 sketches the mass contributions potentially available for meeting the

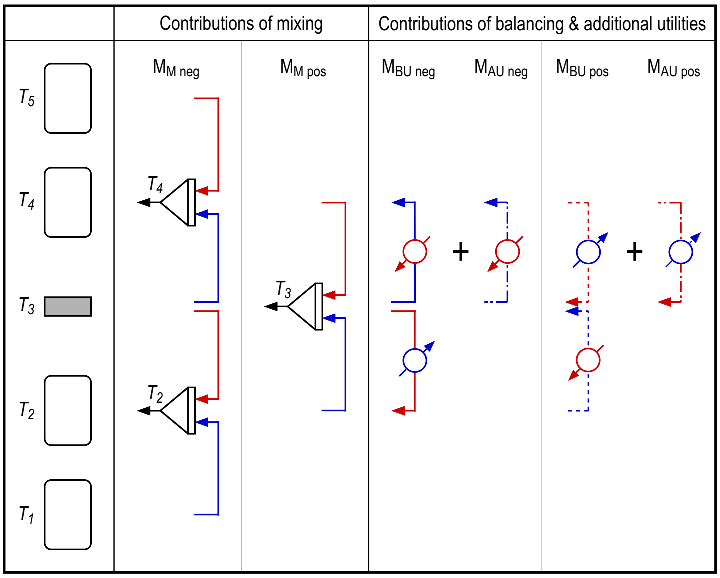

Figure 5-8 Mass transfer contributions around the *PW HSU* to meet the related flowrate constraints.

inequality constraints of Equation 5-22 :

1. the mixing mass contributions ($M_{M\ neg}$ and/or $M_{M\ pos}$);
2. the balancing utility mass contributions ($M_{BU\ neg}$ and/or $M_{BU\ pos}$);
3. the additional utility mass contributions ($M_{AU\ neg}$ and $M_{AU\ pos}$).

The subscripts $_{neg}$ and $_{pos}$ refer to the direction of the mass transfer from the *PW HSU* standpoint [52]. The $M_{AU\ neg}$ contribution is required if $M_{M\ neg}$ and/or $M_{BU\ neg}$ contributions do not exist, or are too limited, to ensure that all inequality constraints of Equation 5-22 are met. But $M_{AU\ neg}$ introduces a mass imbalance which has to be compensated by an equivalent mass $M_{AU\ pos}$ back to the *PW HSU* during uncritical time slices.

52. With positive sign direction corresponding to mass coming into the *PW HSU*.

Figure 5-9 illustrates the scheduling procedure on a simple example. The time slices

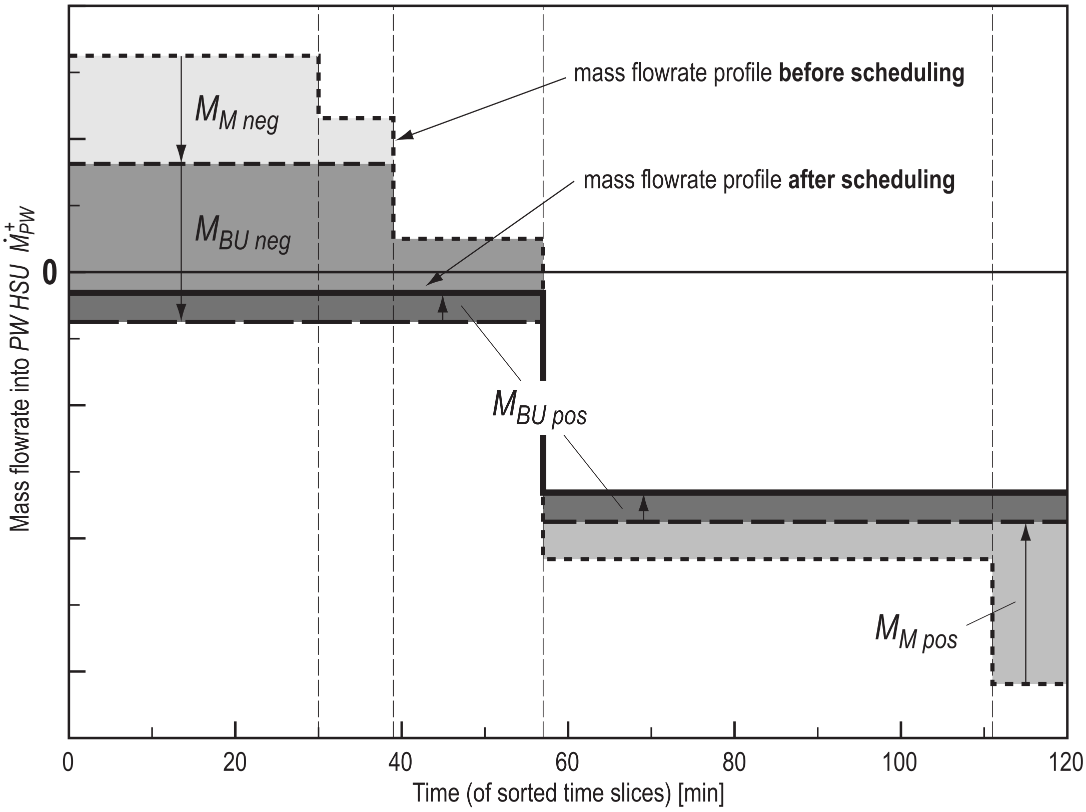

Figure 5-9 Example of scheduling of the rebalancing mass flowrates to meet the flowrate inequality constraints.

have been sorted in decreasing order of incoming flowrate values.

The scheduling procedure aims at meeting the flowrate inequality constraints while minimizing the corresponding utility costs and the capital costs of the related *HEX* units (as already mentioned, the effect on the capacity of *HSUs* is not addressed). To do so, the following features are taken into account :

1. the mixing mass contributions $M_{M\ neg}$ and/or $M_{M\ pos}$ provide with the greatest flexibility at almost no cost (neither energy nor significant capital costs), hence they should be used in priority. The beneficial mixing mass contributions $M_{M\ neg}$ are scheduled according to a peak-shaving strategy to level out the mass flowrates during critical time slices. The detrimental mixing mass transfer $M_{M\ pos}$ is scheduled according to a hollow-filling strategy [53]. These strategies smooth the flowrate profile in anticipation of the scheduling of $M_{BU\ neg}$ and $M_{AU\ neg}$.

53. Note that if the *PW HSU* is the coldest *HSU*, $M_{M\ pos}$ cannot exist.

2. the $M_{BU\ neg}$ and/or $M_{BU\ pos}$ contributions are associated with both energy costs (fixed, independent of scheduling) and *HEX* capital costs (dependent on the heat rate). Since $M_{AU\ neg}$, and hence $M_{AU\ pos}$ in return, are associated with energy and possibly with *HEX* capital costs (if a utility *HEX* unit does not already exist yet), they should be minimized. But in order to minimize the energy cost (the minimum mass $M_{AU\ neg}$ being given), the *HSU* featuring the temperature closest to the *PW HSU* should be selected for temporary storage of $M_{AU\ neg}$.

   Depending on whether $M_{AU\ neg}$ is needed or not, the scheduling of these contributions ($M_{BU\ neg}$ and/or $M_{AU\ neg}$ considered together, and $M_{BU\ pos}$ and/or $M_{AU\ pos}$ also together) applies a minimum heat rate strategy, or a peak-shaving strategy for $M_{BU\ neg}$ and a minimum heat rate strategy for $M_{BU\ pos}$. In the latter case in particular, the strategy should address the scheduling of $M_{BU\ neg}$ and $M_{BU\ pos}$ simultaneously to actually minimize the costs of the two contributions [54].

The flowrate profiles after account of each properly scheduled rebalance contribution are represented on Figure 5-9. In this case, $M_{BU\ neg}$ is in excess so that $M_{AU\ neg}$ is not needed. As suggested, the peak-shaving and hollow-filling strategies smooth the profile by cutting peaks and hollows respectively; the minimum heat rate strategy suppresses by starting from the base and shifts the baseline (as is the case for $M_{BU\ pos}$).

The integral, over the time slices, of the finally obtained flowrate profile (i.e. after $M_{BU\ pos}$ scheduling in the case of Figure 5-9) yields the total mass M_{PW} supplied by the *PW HSU*.

5.5 Optimization Related Issues

The principles of *GA* based optimization and the main features of the *Struggle GA*, originally developed for multimodal optimization of continuous functions, have been described in Section 3.7. This Section summarizes the main difficulties encountered while using *Struggle* in a single-level optimization scheme, and the remedial actions taken. More insight into the difficulties and a detailed description of the techniques implemented to circumvent these may be found in Appendix D.

54. And not sequentially as presently; however, this issue is not considered yet.

5.5.1 Limited Search Capability for Large Heat Recovery

Early optimization trials with the simple *IHRS* model of example process *EP-1* [55] were scarcely able to explore solutions featuring high levels of heat recovery (*HR*) and were stuck to sub-optimal solutions (i.e. at inferior levels of *HR*). This limited search capability seemed inconsistent with the advocated robustness of *GAs*.

This problem has been traced back to a mismatch of the replacement strategy of *Struggle* with the penalty induced by the *HSU* mass imbalances. Individuals featuring a potentially large *HR* but temporarily not able to compete with existing good individuals [56] are prematurely rejected (i.e. not kept in population) before they can improve and develop their full capability.

To bypass this shortcoming, the *HR* is maximized (actually $OF = -HR$ is minimized) during a first phase to allow for large *HR* individuals to develop in the population [57]. After this first phase, $OF = TBCs$, as usually [58].

This strategy aims at providing large *HR* individuals more chances to develop, and has been found to perform well.

5.5.2 Loss of Structural Diversity & Two-levels Optimization Scheme

Using the single-level optimization scheme and the distance function as defined in Sub-section 5.2.8, optimization runs could not identify the known best *IHRS* solution for the simplified brewing process *EP-3* [59]. Unlike expectations, structural diversity was not present in the final population, and the temperatures of *HSUs* showed little individual-to-individual variations.

The distance function (based on cut-off temperatures of process streams exclusively) mixes various distance contributions together and is unable to make a clear distinction between structural and parametric differences. The structural dimension of the similarity measurement between individuals is introduced by

55. These trials aimed at minimizing *TBCs*, while solutions previously obtained with the heuristic method were used as upper bound target values.
56. Because of still inaccurately adjusted mass contributions of process streams to the *HSUs*.
57. It is necessary, during the first phase, to add a constant value to the *OF* to ensure that individuals generated during the first phase be quickly replaced by better offsprings during the second phase.
58. To avoid the risk of early disappearance of large *HR* individuals by a too abrupt change, intermediate steps minimizing a blend of *TBCs* and *HR* may be used.
59. Instead, a *IHRS* structure quite similar (but yet different) to the one of the known best solution was returned.

accounting for the set of binary *DVs* in the distance function, and selecting a weight large enough to prevail over the parametric contributions to the distance. In this way, individuals of different structures are spread apart in the distance space, excluding possible overlap in the parametric distance ranges of different structures.

The use of this new distance definition with the single-level optimization scheme clearly demonstrated, as expected, that the structural diversity is preserved, but the *GA* failed to address the parametric optimization. With at best one individual per structure and no chance for increasing this number [60], the improvement of the *OF* of a structure by crossover of structurally different individuals is very inefficient indeed ! [61].

The only reasonable solution is a two-levels optimization scheme [62], as depicted on **Figure 5-10** :

- the upper level addresses the optimization of the structure (defined by the set of streams to be (potentially) integrated - vector *Y* of binary variables) [63];
- at the lower level, the parametric optimization (vector *X* of continuous *x* variables) of a given structure is performed. A preliminary phase of *HR* maximization is applied anyway.

To ensure the preservation of the population diversity at the lower level, the distance function must account for both the cut-off temperatures (parametric distance contribution) as well as the k_{max} & k_{min} integer values (refer to Sub-section 5.2.6) which describe the structure of actually feasible matches (low-level structural distance contributions).

This is still an hybrid solution where structural issues are not limited to the upper level, but extend to the lower level as well [64]. An extended *IHRS* model suitable for a complete segregation of the *DVs* (i.e. all structural issues addressed at the upper level) and allowing the optimization of the connections to intermediate *HSUs* is proposed in Appendix E.

60. If an offspring has the same structure but a worse *OF*, the existing individual is kept; in the opposite case, it is replaced by the offspring; in both cases, only one individual remains.
61. Improving the parametric features of an individual requires a blend crossover of structurally similar individuals: the probability of mating two such individuals quickly decreases as the number of possible structures becomes of the order, or exceeds, the population size N_{Pop}. Increasing the number of generations to compensate for this decrease is illusory and globally inefficient.
62. Unless the structural dimension can be restricted to a few structures by a preliminary analysis.
63. Refer to comments of Sub-section 5.3.6.
64. Resorting to this hybrid, short term solution was conditioned by earlier choices and implementations of the models - the modifications required to implement the model proposed in next Section were too significant.

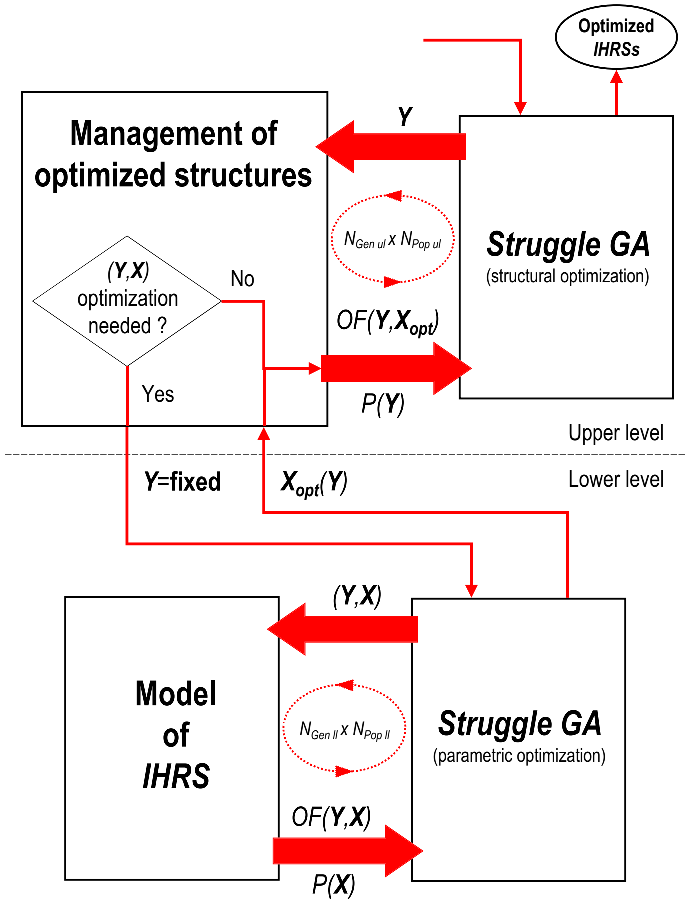

Figure 5-10 Two-levels optimization scheme.

5.6 Summary

Two models of indirect heat recovery schemes (*IHRSs*) using fixed temperature / variable mass (*FTVM*) heat storage units (*HSUs*) suitable for a *GA* based optimization have been developed and implemented in *Matlab*. A first model considers a closed storage system (i.e. the standard case, where storage fluid is confined in the *HSUs*), while the second is based on an open storage system, in which the storage fluid is a process fluid (most generally process water) which enters the storage system, is heated (or cooled) and leaves the *HSUs* whenever these process streams are required.

Designed to deliver practice relevant solutions for real processes and to account for their constraints, the implemented models are detailed with respect to :

- the process streams features which may be taken into account (multi-segments, multi-periods, soft-temperature segment, time discretization of non-flowing streams accounting for the re-use of *HEXs*);
- the utility streams features (multi-segments, variable temperature utilities (e.g. chiller) accounting for the variation of the efficiency, of the specific cost, and of the capital costs, if need be);
- *HEX* types and costs functions (match-wise *HEX* type specifications, multiple costs functions depending on size ranges, proper account for the possibility of mounting several groups of heat exchange on a single frame in the case of plate & frame *HEXs*);
- *HSU* types and cost functions.

The models postulate a heat exchange match between each process stream and each storage sub-system (*SSs*), subject to the constraints of feasible temperature driving forces. A technique called *RMFD* (relative mean flowrate deviation) has been tentatively introduced to account for the possibility of bypassing an intermediate *HSU* and grouping several *HEXs* in serie into a single *HEX*.

The mass balance of the *HSUs* over a period of analysis are not necessarily met solely by the contributions of process streams. Prior to resorting to utilities, the opportunities for mass rebalancing by mixing of storage fluid from different *HSUs* are exhausted, for which a systematic procedure using the Grand Composite Curve representation has been developed to calculate the optimal mixing contributions.

The model based on an open storage system inheritates most of the features of the closed storage system; in addition, the process water supply network is included in the storage system as a special *HSU* featuring a "single-way capacity", i.e. it can supply a net flowrate at any time, but cannot accept a net flowrate into it. This property results in a set of mass flowrate inequality constraints (one for each time slice), which are solved by a sound heuristic scheduling strategy of the mass rebalancing contributions (mixing, balancing utility and additional utility). Process water streams can be prepared by a simple deterministic mixing of the *HSUs* which temperatures surround their target temperature, or by a more complex mixing controlled by optimization variables.

The decision variables (*DVs*) to be optimized are :

- the decision which process streams should preferably be integrated and which should not;
- the operating temperatures of *HSUs*;

- the heat contribution of each process-storage match.

The number of *HSUs* is selected by the user and can only be optimized by repeated optimization runs. The scheduling of rebalancing mass flowrates (in both models) relies on a heuristic best guess strategy but are not actually optimized, unlike the above variables.

Because the bounds on the *HSU* temperatures as well as on the stream cut-off temperatures are variable (depending on the values of more upwards variables), the above optimization variables could not be handled at the *GA* level. Instead, dimensionless variables (which express a ratio of the actual value over the maximum possible value of the corresponding variable) have been used. The hierarchical dependence links resulting from the cause to effect relationships inherent in the *IHRS* models was originally a cause for concern, but has not led to significant optimization difficulties.

From previous experience of other researchers, the *Struggle GA* and a single-level optimization scheme have originally been advised, in spite of the large structural dimension of the problem. Major difficulties with the optimization itself were not expected in view of the robustness of *GAs*. Optimization runs on processes *EP-1* and *EP-3* (refer to Chapter 6) have resulted in a better understanding of the replacement strategy of *Struggle* and in particular of the way the distance function could account for both structural and parametric variables at the same time. When using *Struggle* for the *IHRS* design problem, the structural variables cannot be mixed with the parametric variables in the distance function and efficiently optimized at a single level, unless the number of structural alternatives is restricted to a number much smaller than the number of individuals in the population.

This condition can sometimes be met after a preliminary analysis (e.g. using the targeting method) and/or simplified optimization runs, which allow to focus on some alternatives and to leave out unpromising structures. Structural variables in the distance function should be given a weight large enough so that structural differences result in distance contributions much larger than that resulting from parametric differences.

To avoid the prerequisite of a very restricted number of alternatives, a two-levels optimization scheme has also been implemented and performs satisfactorily, except that the *CPU*-time becomes excessively large because the implemented *Matlab* code is still interpreted. But experience indicates that a speed-up factor of the order of 1000 could be expected using compiled code (either from *Matlab*, or from *C++*), reducing an optimization run to a couple of hours on a typical present day generation *PC*.

When the total batch costs (*TBCs*) are used as the objective function throughout the optimization process, the replacement strategy applied by *Struggle* prevents the development and the progressive improvement of individuals featuring a high heat recovery (*HR*), so that the delivered solutions actually stick at sub-optimal regions. A preliminary step of *HR* maximization or a reduced penalty associated to mass imbalances of *HSUs* solve this issue. The *RMFD* technique fails to simultaneously keep trace of several opportunities to bypass connections to intermediate *HSUs*. An extended *IHRS* model is proposed in order to allow a direct control over the connections to *HSUs* and the full specification of the structural issues at the upper level.

Chapter 6

APPLICATION RESULTS & CONCLUSIONS

6.1 Overview & Preliminary Comments

This Chapter presents the prominent results obtained for the test case *EP-1* (**Section 6.2**) and for the simplified brewery process *EP-3* (**Section 6.3**) using the indirect heat integration methods presented in Chapters 4 and 5.

In addition, issues and proposals which arose during a preliminary indirect heat integration study of a grassroot multi-purpose batch plant in the pharma industry are summarized in **Section 6.4**.

Finally, **Section 6.5** draws the main conclusions pertaining to the indirect heat integration methods developed in this work.

Guidelines for selecting the key optimization parameters (e.g. the number of individuals N_{Pop} and the number of generations N_{Gen}) of the current implementation of the *GA* optimization scheme (in which structural and parametric variables still coexist at the lower level) may be found in Appendix F.

The heuristic targeting method has not been implemented in a dedicated software programme; it has only been applied to *EP-1* using a spreadsheet based approach.

As described in Chapter 5, three indirect heat recovery scheme (*IHRS*) models have been implemented, and the *GA* based optimization of *IHRSs* has significantly evolved with respect to both the optimization strategy and the definition of the distance function. The following summary information is therefore provided with each result :

1. the model *Mdl* (simple *IHRS* / improved *IHRS* / open storage system) [1];
2. the optimization scheme *OS* (single level / two levels);

3. the distance function *DF* (*CoT* / *BDV* / *CoT*&*BDV* / *CoT*&k_{max}&k_{min}) [2];

4. the number of individuals N_{Pop} ;

5. the number of generations N_{Gen} ;

6. the strategy *Sty* (*TBCs* dir / *MBU* red / *HR* max) [3].

Note that the characteristics 3) to 6) are specified for each optimization level; in case of two levels, subscript *ul* denotes the upper level, and *ll* the lower level.

All optimization runs have used the total batch costs (*TBCs*) as the objective function.

The *TBCs vs HR* diagram obtained by the *GA* based approach represents the lowest *TBCs* individuals out of the $N_{Pop} \times N_{Gen}$ generated individuals, as a function of the heat recovery (*HR* - actually discretized in small ΔHR increments). In the vicinity of "optimized optima" [4] the curve represents the lowest achievable *TBCs*(*HR*) with confidence because during the optimization process, a significant number of good individuals (solutions) have been generated in these regions [5].

The solutions delivered by the *GA* and reported below are near-optimum solutions which could be further improved by mathematical methods to accurately adjust the continuous *DVs*. This has not been performed in this work; considering the low consumption of mass rebalance utilities (an indicator of how well the mass balance equality constraints are met) and the known best reference solutions, the improvement potential is expected to be very small, and probably significantly smaller than the errors resulting from fluctuations of the schedule and from the inaccuracies of the model.

In spite of these inherent errors, most of the numerical results reported in this Chapter have not been rounded to their meaningful degree of precision in order to allow future comparisons and use as a benchmark problem.

1. Description of the models in Sections 5.2 (simple *IHRS*), 5.3 (improved *IHRS*) and 5.4 (open storage model).
2. *CoT* = cut-off temperatures (refer to Sub-section 5.2.8), *BDV* = binary decision variables (refer to Sub-section 5.3.6), k_{max}&k_{min} = low level structure (refer to Appendix D).
3. *TBCs* dir = *TBCs* is minimized from the very beginning, *MBU* red = *TBCs* is minimized but the cost of mass balancing utility needs is reduced during a preliminary stage, *HR* max = *TBCs* is minimized but only after a preliminary stage maximizing the heat recovery (for these latter modes, refer to Appendix D).
4. By "optimized optima", it is meant local optima which correspond to different *IHRS* structures, provided that the structural differences are explicitly taken into account in the distance function, ensuring that each structure is optimized independently of the others.
5. This is not necessarily the case away from these optima, since a detailed optimization does not occur there; the curve does not provide a reliable lower bound of *TBCs* over the whole heat recovery range !

6.2 Test Case *EP-1*

EP-1 is a simple, imaginary process (described in Section A.1) originally set up to validate the *multiple base case* (*MBC*) targeting for direct heat exchanges (refer to Chapter 7). It is has been used for testing the indirect heat integration methods as well, and therefore allows for a comparison of the different approaches.

The results obtained with the heuristic targeting method have already been presented in Chapter 4 to illustrate the procedure. They are recalled on **Figure 6-1** for comparison with the results obtained with the *GA* optimization approach. Optimization runs have been carried out for 3 and 4 heat storage units (*HSUs*).

In both cases, the *GA* takes advantage of the additional degrees of freedom and provides solutions featuring *TBCs* improvements of 2.6 % (for 3 *HSUs*) and 5 % (for 4 *HSUs*) compared to the corresponding solutions derived from the assumption of the vertical model.

6.2.1 *GA* Optimization with 4 *HSUs*

With 4 *HSUs*, the following best solution has been obtained [6]:

- *TBCs* = 27.4 *CHF*/batch; *HR* = 292 *kWh*/batch

Compared to the related best solution obtained by targeting, the *TBCs* improve by 5 %, while the *HR* decreases by 1.4 %. The optimum region features an extended *HR* range, and small differences in *HR* are not meaningful; additional optimization runs have resulted in similar values featuring an identical structure of the matches :

- *TBCs* = 27.46 *CHF*/batch; *HR* = 294 *kWh*/batch;
- *TBCs* = 27.5 *CHF*/batch; *HR* = 291 *kWh*/batch.

Table 6-1 provides detailed numerical values to compare the optimum *4 HSUs* solutions obtained by the heuristic targeting (refer to the *IHRS* represented on Figure 4-3) and the *GA* based method, respectively. It appears that :

1. the differences between corresponding temperatures of *HSUs* are within the range 1.5 .. 4.3 °*C*, i.e. quite close to each other. More importantly, the *HSU* temperatures define identical k_{max} & k_{min} set of values;

6. *Mdl* = simple / *OS* = single / *DF* = *CoT* / N_{Pop} = 75 / N_{Gen} = 10000 / *Sty* = *HR* max during 5000 generations.

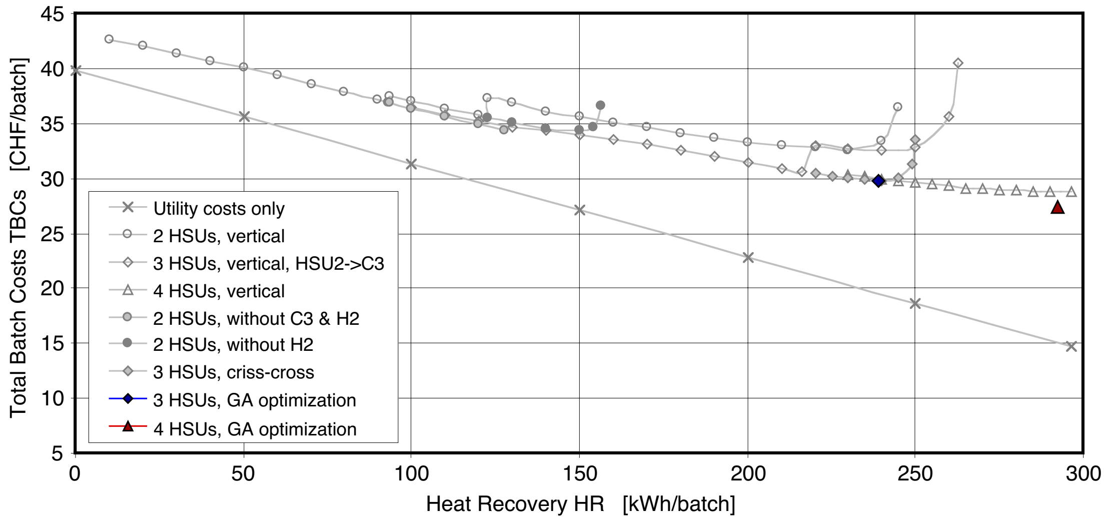

Figure 6-1 Solutions obtained for process *EP-1* on a *TBCs vs HR* diagram.

2. the striking difference between the two solutions relates to the capacities of the *HSUs*. The relaxation of the constraint of a vertical definition of *HR* ranges (and cut-off temperatures) provides with an important additional degree of freedom : by allowing the cut-off temperatures of streams to be independently adjusted, the trade-off between the *HEX* areas and *HSU* capacities is optimized in a much extended search space. The solution identified by the *GA* efficiently benefits from it. While stream H_3/H_4 is only matched with storage sub-system n° 3 (SSs_3) in the targeting solution, matches with SSs_1 to SSs_3 exist in the *GA* solution; this accurate adjustment of mass supply and mass extraction results e.g. in the very small capacity of HSU_2;
3. the reduction of the *HSU* capacities is actually helped by assuming no fixed cost for the *HSUs* [7] as well as assuming plate & frame *HEXs* allowing for the total area on a process stream to be split into several area units without cost penalty (refer to Appendix A). Nevertheless, it demonstrates the capability of the *GA* to exploit these beneficial features whenever provided;

COSTS	HEN Costs	HSU Costs	Utility Costs	TBCs	**Rel. Costs**
Method	[CHF/batch]	[CHF/batch]	[CHF/batch]	[CHF/batch]	**[%]**
Heuristic	10.17	3.93	14.71	28.81	**100**
GA Optim.	10.81	1.51	15.05	27.37	**95**

Table 6-1 Heuristic targeting vs *GA* optimized *IHRSs* for *EP-1* with 4 *HSUs*.

7. This assumption can be questioned but introducing a fixed cost term would not decrease the validity of the approach.

SIZES Method	HR [kWh/batch]	HEN Area [m2]	HSU Capac. [m3]	HU [kWh/batch]	CU [kWh/batch]
Heuristic	296.25	**119.0**	**6.30**	180.00	61.35
GA Optim.	292.16	**132.5**	**1.68**	184.09	65.44

HEN Temp. [°C]		H1	H2	H3/H4	C1	C2	C3
Heuristic	T4	135.0	100.0	165.0	100.0	130.0	105.0
	T3	100.0	100.0	125.0	89.5	130.0	89.5
	T2	95.9	95.9	125.0	80.0	130.0	80.0
	T1	51.0	95.0	125.0	25.0	130.0	80.0
GA Optim.	T4	135.0	100.0	165.0	99.2	130.0	104.6
	T3	104.4	100.0	147.8	92.2	130.0	94.5
	T2	94.7	96.1	126.3	79.1	130.0	80.0
	T1	52.5	95.0	125.2	25.0	130.0	80.0

HEXs Areas [m2]		H1	H2	H3/H4	C1	C2	C3
Heuristic	Hot Util.	–	–	–	–	10.48	–
	SSs3	12.23	–	8.26	1.51	–	12.69
	SSs2	1.23	22.42	–	3.69	–	18.46
	SSs1	9.15	1.35	–	12.71	–	–
	Cold Util.	4.80	–	–	–	–	–
GA Optim.	Hot Util.	–	–	–	0.02	10.48	0.05
	SSs3	9.32	–	3.11	1.04	–	10.51
	SSs2	2.80	29.15	3.38	4.24	–	32.32
	SSs1	8.05	1.67	0.26	11.43	–	–
	Cold Util.	4.88	0.02	0.01	–	–	–

HSUs	HSU1		HSU2		HSU3		HSU4	
Method	T [°C]	V [m3]	T [°C]	V [m3]	T [°C]	V [m3]	T [°C]	V [m3]
Heuristic	41.3	0.24	83.9	1.61	96.0	3.15	125.6	1.30
GA Optim.	37.0	0.21	86.3	0.04	97.5	0.82	127.4	0.62

Table 6-1 Heuristic targeting vs *GA* optimized *IHRSs* for *EP-1* with 4 *HSUs.*

4. the HSU_2 capacity is small but its presence is needed by stream C_3 ($T_{S\,3} = 80\ °C$) which otherwise could not cool the storage fluid down to $T_1 = 37\ °C$;

5. the extent to which the capacities of *HSUs* can be reduced is a measure of the opportunity to match hot and cold stream contributions within each *SSs* in order to maximize the proportion of heat which could be transferred by a direct *HEN* [8].

8. The larger the specific cost of the *HSUs* with respect to that of *HEXs*, the stronger the trend to maximize direct heat exchanges. The significance and consequences of this observation to identify beneficial direct matches, and the comparison with the direct batch *HEN* obtained by *MBC* targeting (refer to Chapter 7) have not been analysed in this work. In any case, the schedule variations likely to occur should first be accounted before meaningful information could be drawn.

6.2.2 *GA* Optimization with 3 *HSUs* & Structural Diversity

With 3 *HSUs*, the best solution among the optimized structures features [9]:

- *TBCs* = 29.83 *CHF*/batch; *HR* = 239 *kWh*/batch

Compared to the related best solution obtained using the vertical model, the *TBCs* improve by 2.6 %, while the *HR* increases by 10.6 %. However, compared to the optimum solution obtained by targeting but allowing for criss-cross heat exchanges [10], the *GA* solution is nearly identical in all respects. Accounting for k_{max}&k_{min} in the distance function allows to keep the structural diversity, i.e. to identify the corresponding local optima; other local optima returned by the *GA* include :

- *TBCs* = 30.4 *CHF*/batch; *HR* = 224 *kWh*/batch
- *TBCs* = 34.0 *CHF*/batch; *HR* = 150 *kWh*/batch

6.2.3 Conclusion

Results obtained for the simple *EP-1* demonstrate the capability of the *GA* to take advantage of the degrees of freedom, in particular of the schedule and heat contributions of streams, to significantly reduce the capacity of *HSUs*. At the same time, for "reasonable" processes (e.g. limited simultaneity of streams, limited temperature driving forces), the targeting approach assuming a vertical definition of the *HR* ranges and cut-off temperatures provides targets of acceptable precision (the smaller the temperature driving forces available for heat exchanges, the more restricted the opportunities for criss-cross heat exchanges to minimize the capacity of *HSUs* without significant *HEX* area penalty).

9. *Mdl* = improved / *OS* = single / *DF* = *CoT*&k_{max}&k_{min} / N_{Pop} = 250 / N_{Gen} = 2000 / *Sty* = *HR* max during 600 generations. Unlike the case with 4 *HSUs*, which has let all heat contributions of process streams be optimized, in this case $x_{i,1}$ = 1 for streams H_2 and H_3/H_4 to explicitly specify that the target temperature of these streams has to be ensured by heat integration solely, without utility coolers. This is a reasonable constraint, instead of letting the GA progressively approach this condition (e.g. see cut-off temperatures of H_2, H_3/H_4, C_1 and C_3 in Table 6-1). This technique is particularly relevant for *HEX* cost functions featuring a large fixed cost.
10. This solution which deviates from the vertical model (refer to Sub-section 4.5.4) was simple to devise because of the simplicity of the process; this is seldom the case for processes including a larger number of streams !

6.3 Case Study *EP-3*

Process *EP-3* is a brewing process studied by *Mikkelsen* (1998) and described in Section A.3. *EP-3* actually includes 12 process streams (C_1, C_2, C_3, C_4, C_5, C_6, C_7, C_8, C_{13}, H_9, H_{10}, $H_{11/12}$) and hence 12 binary *DVs* are required for a full structural optimization with the presently implemented models (refer to Appendix D) [11]. A closed storage *IHRS* model including 3 *HSUs* requires 27 continuous *DVs* (3+12x(3-1)), while an open storage *IHRS* model including 3 *HSUs* (excluding the *PW HSU*) requires 39 continuous *DVs* (3+12x(4-1)).

The known best solutions from his work provide a useful reference for checking and improving the *GA* based approach. Inspired by features of *EP-4* (an actual brewing process at the *Brasserie du Cardinal*), *EP-3* has also been slightly modified to check the validity of the open storage system *IHRS* model, and to carry out a preliminary assessment of the sensitivity of the optimal solutions to variations of the batch repeat time.

The *GA* optimization runs have provided significant insight into the structural issues and have resulted in the improvements of the optimization scheme presented in Section 5.5. Because of the *CPU*-time constraints associated with the use of non-compiled *Matlab* models, the full structural optimization could not performed. But simple insight into the process has allowed to set some of the binary *DVs* and to focus the structural considerations on 3-4 streams only out of the 13 streams.

All runs have considered 3 *HSUs*. Both closed storage and open storage system models have been used :

- for the closed storage system, the known best solution integrating 6 streams (C_1, C_4, C_7, C_{13}, H_9, H_{11}, reported in *Mikkelsen*, 1998) has been searched for and optimized. Very close solutions have been obtained by the *GA* approach; the small differences in the models (*HEX* matches and costs, and non-perfect parametric adjustment achieved by the *GA)* explain the small discrepancies;
- the open storage *IHRS* model of *EP-3* has been optimized assuming that C_7 be the single process water stream. Solutions obtained are significantly cheaper and achieve a larger HR; the introduction of the *PW HSU* relaxes the constraints on the temperature assignment of the *HSUs*, explaining that the actual cost savings are much larger than the *HEX* capital cost savings contribution alone.

11. The extended *IHRS* model proposed in Appendix E would involve a larger number of binary *DVs*.

6.3.1 Closed Storage System

The *GA* optimization [12] of the C_1, C_4, C_7, C_{13}, H_9, H_{11} set of integrated streams has resulted in a *IHRS* very similar to the 6-streams optimum solution developed by *Mikkelsen* (see **Figure 6-2** and **Table 6-2**). These two solutions are worth the

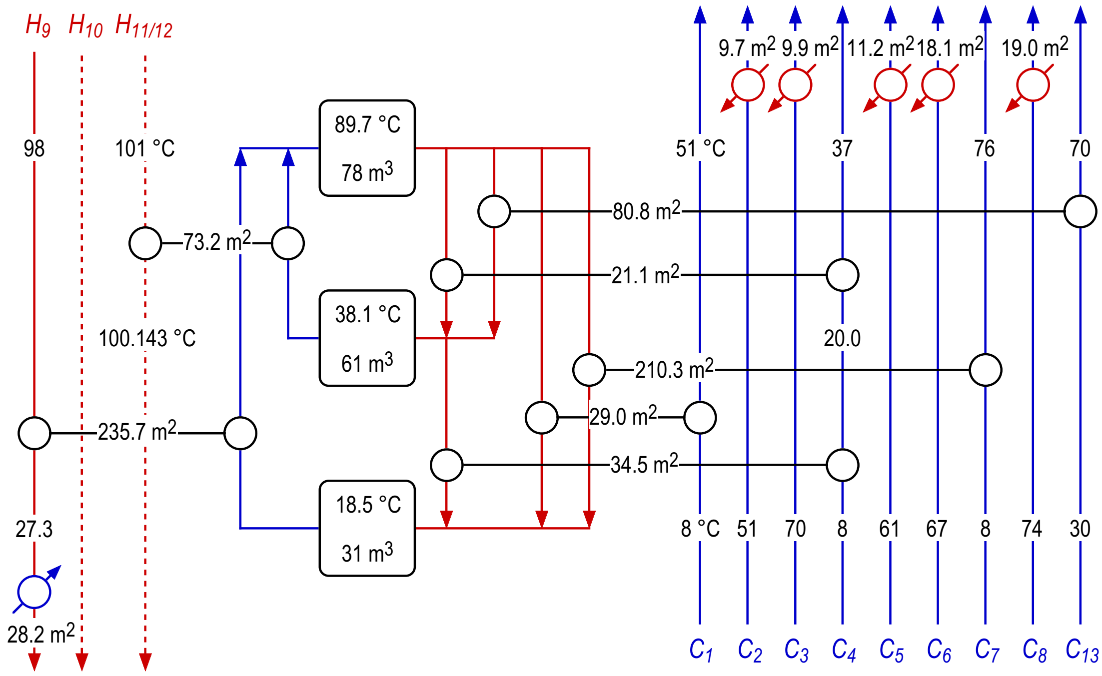

Figure 6-2 *Mikkelsen's* best *IHRS* solution integrating 6 streams (H_{10} & $H_{11/12}$ in dotted line are heat recovery streams, *EP-3*, 3 *HSUs*, closed storage system).

following comments :

1. both solutions achieve the same *HR*, but the utility costs of the *GA* solution are slightly higher, owing to the 35 *kWh*/batch cold utility for mass rebalance. Actually, this results from 35 *kWh*/batch of excess heat being recovered on H_{11} (a heat recovery stream) which are finally left out in cold utility, explaining why the actually achieved *HR* is not influenced;
2. low-level structural differences are present: *Mikkelsen* postulates no connection to intermediate *HSUs*, but still introduces them when beneficial (e.g. on C_4). In the *GA* solution, inherent to the model, intermediate connections exist on C_1,

12. *Mdl* = improved / *OS* = single / *DF* = *CoT* / N_{Pop} = 100 / N_{Gen} = 1000 / *Sty* = *HR* max during 300 generations; the match variables with SSs_2 on C_1, C_4, C_7 and C_{13} were set to $x_{j,2} = 1$ to avoid considering utility heaters. However, this insight into the problem is not a prerequisite condition, the *GA* being able to automatically identify these conditions thanks to the exponential multiplying function mentioned in Sub-section 5.2.4.

COSTS Method	HEN Costs [DKK/batch]	HSU Costs [DKK/batch]	Utility Costs [DKK/batch]	TBCs [DKK/batch]	Dev. TBCs [%]
Mikkelsen	507.2	136.2	632.7	**1276.1**	**100**
GA Optim.	515.9	133.5	639.3	**1288.7**	**101.0**

SIZES Method	HR [kWh/batch]	HEN Area [m2]	HSU Capac. [m3]	HU [kWh/batch]	CU [kWh/batch]
Mikkelsen	14510	780.8	170	5766	1931
GA Optim.	14510	783.4	166.3	5766	1966

Cut-off T [°C]	Mikkelsen			GA Optimization		
	T1	T2	T3	T1	T2	T3
H9	27.3	–	98.0	27.9	**48.5**	98.0
H10	–	–	–	–	–	–
H11	–	100.143	101.0	100.095	100.109	101.0
H12	–	–	–	–	–	–
C1	8.0	–	51.0	8.0	**25.3**	51.0
C2	–	–	–	–	–	–
C3	–	–	–	–	–	–
C4	8.0	**20.0**	37.0	8.0	**13.6**	37.0
C5	–	–	–	–	–	–
C6	–	–	–	–	–	–
C7	8.0	–	76.0	8.0	**30.6**	76.0
C8	–	–	–	–	–	–
C13	–	30.0	70.0	–	30.0	70.0

HEXs [m2]	Mikkelsen				GA Optimization			
	CU	SSs1	SSs2	HU	CU	SSs1	SSs2	HU
H9	28.2	235.7			28.9	65.9	152.3	
H10								
H11			73.2			0.2	72.0	
H12								
C1		29.0				20.1	15.6	
C2				9.7				9.7
C3				9.9				9.9
C4		34.5	21.1			12.9	25.2	
C5				11.3				11.3
C6				18.1				18.1
C7		210.3				84.6	159.6	
C8				19.0				19.0
C13			80.8				78.2	

Mass rebalance contributions (for GA optimized solution only)	
Mixing:	1280 kg from HSU1 to HSU2 & 520 kg from HSU3 to HSU2
Utility:	cooling 616 kg from HSU3 to HSU2 (35.3 kWh/batch)

HSUs	HSU1		HSU2		HSU3	
Method	T [°C]	V [m3]	T [°C]	V [m3]	T [°C]	V [m3]
Mikkelsen	18.5	31	38.1	61	89.7	78
GA Optim.	19.2	27.7	39.4	58.4	88.6	80.2

Table 6-2 *Mikkelsen vs GA* optimized *IHRS* solutions for *EP-3* with 3 *HSUs* (closed storage system).

C_4, C_7, H_9, H_{11}; however, the benefit of removing the one on H_9 is identified by the *GA* (remaining mass flowrate deviation *RMFD* = 0.011), while the match on H_{11} with SSs_1 could be left out because of its very small contribution. Opportunities for improvements are found by insight;

3. in the *GA* solution, a fixed cost per header (inlet/outlet connection) has been introduced in the *HEX* cost function (refer to Sub-section 5.3.2) to account for the costs associated to an intermediate connection, while such a penalty does not seem to be accounted in *Mikkelsen's* best solution (the cost of the *HEX* on C_4 ignores the fact that the *HEX* area is actually split). The penalty for the 5 intermediate connections of the *GA* optimized *IHRS* contributes to 1/3 of the difference between the two solutions (i.e 0.34 % of the *TBCs*);
4. the *GA* solution still includes a small utility contribution to the mass rebalance of the *HSUs*; the utility costs and the capital costs of the utility *HEX* amount to 46 % of the *TBCs* difference between the two solutions (i.e. 0.46 % of *TBCs*) though quite small, a mixing contribution for mass rebalance still exists; this is likely only due to the limited capability of the *GA* for very accurate adjustment of continuous parameters (real *DVs*). This reveals an additional potential to decrease the *HEX* areas by an improved distribution of the temperature driving forces;
5. though quite small, a mixing mass contribution still exists; this is likely due to the limited capability of the *GA* to achieve a very accurate adjustment of continuous parameters (real *DVs*) and reveals an additional potential to decrease the *HEX* areas by an improved distribution of the temperature driving forces;
6. the *HSU* capacity of the *GA* solution is 2 % smaller. Knowing that splitting of *HEX* units (i.e. introducing intermediate connections) provides the optimization with additional degrees of freedom, and provided that the intermediate connections are free of cost penalty (as apparently assumed by *Mikkelsen*), *IHRSs* cheaper than the *Mikkelsen's* best solution could potentially be identified. In this case the improvement is likely to be negligible, but the above considerations support the idea of explicitly including the intermediate connections in the optimization, as proposed in Appendix E.

6.3.2 Open Storage System

A brewing process alone often includes two process water streams: the water for mashing, and the sparging water (refer to the description of *EP-4* in Appendix A). Large amounts of hot water are needed outside the brewhouse too. To verify the interest of the open storage system for *EP-3*, stream C_7 (i.e. the preparation of the sparging water) has been specified as a process water stream [13]. Three cases have been considered and the optimized solutions are reported and commented below :

1. a set of 9 process streams to be optimally heat integrated over the standard 200 *min* repeated batch cycle;
2. the optimization of the indirect heat integration of the same set of 9 streams, but over a period of 10 batches, including the start-up and shut-down phases (i.e. phases of non-cyclic conditions) and variations of the batch cycle times;
3. a search for an optimum open storage *IHRS* integrating all 13 process streams.

Warning ! Unlike the closed storage *IHRS* described in the previous Sub-section, the 3 optimized open storage *IHRSs* presented below now include one or several non-flowing streams (C_2, C_3, C_5, C_6 - refer to Section A.3). According to the comments of Section A.4 concerning the modelization of these streams, further optimization runs must be performed to ensure the actual feasibility of these *IHRS* solutions, but this issue has not been addressed yet.

6.3.2.1 9-Streams, Single Batch Cycle

Preliminary optimization runs indicated that the set of integrated streams C_1, C_2, C_4, C_7, C_8, C_{13}, H_9, $H_{11/12}$ lead to a cost-optimum open storage *IHRS*. The optimization [14] of this "high-level structure" has resulted in the *IHRS* represented on **Figure 6-3**. The *PW HSU* is the first (i.e. coldest) *HSU* of the system so that the balance of mass flowrates around it is quite simple, but it could also be the second one, while the coldest would store the cold utility to cool H_9 [15].

With respect to the known best *IHRS* for the closed storage model (refer to Figure 6-2), both the *TBCs* and the *HR* are significantly improved, by 13.2 %, and 11.5 % respectively. **Table 6-3** summarizes the main characteristics of the two *IHRSs* [16].

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13. This is a pessimistic assumption since the additional potential benefit of reduced *HEX* units and *HEX* area associated with other process water streams is not accounted for.

14. *Mdl* = open storage system / *OS* = single / *DF* = *CoT*&k_{max}&k_{min} / N_{Pop} = 200 / N_{Gen} = 2000 / *Sty* = *HR* max during 300 generations / selected streams C_1 C_2 C_4 C_7 C_8 C_{13} H_9 $H_{11/12}$ / 3 *HSUs* + *PW HSU*.

15. The supply temperature of the process water streams is often equal to the cold end temperature of the cold composite, but the open storage system can deal with any other case featuring a more complex balance of flowrates around the *PW HSU*.

16. Considering Table 6-3, remember that the utility costs are proportional to the utility consumption (Q_{HU} = *4091* kWh/batch, Q_{CU} = 1778 *kWh*/batch) and not to the heat recovery; the fact that the relative increase of the *HR* (11.5 %) is significantly smaller than the relative decrease of the utility costs (24.6 %) is therefore not surprising.

The comparison further indicates that :

1. the reduction of the *TBCs* does not solely result from the *HEX* on C_7 being left out (C_7 prepared by mixing, see Figure 6-3);
2. the *HR* is significantly increased by the integration of C_2 and C_8; these two streams require an intermediate *HSU* (HSU_3) at a temperature $T_3 > 51\ °C$ (for C_2), and $T_3 > 74\ °C$ (for C_8);
3. the above condition can be met by the open storage *IHRS* because the existence of the *PW HSU* sets one *HSU* free to match this temperature condition, relaxing the conflicting conditions which prevail for closed storage system. In the latter case (refer to Table 6-2), only one intermediate *HSU* is available : its operation at about 40 *°C* is globally more profitable than an operation above 75 *°C*, with the consequence that C_2 and C_8 cannot be integrated;
4. the *PW HSU* comes with the constraint of a fixed temperature, and with the additional conditions that the mass contributions around this *HSU* need to be adjusted to meet the flowrate inequality constraints, potentially increasing the *HEX* area and/or the *HSU* capacity. But the *PW HSU* is free;
5. unlike closed storage systems, for which the mixing mass rebalance contributions were expected to be small in optimized *IHRSs*, the mixing contributions may be large in optimized open storage *IHRSs* (see Figure 6-3) as a result from the need to meet the flowrate inequality constraints without resorting to rebalancing utilities. In the light of this observation, the heuristic simple scheduling strategy of mixing mass contributions (refer to Sub-section 5.3.5) should be revisited;
6. the open storage system is expected to be more sensitive to schedule variations of streams than their closed storage counterpart, because of the time-related flowrate inequality constraints. This effect has not been assessed.

Beyond the bare savings on *HEX* units, an open storage system allows the number of (actual) *HSUs* to be decreased by one unit without major *TBCs* and/or *HR* penalties. Or, reversely, for the same number of (actual) *HSUs*, the *HR* may be significantly increased ... as long as the number of *HSUs* is limiting. The actual cost benefit of an open storage system is very much process dependent and the benefits demonstrated on the brewery process should not be extrapolated. The large temperature driving forces available in this process provide the optimization with an extended room for adjustment without incurring significant *HEX* area penalty.

6.3.2.2 9-Streams, 10-Batches

The heat integration problem consisting of the 9-streams set just described has been re-optimized [17] over a period including 10 batches [18] and accounting for the non-periodic part of the brewing process (0 to 582 *min* and 1970 to 2436 *min*).

This optimization run aimed at checking whether the optimized *IHRS* designs obtained considering only the repeated part (i.e. the 200 *min* batch cycle time) of the actual brewing process provide good approximations of the actually optimum *IHRS* or not. The following conditions have been considered for the optimization :

- stream C_{13} (hot water need outside the brewhouse, e.g. for washing the kegs) has been modelled as a constant mass-flowrate over the whole period of analysis (0-2436 *min*), in the same way this is done in the standard *EP-3* specification [19];
- variations of the batch cycle time have been introduced, to account for the need of a regular cleaning of heat transfer equipment units [20]. The actual starting times of the batches are: 0 / 194 / 388 / 582 / 776 / 1000 / 1194 / 1388 / 1582 / 1776 *min*, corresponding to a mean batch cycle of 200 *min*, but modelled as a serie of four batches starting at 194 *min* interval, followed by a fifth batch starting after 224 *min* to account for a 30 *min* cleaning cycle, etc.);
- due to the "start-up" time to reach the pseudo-cyclic operation conditions, to the assumed variations of the batch cycle times, and to the shut-down phase, the different periods of existence [21] of the process streams face different operating conditions of the *IHRS* [22]. One would therefore expect that the optimal heat recovery on any stream during each time period could be different from that during the other time periods, owing to the effect on the capacity of *HSUs*. In spite of these possible effects, the heat contributions of any process stream to each storage sub-system (i.e. the $x_{i,k}$, $x_{j,k}$ *DVs*) have been assumed to be independent of the time period (batch) [23];

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17. Using identical parameters: *Mdl* = open storage system / *OS* = single / *DF* = *CoT*&k_{max}&k_{min} / N_{Pop} = 200 / N_{Gen} = 2000 / *Sty* = *HR* max during 300 generations / selected streams C_1 C_2 C_4 C_7 C_8 C_{13} H_9 $H_{11/12}$ / 3 *HSUs* + *PW HSU*.
18. The restriction to 10 batches (brews) instead of 25 batches (a typical production week) has only been motivated by computing time reasons: the computing time is approximately proportional to the number of time slices, itself proportional to the number of batches. 10 batches already include 149 time slices !
19. To be more realistic, the night/day schedule of this stream could have been modelled, refer to Section A.4.
20. E.g. for wort boiling, refer to process *EP-4* described in Section A.4.
21. 10 periods for all process streams but C_{13}.
22. In particular, different inventory states of the *HSUs*.

- the mass balance constraints apply to the "macro-batch" including all 10 batches.

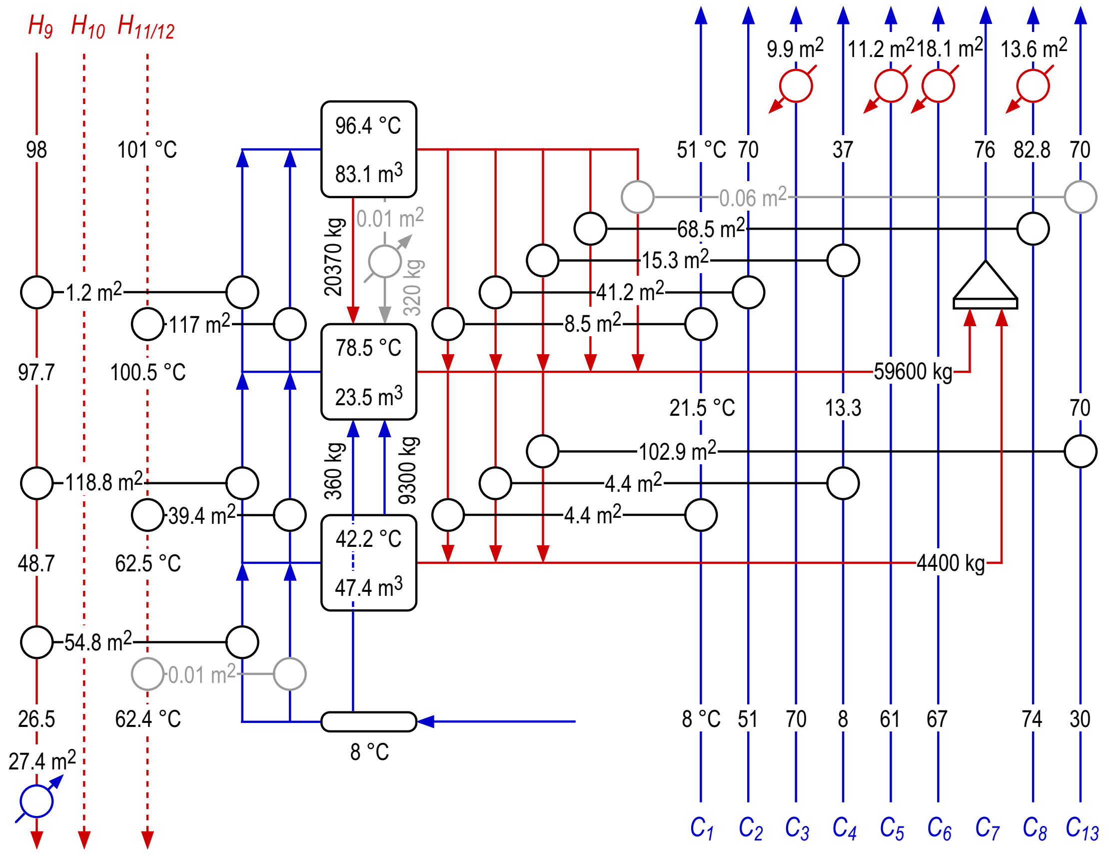

Figure 6-3 Open storage *IHRS* obtained by *GA* optimization over one batch cycle (H_{10} & $H_{11/12}$ in dotted line are heat recovery streams, *EP-3*, 3 *HSUs*).

MAIN FEATURES

Model	HR [kWh/batch]	HEXs [m2]	HEXs [DKK/batch]	HSUs [m3]	HSUs [DKK/batch]	Utility Costs [DKK/batch]	TBCs [DKK/batch]
Closed storage system	**14510**	781	**507.20**	170	**136.15**	**632.70**	**1276.05**
Open storage system	**16185**	656	**505.90**	154	**124.90**	**477.00**	**1107.80**

Table 6-3 Main features of the best solution of an open storage *IHRS* compared to the optimum closed storage *IHRS* (*EP-3*, 3 *HSUs*).

Table 6-4 provides a short-form comparison of the *IHRS* solution obtained by the optimization using the actual schedule of 10 batches [24] with respect to the one

23. With this assumption, the number of continuous *DVs* remains equal to that of the single batch cycle optimization, while the delivered *IHRS* solutions may possibly be sub-optimal.
24. Since the "macro-process" defined in this case corresponds to 10 batches, all extensive variables (costs per batch, heat recovery) have been divided by 10 to get comparable mean values per batch.

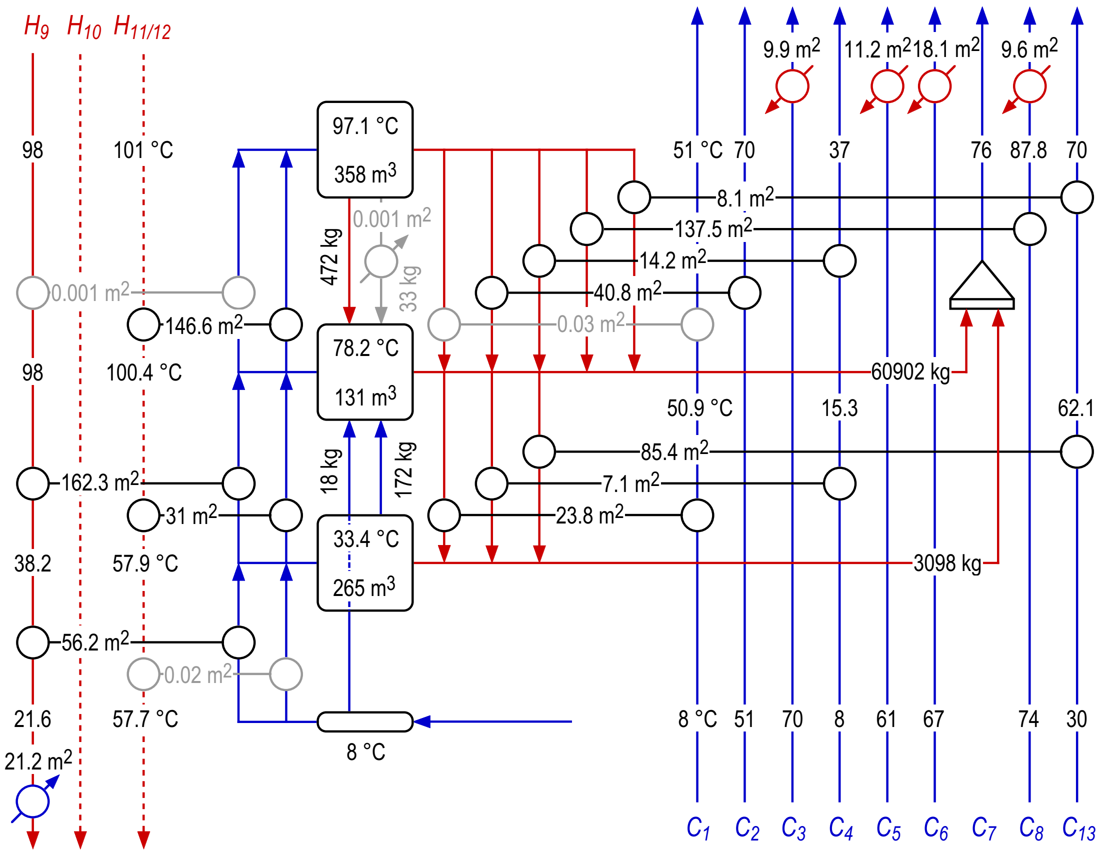

Figure 6-4 Open storage *IHRS* obtained by *GA* optimization over a period of 10 batches (H_{10} & $H_{11/12}$ in dotted line are heat recovery streams, *EP-3*, 3 *HSUs*).

MAIN FEATURES	HR	HEXs		HSUs		Utility Costs	TBCs
Model	[kWh/batch]	[m2]	[DKK/batch]	[m3]	[DKK/batch]	[DKK/batch]	[DKK/batch]
Single batch cycle	**16185**	656	**505.90**	154	**124.90**	**477.00**	**1107.80**
10 batch period	**16819**	783	**558.00**	753	**352.03**	**385.10**	**1295.15**

Table 6-4 Optimized open storage *IHRSs*: 10-batches *vs* single repeated batch model (*EP-3*, 3 *HSUs* + *PW HSU*, 9-stream set C_1, C_2, C_4, C_7, C_8, C_{13}, H_9, $H_{11/12}$).

delivered by the single repeated batch model described under 6.3.2.1. The detailed *IHRS* is represented on **Figure 6-4**, and the evolution of the mass inventories of the 3 *HSUs* over the period of analysis is given on **Figure 6-5**. The following differences are observed :

1. the required storage capacity is almost 5 times larger, but thanks to the scale effect, the *HSUs* are only 2.8 times more expensive. Considering the mass inventory of HSU_1 and HSU_3 (Figure 6-5) it clearly appears that their large capacity increases are due to the "start-up" and "shut-down" phases, characterized by large global heat imbalances [25] [26]. Hence, a large proportion of

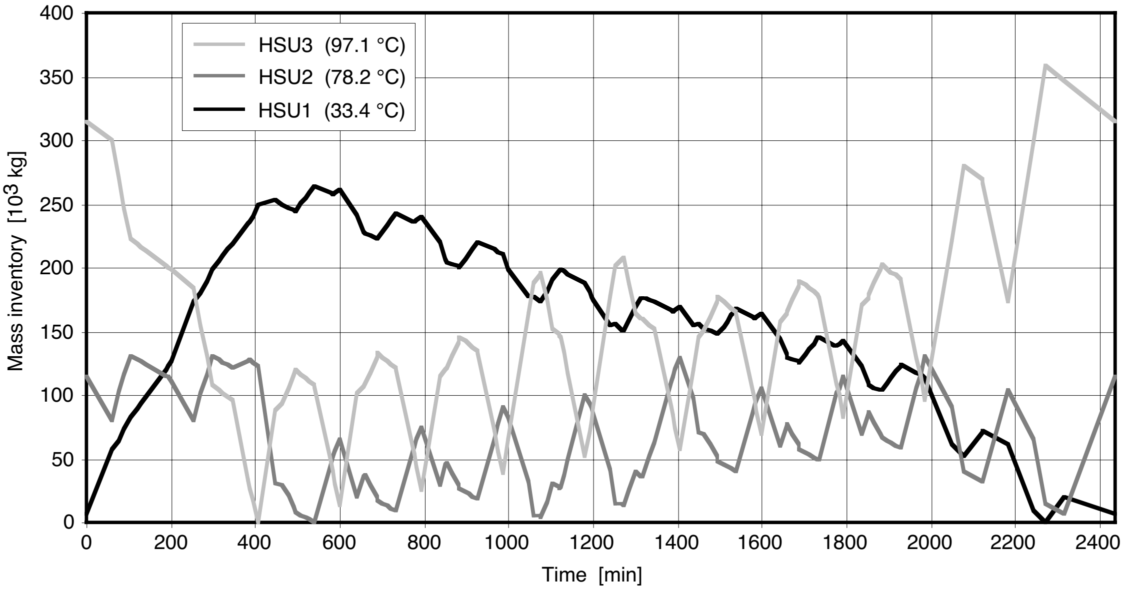

Figure 6-5 Mass inventories of the *HSUs* during the period of analysis (*EP-3*, 3 *HSUs* + *PW HSU*, 9-stream set C_1, C_2, C_4, C_7, C_8, C_{13}, H_9, $H_{11/12}$).

the capacity of *HSUs* is used to store heat during the "shut-down" phase of one week to supply heat during the "start-up" phase of the next week [27]. The capacities should be essentially similar if the period of analysis would include 25 batches instead of 10. In comparison, if the actual day/night cycles of C_{13} were taken into account, the effect on the required capacities of *HSUs* is expected to be small [28], as does the contribution of the variation of the batch cycle time (except on HSU_2, which is more sensitive to these variations);

2. the temperatures of HSU_2 and HSU_3 remain almost unchanged, while HSU_1 operates at a 14 °*C* lower temperature. This is closely related to the increased *HR* (by 4 %) obtained with a quite different distribution of the heat contributions of process streams to the *SSs* meeting the conditions of mass balance of the *HSUs*. The 10 % increase of the *HEX* costs mainly arise from the larger heat transfer from H_9, and to C_8, respectively. Unlike the optimization over one batch cycle, the mixing contributions to mass rebalance are very small indeed; the mass rebalance utility requirement is negligible too, indicating an almost perfect parametric optimization of the *IHRS* [29];

25. "Start-up" features heat needs for brewing and for C_{13}, while heat supply from the hot streams H_9 and $H_{11/12}$ is not provided yet (H_9 appears after 540 *min*, and $H_{11/12}$ after 405 *min*). The opposite phenomenon occurs during the "shut-down" phase.

26. HSU_2 is essentially a buffer capacity between the two *SSs*.

27. This means about 50 charge/discharge cycles per year only.

28. Except if the bottling and/or kegging facilities operate one or more days after the brewing has been stopped.

3. the multiplying exponential function $[1 - \exp(-(A/A_{min})^2)]$ applied to the cost function of heat exchangers efficiently provides the *GA* with the ability to cancel a heat contribution, whenever this decision is beneficial, as demonstrated on H_9 (first heat contribution) or on C_1 (last heat contribution);
4. the increased *HR* cannot compensate for the very significant increase of the capital costs, resulting in a 17 % increase of the *TBCs* [30].

6.3.2.3 13-Streams, Single Batch Cycle

Figure 6-6 represents the *TBCs vs HR* diagram obtained by *GA* optimization of an open storage system potentially integrating 13 streams [31] instead of 9 only. Several local optima obviously exist in the *HR* range from 14'000 to 18'000 kWh/batch. Each corresponds to a different set of k_{max}&k_{min} values [32], as can be seen in **Table 6-5** listing only the 4 most obvious local optima of Figure 6-6. Actually, 80 different match structures (i.e. sets of k_{max}&k_{min}) have been found among the lower-level population ($N_{Pop\ ll}$ = 200), the number of individuals featuring the same structure ranging from 1 to 29, depending mainly on the extension of the *HSU* temperature ranges corresponding to each match structure. The match structure of the best optimum (n° 4) is only represented by 2 individuals, whereas competing structures (n° 1 to n° 3) benefit from a much larger representation in the population. It can be concluded that :

1. a potential for further improvement of the best optimum (n° 4) very likely exists [33], and this potential is likely to be higher than that of the local optima listed in Table 6-5, because the latter have benefited so far from a significantly larger number of improvement opportunities;
2. observing that the actual best match structure can be poorly represented compared to competing structures, the identification of the actual best structure

29. It may however be a local optimum. A global optimization allowing for all match structures to be evaluated has not been achieved; for comparison purposes, the search has been limited to the 9-streams set obtained by single batch cycle optimization. 23 individuals among the 200 individuals of the population feature this structure, meaning that about 46000 individuals have been evaluated to reach this parametric optimization, what is expected to take about 5 min on a PC with 700 *MHz* processor frequency and a compiled *C*++ code.
30. The requirement for a larger storage capacity was foreseen, due to the batch processing time being 3.5 time the batch cycle time, but more importantly, owing to the fact that the heat needs and the heat releases are fully out-of-phase (all heat needs first, then heat releases). A rough calculation of the additional capacity requirements due to the non-periodic phases might be proposed, but a detailed sizing can only be made by simultaneous optimization as reported here, since the capacities depend on the temperatures of the *HSUs*, themselves linked to the heat contributions through the mass balance constraints of the *HSUs*.
31. *Mdl* = open storage system / *OS* = single / *DF* = *CoT*&k_{max}&k_{min} / N_{Pop} = 200 / N_{Gen} = 2000 / *Sty* = *HR* max during 300 generations / all streams selected / 3 *HSUs* + *PW HSU*.
32. I.e. match structure, resulting from the *HSU* temperatures being included in different *HSU* temperatures ranges.

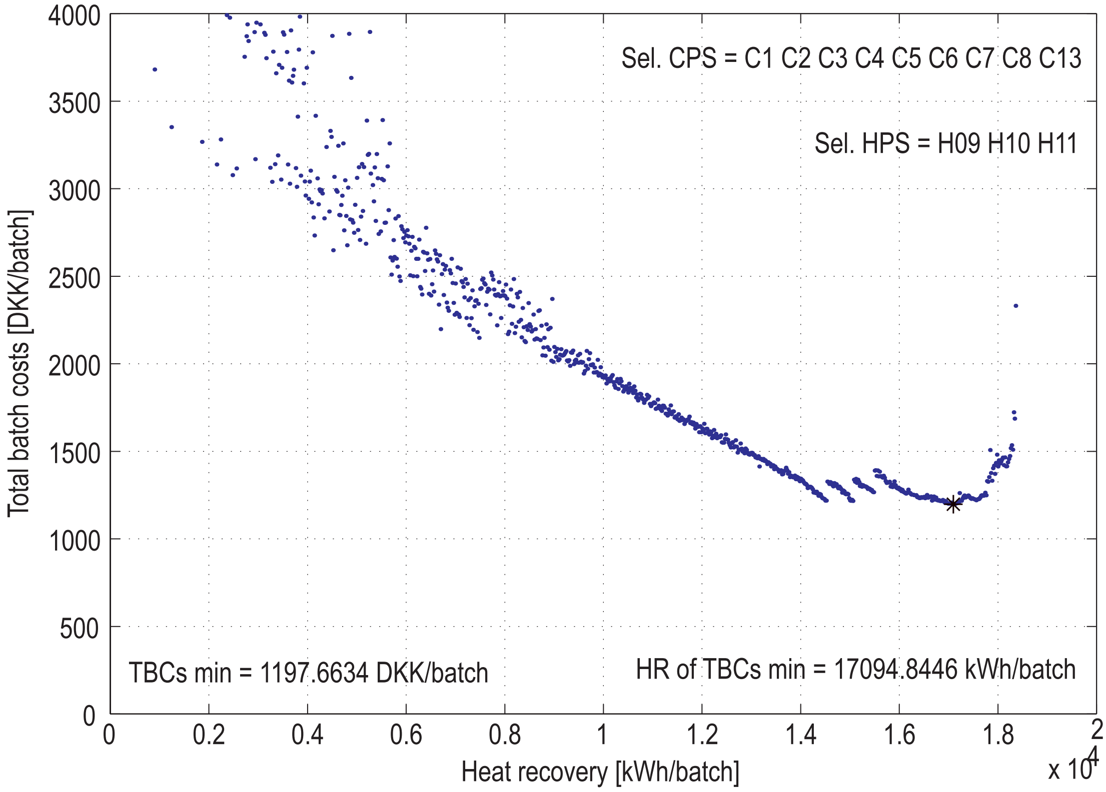

Figure 6-6 *TBCs vs HR* of all individuals generated during a *GA* optimization of an open storage system (potentially) integrating all streams (*EP-3*, 3 *HSUs*).

may be impossible since the comparison of the *TBCs* of several, unequally represented structures (yet featuring very close *TBCs* values) can be misleading. In other terms, even if the number of match structures is restricted, the present implementation of the lower-level optimization may fail to identify the actual optimum (refer also to Appendix F).

33. This statement has been verified by constraining the temperatures of *HSUs* so that all individuals of the population feature the same match structure (i.e. 37 < T_1 < 51 °C; 76 < T_2 < 98 °C; 98 < T_3 < 99 °C). With *MdI* = open storage system / *OS* = single / *DF* = *CoT*&k_{max}&k_{min} / N_{Pop} = 100 / N_{Gen} = 1000 / *Sty* = *HR* max during 150 generations / all streams selected / 3 *HSUs* + *PW HSU* / the optimum features *TBCs* = 1161 *DKK*/batch, *HR* = 17512 *kWh*/batch, i.e. a 3 % improvement of the *TBCs* and a 2.5 % increase of the *HR* compared to the approximate value (*TBCs* = 1198 *DKK*/batch, *HR* = 17085 *kWh*/batch) obtained without control of the match structures of the individuals of the population.

<table>
<tr><th>Local Optim.</th><th>HR [kWh/batch]</th><th>TBCs [DKK/batch]</th><th>Hot Streams k max [H9 H10 H11/12]</th><th>Cold Streams k min [C1 C2 .. C8 C13]</th><th>Nb. of Indiv. in Popul.</th></tr>
<tr><td rowspan="2">n° 1</td><td rowspan="2">14510</td><td rowspan="2">1218</td><td>4 4 4</td><td>2 4 4 2 4 4 2 4 3</td><td rowspan="2">13</td></tr>
<tr><td colspan="2">8 < T1 < 30; 30 < T2 < 98; T2 < T3 < 98</td></tr>
<tr><td rowspan="2">n° 2</td><td rowspan="2">15064</td><td rowspan="2">1217</td><td>4 4 4</td><td>2 3 4 2 4 4 2 4 2</td><td rowspan="2">12</td></tr>
<tr><td colspan="2">30 < T1 < 51; 51 < T2 < 98; T2 < T3 < 98</td></tr>
<tr><td rowspan="2">n° 3</td><td rowspan="2">15479</td><td rowspan="2">1275</td><td>4 4 4</td><td>2 3 4 2 3 4 2 4 2</td><td rowspan="2">5</td></tr>
<tr><td colspan="2">30 < T1 < 51; 61 < T2 < 98; T2 < T3 < 98</td></tr>
<tr><td rowspan="2">n° 4</td><td rowspan="2">17095</td><td rowspan="2">1198</td><td>3 4 4</td><td>2 3 3 2 3 3 2 3 2</td><td rowspan="2">< 3</td></tr>
<tr><td colspan="2">37 < T1 < 51; 76 < T2 < 98; 98 < T3 < 99</td></tr>
</table>

Table 6-5 Some local optima obtained by *GA* optimization of an open storage system (potentially) integrating all streams (*EP-3*, 3 *HSUs*). Unlike local optima n° 1 to n° 3, optimum n° 4 actually integrates all 13 streams.

6.4 Heat Integration Study of a Multi-Purpose Batch Plant

6.4.1 Context and Objective

In the course but independently of this research work, a preliminary heat integration study of a grassroot, multi-purpose batch production plant has been achieved (*Krummenacher* & *Mayor*, 2000). The study aimed at identifying major energy savings opportunities to be taken into account by the engineering firm during the layout and design of the plant.

The production pieces of equipment include 18 batch reactors, 6 spin-dryer, 5 dryers of different types, buffer tanks, etc. Although some equipment units are made of special materials to withstand highly corrosive conditions or cryogenic temperatures, the equipment units are essentially multi-purpose and the key requirement is flexibility. The company operating the plant produces proprietary active pharma products, as well as other pharma products under license subject to very stringent external quality controls.

Utilities available on site are steam (at 6 bars), industrial cooling water (10 °C), and ethylene glycol-water mixture (-35 °C). Most heating and cooling operations occur in vessels (reactors, dryers) using an intermediate (secondary) fluid. A standardized energy module interfaces the primary utility networks with the secondary fluid loop.

The observations and conclusions with respect to the indirect heat integration opportunities and the suitability of the fixed temperature storage for multi-purpose batch plants are summarized below.

6.4.2 Observations

Unlike brewing processes, producing large volume, low cost consumer goods, the pharma processes produce low volume, high added value goods for which energy costs amount to a very small part of the production costs. Despite the large number of detrimental features listed below, heat integration solutions of side processes (distillation of mother liquors) could be implemented. Detrimental or problematic features (from a heat integration point of view) can be classified with respect to :

1. **process & heat transfer equipment**

- low heat transfer coefficient of process equipment units (enamel-lined vessel, stainless steel vessel);
- intermediate fluid and heat transfer module, adding to the already large loss of temperature driving forces across the wall of reactor / dryer for heat recovery;
- low spacial energy intensity, distributed quite evenly over the plant, resulting in significant piping costs of the intermediate networks compared to that of *HSUs*;
- need for very expensive corrosion-resistant materials for overhead condensers (tantalum, polymer-graphite) to withstand the most aggressive vapours.

2. **processes**

- in-vessel heating and cooling steps, generally at high or maximum transfer rate [34] for productivity reasons (although the task may not be on the critical path) or owing to product stability;
- small or no initial heating step at all, preventing the use of a pre-heating during loading strategy;
- all significantly exothermic reactions achieved at low temperature, the rate of feed being limited by the maximum cooling rate;
- trend towards a "risky chemistry" at cryogenic temperatures;
- long batch cycle (typically 2 days) with relatively small mean energy intensities (limited number of charge/discharge cycles of a heat storage system);
- production planning accounting for the heat integration potential (symbiosis) of processes not desired;

34. Except crystallization cooling which is conducted at a slow, controlled rate.

- external quality control, compliance with GMP rules, and concern about justifying batch-to-batch variations of the time-temperature profiles, as a result from applying heat integration or not.

6.4.3 Synthesis

Several heat storage systems have been compared [35] in the context of this multi-purpose batch plant; the following conclusions can be drawn regarding the indirect heat integration :

- for multi-purpose operations, the variable temperature mixing heat storage features the capability (unlike *FTVM HSUs*) of automatically adjusting its mean operating temperature to the processes being connected and is much simpler with respect to valving and piping (only one network loop is needed);
- in presence of non-flowing streams solely, the heat recovery potential is not more limited when using a mixing heat storage instead of a *FTVM* or a stratified heat storage;
- the larger the contribution of flowing streams among the streams to be integrated, the more attractive a *FTVM* heat storage compared to a mixing heat storage, and the larger the heat recovery potential;
- owing to the significant fixed costs associated to piping and valving, and to variable costs of overhead condensers, a trade-off effect exists with respect to the number of reaction groups integrated together. Without adverse effect on the flexibility, a local integration of some reactor groups can be significantly more cost effective, provided that energetically complementary processes are assigned in priority to these reactor groups;
- side-processes such as the distillation of the mother liquors represent a major heat integration opportunity, provided that a dedicated distillation group is used to treat these liquors, instead of being distillated in a side reactor close to the related process;
- the optimal sizing of the *HSU* capacities does not only rely on known process data and schedule, but also depends on the relative, essentially uncertain scheduling of the integrated processes, resulting in the risk of oversizing or undersizing and in a poor economical performance;

35. Using simple calculations, without considering any *GA* optimization - the available process data were quite approximate (confidentiality issues).

♦ for these types of processes, cooling is a key issue and a trade-off exists between industrial water, ethylene glycol-water and time. From the energy integration point of view, the in-vessel cooling operation represents a major bottleneck.

6.5 Conclusions

The main features of the proposed tools & methods for targeting, as well as the developed models of indirect heat recovery scheme (*IHRS*) & the *GA* based optimization strategy are summarized in Sections 4.6 and 5.6 respectively. This Section focuses on conclusions with respect to the capabilities and limitations of these methods & models which can be established from their application to the *EP-1* and *EP-3* processes.

The graphical tools and methods developed for targeting provide valuable insight into the main structural issues and deliver good first-order solutions. Inherently, the vertical model cannot properly explore the *HSU* capacity – *HEX* area trade-off, which allows the total batch costs (*TBCs*) to be improved (i.e. decreased) by several *percent*, while the main difference lies in the significantly decreased overall capacity of the *HSUs*. In spite of this limitation, the smaller the temperature driving forces between the *TAM* composite curves and the smaller the simultaneity of the streams, the better the quality of the solutions provided by targeting [36].

Applied to the *EP-3* simplified brewery process, the *GA* based *IHRS* synthesis framework (consisting in both the closed and the open storage *IHRS* models in the two-levels *GA* optimization scheme) delivers state-of-the-art and practice relevant solutions. These results demonstrate both the suitability of the developed models and the capability of the *Struggle GA* (after improvement of the optimization strategy) to optimally exploit complex trade-off effects. Within these models, the systematic procedures developed for calculating the optimal mixing of storage fluid and for scheduling the rebalance mass flowrate contributions work successfully.

The *IHRS* model built around an open storage system has a high relevance for a brewery process like *EP-3* and, by extension, probably for any process including a significant proportion of process water streams as well. It allows both a significant decrease of the *TBCs* and an increase of the *HR*. It is further demonstrated that optimum *IHRS* solutions obtained by optimization over a period of analysis of one week (including the non-periodic "start-up" and "shut-down" phases) [37] are more realistic and significantly deviate in all respects [38] from the solutions obtained when

36. Or, reversely, the smaller the improvement potential by relaxing the vertical model assumption.

optimizing on a batch cycle time (corresponding to the usual practice). Considering these differences, it can be stated that short-cut calculation methods to extrapolate to one week operation solutions obtained on a batch cycle time basis would certainly miss the actually optimum solutions.

The application of the *GA* approach to the test cases *EP-1* and *EP-3* has contributed to an improved understanding of the optimization issues and results in a significantly improved and robust optimization strategy. Considering the small mass rebalance utility consumption existing in the delivered solutions and the complex trade-off effects involved, *Struggle* is a first choice *GA* for parametric optimization. Owing to the large structural dimension involved in the *IHRS* synthesis, and to the difficulties to define a meaningful distance function including both structural and parametric variables, a two-levels optimization scheme is absolutely necessary. Moreover, the upper-level optimization must address all structural issues, and the lower level the parametric variables solely (i.e. complete segregation of variables).

The present implementation of the *GA* based *IHRS* synthesis framework involves three main limitations :

1. the optimization of the connections to intermediate *HSUs* is imperfectly addressed using the remaining mass flowrate deviation (*RMFD*) technique; the delivered solutions might be sub-optimal in cases of large fixed costs associated to the intermediate connections (costs for temperature control, etc.);
2. the involvement, in the lower-level optimization, of both structural and parametric issues slows down the convergence; moreover, the delivered solutions generally feature an unequal quality (degree) of optimization, which depends on the relative proportion, in the population, of individuals featuring a given match structure;
3. the non-compiled *Matlab* implementation of the *IHRS* models makes a complete structural and parametric optimization run excessively long (several hundred hours).

The two first limitations are actually removed by the new *IHRS* model proposed in Appendix E : the model provides a direct control over the structure of process-storage matches and ensures a full segregation of structural and parametric issues.

37. Whenever the brewing and bottling facilities are operated on a weekly basis, which is the operation mode usually encountered in swiss breweries.

38. In the global features such as the *TBCs* and the capacity of the *HSUs* mostly, but also in the *HR*, the *HEX* area and the *IHRS* structure and the operating temperature of *HSUs*.

Furthermore, this model allows for the opportunity to relax the feasible temperature driving forces constraints on process-storage matches and potentially increases the profitability of integrating a larger number of process streams.

The third limitation is actually not a fundamental limitation since the compilation of the *Matlab* code or the direct coding in *C++* are known to provide, in conjunction with the optimization of the code of the model itself, with a speed up factor of the order of 1000. Alternatively, the insight into the structural issues gained using the proposed targeting tools may help to significantly restrict the structural search domain.

Finally, a preliminary heat integration study of multi-purpose batch plants indicates that the models described in Chapter 5 can be reasonably used for processes including a significant proportion of flowing streams (in other terms a limited number of non-flowing streams). In addition, in practical designs, piping, valving and temperature control costs may not be neglected and should be accounted in the capital costs of the models. Such improvements, as well as other practice relevant features, may readily be included in the *IHRS* models, at the expense of more detailed data specifications and management.

Part III

DIRECT HEAT INTEGRATION

Chapter 7

PINCH BASED TARGETING & DESIGN OF DIRECT BATCH *HENs*

7.1 Motivation & Overview

As pointed out in Chapter 2, the Cascade Analysis inherently requires a single ΔT_{min} pinch value. The Time Slice Model is a simplified Cascade Analysis in which heat is cascaded in temperature (i.e. direct heat exchanges solely) making this model suitable for using slice-wise $\Delta T_{min\ l}$ pinches. In spite of this possibility, a single ΔT_{min} experience value is generally applied (e.g. 20 $°C$ as reported in *Klemes* et al., 1994). For cost targeting [1] of batch processes, a single ΔT_{min} value is not suitable because :

- time slices may feature very different shapes of composite curves, and threshold problems are often found, resulting in different energy-capital costs trade-offs (for example, see Figure A-2);
- the duration of time slices may widely differ within the same batch (a ratio of 1 to 10 is common), resulting in different optimum trade-off values between energy and capital costs;
- the batch *HENs* beneficially resort to *HEX* re-use across time slices to decrease the capital costs, creating links between the energy-capital costs trade-offs between time slices.

A supertargeting methodology able to identify the slice-wise optimal $\Delta T_{min\ l}$ (with subscript l referring to the time slices) is required to identify appropriate energy targets and for a proper initialization of the design of each slice-wise *HEN*.

1. In the context of continuous processes, the ability to set energy and total cost targets prior to any actual design is called *supertargeting*, and this term shall also be used for the energy & costs targeting of batch processes.

Such a methodology has been found to already exist among previous works and this Chapter summarizes the main ideas behind the *Multiple Base Case* (*MBC*) supertargeting and design methodology originally developed by *Jones* (1991) to account for the flexibility in the design of continuous *HENs*. Drawing a parallel between the base cases and the time slices of batch processes guides the way to the required supertargeting methodology for batch processes [2]. This parallel has been drawn independently by *Gremouti* (1991) and *Krummenacher* & *Favrat* (1995).

Although an extensive description of the methodology can be found in *Krummenacher* & *Favrat* (1995) (applied to batch processes) or in *Jones* (1991), it is worth summarizing the key steps of the methodology for the following reasons :

- it provides insight into the different modes of *HEX* re-use across time slices and introduces the problem considered in Chapter 8;
- it demonstrates the capabilities and the limitations of the methodology as applied to the *EP-1* example process; the example provides upper bound values for automated design methods to come later.

The specific issues for the targeting and the design of batch *HENs* are first stated in **Section 7.2**.

Section 7.3 introduces the three possible modes of re-using *HEXs* (conventional, resequence, and repipe design types) for which suitable mathematical solution approaches have been developed.

The principle of area targeting, the concept of area matrix and the available degrees of freedom to manipulate the elements of this matrix are described in **Section 7.4**. The key steps in the calculation of area targets for a resequence and a conventional design are also reviewed.

Section 7.5 deals with a practical technique to optimize the slice-wise pinches $\Delta T_{min\ l}$.

The guidelines developed by *Jones* for *HEN* design are summarized in **Section 7.6**. Results obtained for the *EP-1* example process are also provided and discussed.

Finally, **Section 7.7** highlights the benefits as well as the weak points of the *MBC* targeting & design methodology.

2. In this Chapter, the time slices or base cases are used indifferently as fully equivalent.

7.2 Problem Statement

In a Pinch Analysis context, the design of continuous *HENs* takes place in two main steps :

1. *supertargeting* : based on simplified models, targets for the utility consumption, for the total *HEX* area, for the number of *HEX* units and finally for the total costs are calculated as a function of the pinch ΔT_{min}. The optimum pinch resulting in the lowest total costs can be identified [3];
2. *actual design* : the cost-optimum pinch and the related pinch temperature are used to initialize the *HEN* grid (separation at the pinch temperature, hot and cold utility targets); the *HEN* is designed using heuristic guidelines of the *Pinch Design Method* (*PDM*) while aiming at meeting the target values. Finally, the constraints set by the utility targets are relaxed to explore the parametric optimization of the heat load of *HEXs* using the available degrees of freedom offered by loops and paths (*Linnhoff*, 1994).

Compared to the supertargeting of continuous processes, for which proven methods have been developed (*Linnhoff*, 1994), the supertargeting of batch processes involves the following main difficulties :

- the calculation procedures [4] to target for the overall area (i.e. for the whole batch *HEN*) have to maximize the re-use of *HEX* area across time slices while meeting the constraints set by the design mode;
- the calculation of the target for the minimum number of units involves a similar problem.

Unlike the above two targets, for which dedicated methods are required, the target for the minimum utility consumption (for each time slice) can be readily calculated using standard procedures for continuous processes.

The minimum *HEX* area target and the minimum number of *HEX* units target can only be calculated for the whole batch; the links between the time slices arising from the re-use of *HEX* area (units) make the determination of the cost-optimal slice-

3. The target values are approximations, owing to the simplifying assumptions involved. Nevertheless, for the actual design stage to come next, an exact ΔT_{min} value is not needed as long as the population of streams below and above the pinch are correctly determined, since a *NLP* parametric optimization may be applied.
4. One calculation procedure for each "design mode" or way of re-using *HEX* units across time slices. Refer to Section 7.3 for the description of the three design modes.

wise $\Delta T_{min\,l}$ a L-dimensional simultaneous optimization problem by opposition to a L independent optimization sub-problems.

With respect to the design of batch *HENs*, the problem consists in the introduction, in the *PDM*, of additional guidelines and tools to decide the placement and the size of common matches and their simultaneous optimal re-use in other time slices.

7.3 Three Modes of *HEX* Re-use Across Time Slices

Jones identified three possible ways of re-using *HEX* units across time slices. Each mode results in a different *HEN* design :

1. in a *conventional design*, the *HEX* units remain between the same two streams during the operation of all time slices; in addition, each stream encounters the *HEX* units in the same order (or sequence) whatever the time slices. This default mode of *HEX* re-use is always possible;
2. in a *resequence design*, the *HEX* units are kept between the same two streams, but their order on the streams may be changed, i.e. their sequence be different during different time slices;
3. in a *repipe design*, *HEX* units are given total freedom to be re-used, across time slices, between any two streams.

In a repipe design, the *HEX* units are provided with the highest flexibility, while they are most constrained in a conventional design.

Specific targeting calculation methods have been developed by *Jones* for each of these modes. The repipe design shall not be described in this Chapter, considering that this design mode is less relevant for batch processes, and also because the area and number of units targeting calculations are easily derived (refer to *Jones*, 1991).

7.4 Targeting for the Minimum Heat Exchange Area

Understanding the *MBC* area targeting methods for a conventional, a resequence, and - to a lesser extent - for a repipe design requires that the basics of area targeting (as developed for continuous processes) and the related assumptions are recalled, as well as the concept of area matrix.

Area targeting for a resequence design is considered first, since this type of design makes full use of the area matrix manipulation features, unlike a conventional design, which may be considered as a particular case deriving from resequence design.

7.4.1 Area Targeting

An area target can be obtained for each time slice using the following equation :

$$A_{T\ l} = \sum_n \frac{1}{\Delta T_{LM\ n,l}} \cdot \sum_s \frac{\dot{Q}_{s,\ n,l}}{h_s} \tag{7-1}$$

where:

- $A_{T\ l}$ is the minimum heat exchange area (area target) of time slice l to transfer the heat rate of n enthalpy intervals (subscript T recalls that this is a target value);
- $\Delta T_{LM\ n,l}$ is the logarithmic mean temperature difference of enthalpy interval n during time slice l (see e.g. Figure 7-1 for the graphical meaning of enthalpy intervals);
- $\dot{Q}_{s,\ n,l}$ is the heat exchanged by stream s in enthalpy interval n of time slice l;
- h_s is the heat transfer film coefficient of stream s;
- index s relates to both process as utility streams.

Equation 7-1, known as the *Bath Formula* (originally proposed by *Townsend & Linnhoff*, 1984, for the area targeting of continuous processes), delivers area targets of suitable precision without significant computational burden, provided that the heat transfer film coefficients of the streams are not too dissimilar (typically within a range of ratio of 1 to 10).

The Bath Formula is based on several simplifying assumptions (defining the so-called *vertical model*), which are :

- within each enthalpy interval, heat transfer occurs vertically from the hot to the cold composite [5]; in other words, $\Delta T_{LM\ n}$ is the same whatever the heat transfer matches within each enthalpy interval, this property is explicitly used in Equation 7-1;
- to achieve the above stated vertical heat transfer, counter-current heat exchangers are used;

5. The condition of vertical heat transfer between composite curves leads to the true minimum total area (i.e. the area target) when the heat transfer film coefficients of hot streams are equal, and so are the ones of cold streams.

- and, less importantly, the resistance to heat transfer by conduction across the wall can be neglected with respect to the heat transfer film coefficient of the matched streams (a widely used assumption);

The re-use of heat transfer area across time slices should allow $A_T < \sum_l A_{T\,l}$, where A_T is the overall heat transfer area to be installed.

Intuitively, the area of matches (i.e. heat transfer area between given pairs of streams) common to several time slices should be maximized.

The maximum re-use of area (more specifically the minimization of the overall area A_T, to minimize capital costs) can be targeted in a systematic manner, subject to the constraints relevant to the type of design under consideration - conventional, resequence, or repipe. Optimizing a resequence or a conventional design is formulated as a linear programming (*LP*) problem, which can be readily solved, using e.g. the *Simplex* algorithm.

According to Equation 7-1, $A_{T\,l}$ results from the addition of individual area contribution of streams, without any explicit consideration of hot stream - cold stream matches. Degrees of freedom (*DOF*) and hence scope for optimization appear when $A_{T\,l}$ is written as the sum of elementary area contributions of stream matches within each enthalpy interval (*EI*), as given by the following equations :

$$A_{T\,l} = \sum_n \frac{1}{\Delta T_{LM\,n,\,l}} \cdot \sum_i \sum_j \dot{Q}_{i,\,j,\,n,\,l} \cdot \left(\frac{1}{h_i} + \frac{1}{h_j}\right) = \sum_i \sum_j \sum_n A_{i,j,n,l} \quad \textbf{(7-2)}$$

$$A_{i,j,n,l} = \frac{\dot{Q}_{i,\,j,\,n,\,l}}{\Delta T_{LM\,n,\,l}} \cdot \left(\frac{1}{h_i} + \frac{1}{h_j}\right) \quad \textbf{(7-3)}$$

where:

- $A_{T\,l}$ is the minimum heat exchange area (area target) of time slice l to transfer the heat rate of n enthalpy intervals;
- $\Delta T_{LM\,n,l}$ is the logarithmic mean temperature difference of enthalpy interval n during time slice l;
- $\dot{Q}_{i,\,j,\,n,l}$ is the heat rate transferred from hot stream i to cold stream j in enthalpy interval n of time slice l;
- h_i, h_j are the heat transfer film coefficients of hot stream i and cold stream j;
- $A_{i,j,n,l}$ is the area needed to transfer $\dot{Q}_{i,\,j,\,n,l}$ from hot stream i to cold stream j in enthalpy interval n of time slice l.

Unlike Equation 7-1, the above equations require that the heat rate of the matches, $\dot{Q}_{i,\,j,\,n,l}$, be previously defined. The corresponding match-wise area elements can be organized in a matrix format called the *area matrix*. The significance and the use of the area matrix are described hereafter.

7.4.2 Area Matrix

Consider time slice 4 (*TS 4*) of example process *EP-1* (its process data can be found in Section A.1 of Appendix A). The corresponding composite curves, as well as their decomposition into enthalpy intervals (with a process pinch arbitrarily set at $\Delta T_{min\ 4} = 10$ °*C*), are represented on **Figure 7-1**, with focus on the internal (i.e. process-to-process) heat exchange region.

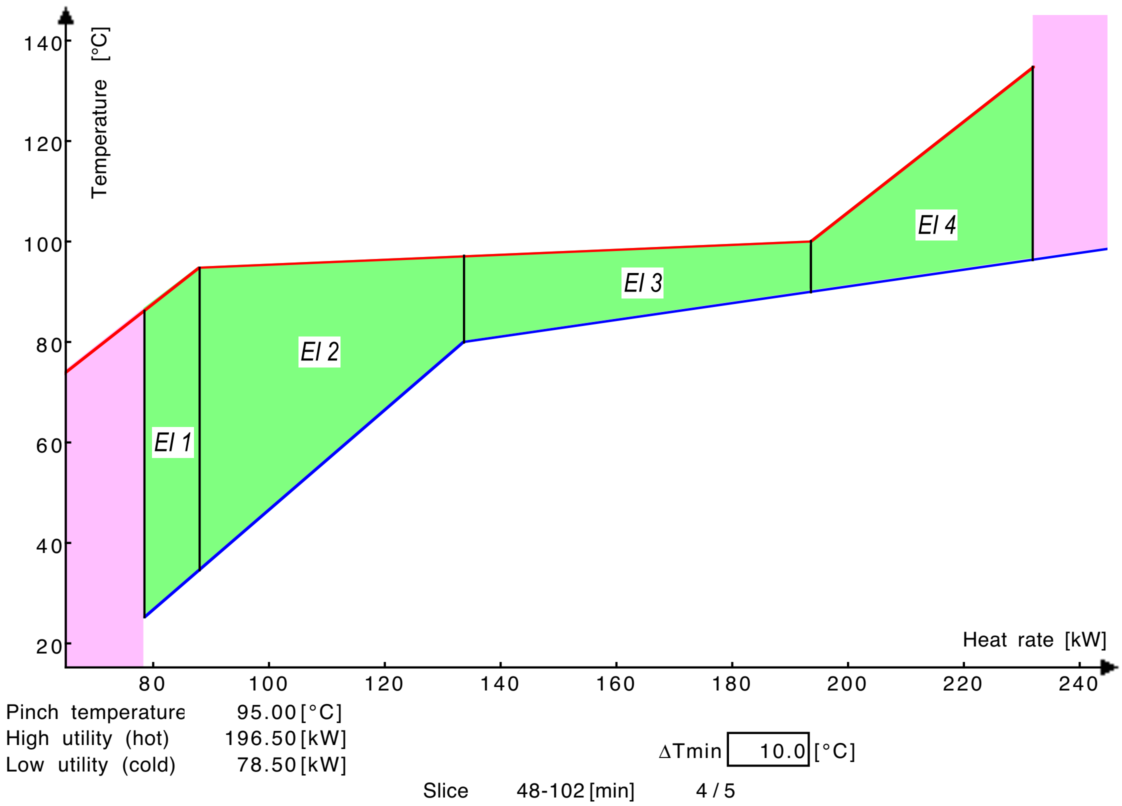

Figure 7-1 Composites curves of *EP-1* / *TS 4*, with focus on the four enthalpy intervals (*EI 1* to *EI 4*) of the internal heat exchange region ($\Delta T_{min\ 4} = 10$ °C).

Enthalpy interval 2 (*EI 2*) includes two hot streams (H_1^2 and H_2^2) and one cold stream (C_1^2), while the heat rate to be transferred amounts to 45.5 *kW* [6]. The area

6. The superscript designates the part of the streams included in the considered enthalpy interval.

elements needed to transfer 2.37 *kW* from H_1^2 to C_1^2 and 43.13 *kW* from H_2^2 to C_1^2 are therefore fully defined, as represented by the following area matrix of *EI 2* (**Table 7-1**).

2.65	H1	H2
C1	0.14	2.51

Table 7-1 Area matrix of enthalpy interval *EI 2* (refer to Figure 7-1); area elements and total area are in given in m^2.

Unlike *EI 2*, *EI 3* includes two hot streams (H_1^3 and H_2^3), and two cold streams (C_1^3 and C_3^3). This provides the designer with some degree of freedom when setting the heat rate (and hence the corresponding heat transfer area) of the four possible matches (H_1^3-C_1^3; H_1^3-C_3^3; H_2^3-C_1^3; H_2^3-C_3^3). This feature may be related to the existence of a loop in the so-called *spaghetti design* (*Townsend*, 1989) as implied by the vertical model. **Figure 7-2** represents such a spaghetti design for *EI 3*, including all four matches mentioned above, and the decomposition of *EI 3* into its constituting streams.

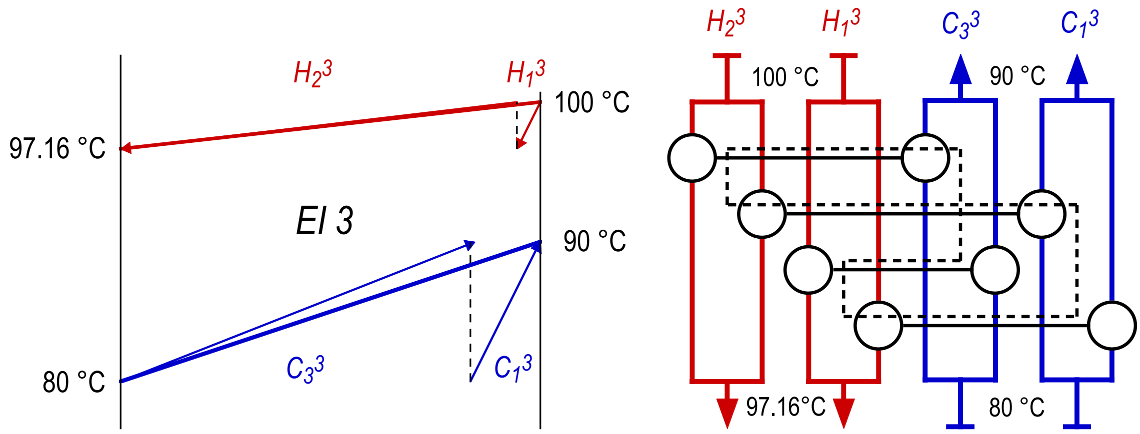

Figure 7-2 Decomposition of the enthalpy interval *EI 3* into elementary stream components, and corresponding *spaghetti design* (refer to Figure 7-1).

Resorting to shifting heat rate around the loop indicated on the spaghetti design [7], the following area matrices may be obtained for *EI 3* (**Table 7-2**) :

- in case a), the heat rate of the match H_2^3-C_3^3 has been minimized (i.e. H_1^3-C_3^3 maximized);

7. This optimization opportunity is commonly used in the Pinch Design Method to improve a *Maximum Energy Recovery* (*MER*) *HEN*.

9.049	H1	H2
C1	0	1.508
C3	0.47	7.071

9.049	H1	H2
C1	0.235	1.273
C3	0.235	7.306

9.049	H1	H2
C1	0.47	1.038
C3	0	7.541

Table 7-2 Three possible area matrices of enthalpy interval *3* (refer to Figure 7-2). Case a) 100 % H_1^3 with C_3^3; case b) 50 % H_1^3 with C_1^3, 50 % with C_3^3; case c) 100 % H_2^3 with C_1^3. Area elements and total area in m^2.

- in case b), 50 % of the enthalpy change of H_1^3 is due to match H_1^3-C_1^3, and 50 % results from H_1^3-C_3^3;
- in case c), H_2^3 has been matched in priority with C_3^3, maximizing the heat transfer area of this match.

All three matrices feature the same overall heat transfer area (9.049 m^2), while the distribution of this area over the 4 matches is different. Note that the sum of area elements over a row (i.e. over a cold stream) or a column (i.e. over a hot stream) is constant, because all heat transfer film coefficients of the streams are equal - but this property does not hold in general.

The area matrix of a given time slice (slice-wise area matrix) is obtained from the area matrices of its enthalpy intervals by summing the area elements match-wise. **Table 7-3** illustrates one such matrix for *TS 4* [8].

33.1	H1	H2	H3/H4	HU1	HU2
C1	1.06	4.02	0	0	0.08
C2	0	0	0	0	10.36
C3	3.5	7.07	0	0	0.96
CU	6.05	0	0	–	–

Table 7-3 One possible slice-wise area matrix for time slice 4 ($\Delta T_{min\,4}$ = 10 °*C,* refer to Figure 7-1). Areas in m^2.

7.4.3 Area Target in Resequence Design

In a resequence design, *HEXs* must stay between the same two streams, but can be resequenced in whatever order as required. In other words, the re-use of match area

8. Note that H_3/H_4 does not require any heat transfer area, since this stream is not active during *TS 4*. Refer to Section A.1 regarding the motivation to group H_3 and H_4 together.

is not limited by match sequence issues. Hence, targeting for the minimum heat exchange area in a resequence design is all about manipulating slice-wise area matrices so as to maximize [9] the area $A_{i,j,l}$ of matches common to several time slices (area is paid once and used across several time slices) and minimize the area of matches specific to one time slice.

However, the area of the common matches may not be independently maximized. This results from the heat rate of matches being subject to constraints of stream individual enthalpy balance within each enthalpy interval [10], while simultaneously satisfying lower and upper boundary values (refer to Appendix G).

Considering that the utility matches are placed at the end of process streams, the re-use opportunities of these matches obey other, simpler considerations and can be dealt with separately :

$$A_{Trs} = A_{Trs\ pp} + A_{Trs\ pu} \tag{7-4}$$

where:

- A_{Trs} is the minimum area to be installed in resequence design;
- $A_{Trs\ pp}$ is the minimum area of process-to-process matches to be installed;
- $A_{Trs\ pu}$ is the minimum area of process-utility matches to be installed;
- the subscript Trs recalls that these are target values assuming a resequence design.

The minimum process-utility area target $A_{Trs\ pu}$ is given by :

$$A_{Trs\ pu} = \sum_n \sum_i Max_l(A_{i,\,n,\,l}) + \sum_m \sum_j Max_l(A_{j,\,m,\,l}) \tag{7-5}$$

where:

- $Max_l(A_{i,\,n,\,l})$ is the maximum, over the time slices, of the match area between the hot process stream i and cold utility n;
- $Max_l(A_{i,\,m,\,l})$ is the maximum, over the time slices, of the match area between the cold process stream j and hot utility m.

The process-to-process area target $A_{Trs\ pp}$ actually includes elements of the overall area matrix which are specifically installed for a time slice, and area elements which

9. Whenever possible, i.e. when the spaghetti design of an enthalpy interval includes loop(s).
10. As a result from the vertical heat transfer assumption.

are common to several time slices. However, $A_{Trs\ pp}$ can be written in a compact form as :

$$A_{Trs\ pp} = \sum_i \sum_j Max_l(A_{i,\,j,\,l}) \tag{7-6}$$

where:

- $A_{i,\,j,\,l}$ is the match area (optimized by linear programming) between hot process stream i and cold process stream j during time slice l.

The optimization of the $A_{i,\,j,\,l}$ (decision variables to be optimized) can be set up as a linear programming (*LP*) problem, consisting in the minimization of $A_{Trs\ pp}$ subject to the constraints arising from :

1. the balance equations of transferred heat rate between hot and cold process streams within each enthalpy interval n and during each time slice l (equality constraints);
2. the lower and upper boundaries on the heat rate transferred by each process stream within each enthalpy interval n and during each time slice l (inequality constraints).

These constraints are formulated in terms of heat rates and not in terms of areas. In addition, the number of heat rate variables is very large. A detailed consideration of the problem has allowed *Jones* to convert these constraints into a reduced set of constraints on areas. Appendix G summarizes the related mathematical developments.

Once set up, the *LP* problem is easily solved using e.g. the *Simplex* algorithm. **Table 7-4** illustrates the overall area matrix optimized for all slice-wise pinches $\Delta T_{min\ l}$ = 10 °C, indicating that a minimum total area of 64.8 *m*^{2} must be installed

64.82	H1	H2	H3/H4	HU1	HU2
C1	11.44	3.71	0.28	3.52	0.08
C2	0	0	12.83	0	10.36
C3	3.2	7.38	4.22	0	1.15
CU	6.05	0	0.6	–	–

Table 7-4 Overall area matrix optimized in resequence design for $\Delta T_{min\ l}$ = 10 °C, whatever *l* (*EP-1*, areas in m^2).

in these conditions for a resequence design [11]. The calculation of the total capital cost target requires that the minimum number of units target be first established. The calculation of the number of units target is based on considerations of the stream population above and below the pinch for each time slice, and is not described below (refer to *Krummenacher* & *Favrat*, 1995).

7.4.4 Area Target in Conventional Design

In a conventional design, the sequence of matches on a stream is fixed and cannot be changed. How many matches on each stream can be re-used, at the same position, across time slices ? The more similar the actual slice-wise *HEX* structures, the larger the number of matches which can be re-used. In absence of a tool able to foresee the similarity of the slice-wise structures, a worst-case assumption should be made.

Jones assumes that one and only one [12] match (called a *candidate match*) can be re-used on each process stream; with this assumption, candidate matches are independent and a sequence of several candidate matches on a stream is never found. On an area matrix, there is at best one candidate match in each row corresponding to a cold process stream, and at best one candidate match in each column representing a hot process stream.

Like for resequence design, the total area can be split into two contributions :

$$A_{Tcv} = A_{Tcv\ pp} + A_{Tcv\ pu} \quad \textbf{(7-7)}$$

where:

- A_{Tcv} is the minimum area to be installed in conventional design;
- $A_{Tcv\ pp}$ is the minimum area of process-to-process matches to be installed;
- $A_{Tcv\ pu}$ is the minimum area of process-utility matches to be installed;
- the subscript Tcv recalls that these are target values assuming a conventional design.

The minimum process-utility area $A_{Tcv\ pu}$ can be calculated using Equation 7-5, since the re-use of utility HEXs is basically of conventional design type, even if a resequence is allowed.

11. The information provided by the optimized individual matches area elements is of less relevance for targeting.
12. This is a realistic assumption for batch processes, for which the time slices feature significantly different stream populations, pinch temperatures, etc.

The problem now consists in optimally selecting the candidate matches of the process-to-process area sub-matrix (subject to the constraints of at best one candidate match per process stream, as well as the constraints given by Equations G-4 to G-6 which are independent of the design type and hence also apply to the conventional design) which minimize the process-to-process area $A_{Tcv\ pp}$ to be installed.

In $A_{Tcv\ pp}$, two categories of match areas must be distinguished ;

- $A_{i,\ j\ cm}$ area elements which are selected as candidate match; in this case, the area to be installed is given by $A_{i,\ j\ cm} = Max_l(A_{i,\ j,\ l})$;
- $A_{i,\ j,\ l\ ncm}$ area elements which are specific to each time slice and complete the slice-wise *HENs*; each of these area elements directly contributes to the total *HEX* area.

In order to minimize $A_{Tcv\ pp}$ to be installed, the area $A_{i,\ j,\ l}$ of candidate matches must be maximized on all times slices [13]; as a result [14], the area elements $A_{i,\ j,\ l\ ncm}$ are minimized.

The maximization of area $A_{i,\ j,\ l}$ of a candidate match allows for area savings (area reduction) $RA_{i,\ j\ cm}$ amounting to the related HEX areas re-used across time slices :

$$RA_{i,\ j\ cm} = \sum_l A_{max\ i,\ j,\ l} - Max_l(A_{max\ i,\ j,\ l}) \tag{7-8}$$

Unlike resequence design [15], in conventional design, the area maximization of the candidate matches can be performed independently for each candidate match, since the maximization of area of a candidate match does not preclude the area of another candidate match (which, by definition, concerns another pair of process streams) to be maximized. Hence, the optimization problem is purely combinatorial and consists in identifying the set of candidate matches allowing for the lowest $A_{Tcv\ pp}$.

Assuming a process including an equal number of hot process streams and cold process streams (*I=J*), *Jones* addresses the combinatorial optimization problem by the exhaustive evaluation of *I!* candidate match matrices. *Peridis* (1991), proposes a new tool called the *area reduction matrix*, and complementary algorithms to identify the optimal set of candidate matches in *4I* evaluations instead of *I!*.

13. The maximum area which may be used in vertical heat transfer is fully defined by Equation G-6.
14. The cumulated *HEX* area for a time slice being constant and independent of the way the area is distributed among the matches of the slice-wise area matrix (according to the vertical model).
15. In which the maximization of common matches cannot be performed independently since trade-off effects exist between common matches corresponding to the same process stream.

The elements of the area reduction matrix are defined by Equation 7-8 above and represent the possible area savings if the corresponding match is selected as a candidate match. **Table 7-5** represents an area reduction matrix.

	H1	H2	H3/H4
C1	11.44	0	0
C2	0	0	0
C3	3.5	0	3.64

Table 7-5 Area reduction matrix for $\Delta T_{min\,l}$ = 10 °C, whatever l (*EP-1*, areas in m^2).

Although generally efficient, the algorithms proposed by *Peridis* may fail to identify the optimal solutions (i.e. set of candidate matches) when some elements of the reduction matrix are almost equal. For this reason, *Krummenacher* & *Favrat* (1995) propose a simple *LP* formulation of the optimization problem, which might not be quicker (this is not so much an issue with current computing capabilities) but features the advantage of being more sound and robust. Given the area reduction matrix, the objective function to be maximized may be written as :

$$RA = \sum_i \sum_j x_{i,\,j} RA_{i,\,j\,cm} \tag{7-9}$$

where:

- RA is the total area reduction (area savings) for the $x_{i,\,j}$ selected candidate matches;
- $RA_{i,\,j\,cm}$ is the $i,\,j$ element of the area reduction matrix (known value);
- $x_{i,\,j}$ is a discrete variable (decision variable): $x_{i,\,j}$ = 1 if the $i,\,j$ element of the area reduction matrix is selected as candidate match, $x_{i,\,j}$ = 0 otherwise.

The $x_{i,\,j}$ variables are subject to the following constraints :

$$\sum_j x_{i,\,j} \le 1 \quad \text{on the columns of the area reduction matrix (for any hot process stream)} \tag{7-10}$$

$$\sum_i x_{i,\,j} \le 1 \quad \text{on the rows of the area reduction matrix (for any cold process stream)} \tag{7-11}$$

$$x_{i,\,j} \ge 0 \quad \forall(i,\,j) \quad \text{(implicit condition of linear programming)} \tag{7-12}$$

Using this formulation, the obtained $x_{i,\,j}$ solutions are non-binary (1/2, 1/3, etc.) only when there are actually several solutions because of equal $RA_{i,\,j\,cm}$ elements. These cases are easily detected and dealt with.

7.5 Search for Cost-optimal Slice-wise $\Delta T_{min\ l}$

Given a set of slice-wise $\Delta T_{min\ l}$, the *MBC* calculation methods deliver targets for the minimum total *HEX* area, for the minimum number of units, for the minimum utility requirements, and for the lowest total costs. What about finding the cost-optimum set of slice-wise $\Delta T_{min\ l}$?

For flexible continuous processes, the number of base cases is often 2 to 4, and the base case-wise optimal pinches are not expected to be very different, so that *Jones* proposes to calculate the above targets for a set of discrete values over a reasonable range of ΔT_{min} for each base case.

Batch processes may feature a much larger number of time slices and the cost-optimal $\Delta T_{min\ l}$ may differ widely, so that the exhaustive calculation of the targets over the whole range of possible slice-wise pinch values is too time-consuming. Instead, a practical approach has been used which consists in sequentially searching for the minimum total cost target with respect to each slice-wise pinch, while the other slice-wise pinches remain constant [16]. Experience on simple example processes such as *EP-1* indicates that going through each time slice three times is generally enough to get good results. Examples of targets obtained for *EP-1* and the comparison with actual values achieved by a conventional design are summarized in Table 7-6 (see next Section).

7.6 *HEN* Design

The *MBC HEN* design methodology developed by *Jones* relies on the proven methods & tools of Pinch Analysis (*Pinch Design Method*, *Remaining Problem Analysis*, etc.), to which specific guidelines & tools have been added (*Area Matrix*, *Pinch Match Matrix*, *Area Reduction Matrix* and *MBC Remaining Problem Analysis*). The description below focuses on the essential steps (principles) of the *MBC HEN* design, while a detailed description can be found in *Jones* (1991).

After *MBC* supertargeting, the cost-optimum slice-wise pinch $\Delta T_{min\ l}$, the pinch temperature $T_{pinch\ l}$ and the cold and hot utility targets are known for each time

16. This optimization technique implicitly assumes the convexity of the total costs target with respect to the slice-wise pinches. Although the technique has worked well for the example processes considered so far, experimental evidence for convexity is lacking ... and could of course need to be revisited when the way structural aspects (i.e. the number of units target) are taken into account is improved. In case of non-convexity, other approaches such as a *GA* based optimization of the slice-wise pinches could be developed.

slice, allowing for the initialization of the grid diagrams of the batch *HEN* (one grid diagram for each time slice). *MBC* design guidelines aim at the optimal re-use of *HEX* area (units) across time slices (i.e. the best possible way of utilising capital across time slices).

In conventional and in resequence design, the *HEX* units remain between the same two streams during the operation of all time slices. In any case, as in the standard Pinch Design Method, the placement of *HEX* matches begins at the pinch (the pinch matches, i.e. matches present at the pinch, are the most difficult matches to place because of the tight temperature driving forces in this region) and proceeds away. Priority should be given to *HEX* matches which are used in the largest number of time slices. The *MBC HEN* design procedure involves the following main steps :

1. identify the possible pinch matches, and select the match concerning the largest number of time slices (build a *Pinch Match Matrix*);
2. determine the maximum possible area to be installed for this match (using a slightly modified *LP* optimization);
3. place match on the time slice requiring the largest area (calculated assuming vertical heat transfer). In some cases, it might be beneficial to install a largest area to form a *tick-off* match [17] in order to minimize the total number of units (either for the time slice under consideration, or for another time slice);
4. re-use the largest fraction of the installed area during the other time slices, even if the maximum area calculated assuming vertical heat transfer should be exceeded [18];
5. verify the efficiency [19] of the placed match using the *Remaining Problem Analysis* (*Linnhoff*, 1994);
6. apply the above steps for the other *HEX* matches, until the target temperature of every stream is satisfied during all time slices;
7. resort to relaxation based on loops and paths to improve the economics.

17. I.e. a match which allows for one of the matched streams to be satisfied and be eliminated from further consideration.

18. In this case, criss-cross heat exchanges take place (i.e. under $\Delta T < \Delta T_{min}$) but this is not a problem since the installed area has already been payed for another, more area-demanding time slice. Thanks to this, the area of the matches to be installed downwards shall be smaller. This is the case of match X_{pp1} during time slice 3 of *EP-1* process (refer to Figure 7-3).

19. With respect to the total batch costs, the total heat transfer area, and the number of *HEX* units.

- When placing the matches, it is recommended to develop similar matches structures in the different time slices in order to minimize the required number of valves and by-pass and to maximize the number of re-used matches. For a conventional design, it is actually possible to use more than one common match on each stream, a possibility which should be exploited.
- The overall *HEN* is obtained by merging of the slice-wise *HENs*, and adding the valves and by-pass to change the sequence of matches according to the requirements of each time slice.
- For a conventional design, the candidate matches should be placed in priority; however, cases exist in which the prioritary placement of candidate matches with both streams present at the pinch is not suitable (owing to their heuristic nature, these design guidelines may fail).

7.6.1 Example

Table 7-6 compares the values actually achieved by a batch *HEN* in conventional design (before and after relaxation) with the targets obtained using the *MBC* supertargeting briefly described above. **Figure 7-3** represents the slice-wise maximum energy recovery (*MER*) *HENs* of *EP-1* in conventional design. The *HENs* have been initialized using the $\Delta T_{min\ l}$ obtained by supertargeting (refer to values given in Table 7-6 and composite curves drawn on Figure A-2) [20] [21].

The common *HEXs* (i.e. the one re-used across one or more time slices) are shaded in gray (X_{pp1}, X_{pp2}, X_{pu1}, X_{pu2}, X_{pu3}); the other *HEXs* (X_{pp3}, X_{pp4}, X_{pp5}, X_{pp6}, X_{pu4}) are specifically installed for one time slice only. The dark gray shaded *HEXs* determine the area to be installed, while the re-use of these *HEXs* in other, less area-demanding time slices are shaded in light gray.

The size of the common *HEX* X_{pp1} is set by time slice 4, while X_{pp1} is re-used during time slices 2 and 3; in the later, X_{pp1} operates with $\Delta T < \Delta T_{min\ 3}$. On the same slice-wise *HEN*, it is observed that X_{pu4} transfers heat across the pinch, owing to the availability of X_{pp1}, X_{pp2}, and X_{pu3} for which it is not advisable to change the structure.

These two observations illustrate that the re-use of *HEXs* units across time slices causes the standard *PDM* guidelines to be relaxed.

20. Although the slice-wise *HENs* have been represented in a *PinchLENI*-like look, the *HENs* have been designed by hand (*PinchLENI* does not provide support for batch *HENs* design yet).
21. Here, *EP-1* has been provided with the two hot utilities HU_1 and HU_2, instead of only *HU* (refer to Section A.1).

TARGETING vs DESIGN		MBC SUPERTARGETING			Convential MBC DESIGN	
		TAM	Conv. Design	Reseq. Design	MER HEN **1)**	Rel. HEN **2)**
Tot. Batch Costs	[CHF/b]	17.03	23.91	23.69	**22.63**	**22.92**
HEX Area	[m2]	34.70	58.99	58.45	**67.13**	**61.56**
HEX Units	[-]	9	12	12	**10**	**9**
Heat Recovery	[kWh/b]	324.3	279.8	279.8	**287.1**	**275.0**
Hot Utility	[kWh/b]	151.9	196.5	196.5	**189.2**	**201.3**
Cold Utility	[kWh/b]	33.3	77.8	77.8	**70.5**	**82.6**
ΔTmin 1	**[°C]**	**7.2 3)**	**– 4)**	**– 4)**	– **4)**	
HU	[kW]	75.96	75	75		
CU	[kW]	16.63	0	0		
ΔTmin 2	**[°C]**	**–**	**35 5)**	**25**	35	
HU	[kW]		0	-11		
CU	[kW]		57	46		
ΔTmin 3	**[°C]**	**–**	**44.5**	**31**	46.3	
HU	[kW]		-6.55	-21.4		
CU	[kW]		65.45	50.6		
ΔTmin 4	**[°C]**	**–**	**4.1**	**4.1**	2.7	
HU	[kW]		160.8	160.8		
CU	[kW]		42.8	42.8		
ΔTmin 5	**[°C]**	**–**	**30 5)**	**30 5)**	30	
HU	[kW]		135	135		
CU	[kW]		0	0		

Notes :
1) Maximum energy recovery HENs for indicated slice-wise pinches (Figure 7.3)
2) Relaxed overall HEN (Figure 7.4)
3) Global value (without reference to time slices)
4) The first time slice includes one cold stream only, the process pinch is undefined
5) Limit pinch value before reverse utility appears

Table 7-6 Targeting versus design values obtained using the *MBC* methodology (example process *EP-1*).

Because the pinch temperature depends on the time slice, matches installed in the below-pinch part may appear above the pinch during another time slice, as illustrated by X_{pp2} (time slices 5 and 3).

Although X_{pp1} installed for time slice 4 is a common match, and that both streams C_1 and H_1 cross the pinch, X_{pp1} should not be placed first (in the opposite case, the area of the match would be significantly larger). X_{pp3} and X_{pp4} have to be placed in priority (the composite curves provide insight into this problem).

Figure 7-4 represents the global *HEN* obtained after merging and relaxation of the slice-wise *MER HENs*. *HEX* X_{pp4} has been suppressed and X_{pu5} had to be introduced because a relaxation path did not exist. In addition, X_{pp6} (time slice 5)

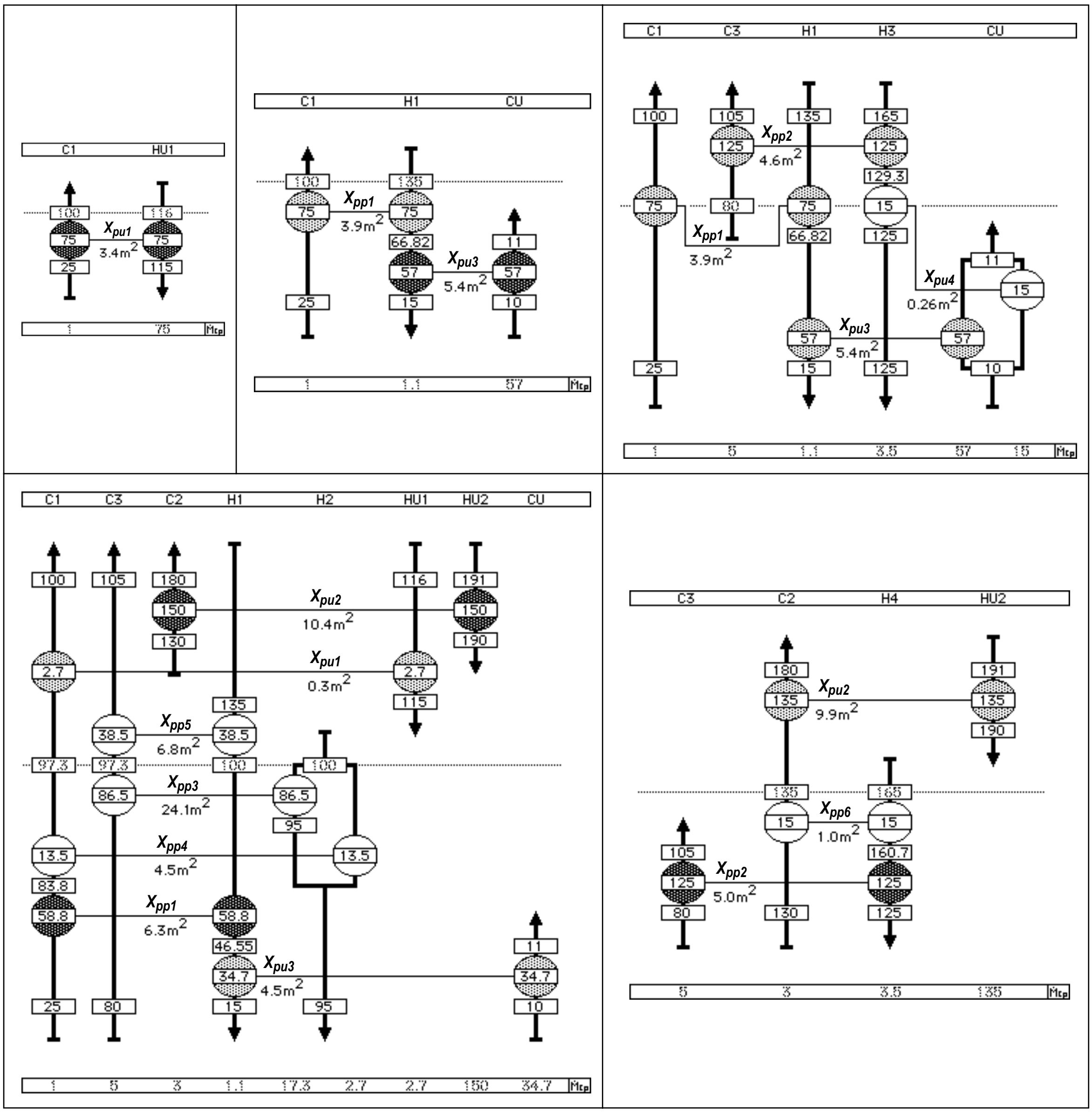

Figure 7-3 Slice-wise maximum energy recovery (*MER*) *HENs* of *EP-1* in conventional design (time slice 1 to 5 from left to right; see text for comments).

has been removed. In this particular case, for which the *HEX* cost function does not include a fixed cost (refer to Section A.1), the *TBCs* of the relaxed *HEN* are actually 1.3 % higher (refer to Table 7-6).

7.7 Summary

The *MBC* targeting methodology [22] has been demonstrated to work reasonably well on simple example processes such as *EP-1*. The analysis of actual *HEN* designs indicates that the re-use of *HEX* units may lead to significant criss-cross heat

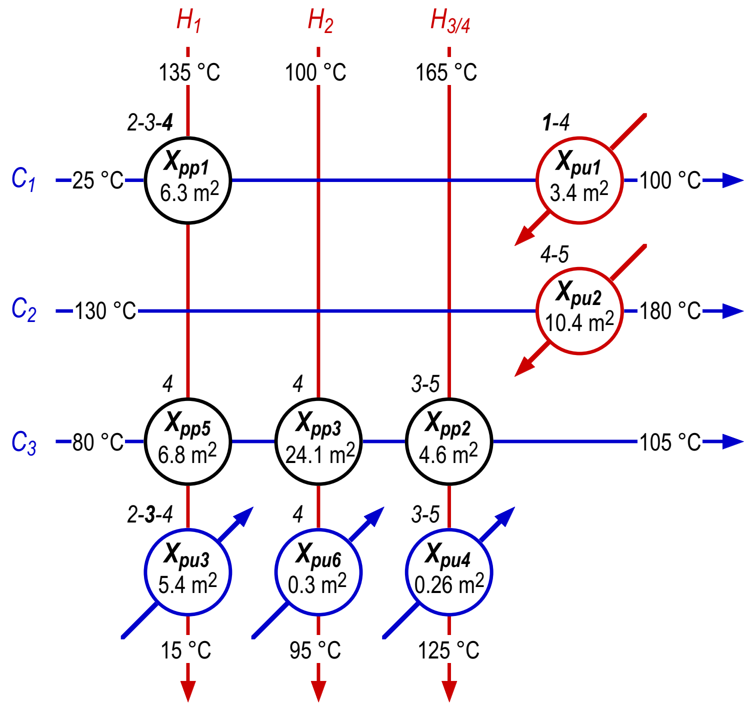

Figure 7-4 Overall relaxed *HEN* obtained from slice-wise *MER HENs* of Figure 7-3.

transfer. Nevertheless, at the targeting stage, the assumption of vertical heat transfer and the decomposition into enthalpy intervals remain very useful in providing with a framework allowing mathematical calculation procedures to be developed.

The cost-optimum slice-wise $\Delta T_{min\ l}$ obtained for *EP-1* demonstrate that both the energy targeting and the *HEN* design of batch processes cannot be properly addressed by considering a single overall process pinch ΔT_{min} as usually proposed. Of course, the actual error resulting from this crude assumption depends on the shape of the composite curves, and in particular on the existence of time slices of the threshold problem type (e.g. time slices 2, 3 and 5 of *EP-1*).

Experience is unfortunately lacking with respect to the capability of the targeting method to address significantly more complex batch processes such as the *EP-4* brewery process (refer to Appendix A) [23]. The complexity of a problem is proportional to both the number of process streams and the number of time slices.

The *MBC HEN* design methodology is time consuming and requires skills, even for a simple process like *EP-1*. An automated design methodology is definitely needed.

22. Including the adaptations/improvements introduced by *Krummenacher* & *Favrat* (1995), to deal with batch processes, and the implementation in the *PinchLENI* software programme.

23. Numerical problems were encountered in the *Simplex* algorithm implemented in *PinchLENI*, which could not be traced in time.

Chapter 8

DESIGN & OPTIMIZATION OF DIRECT BATCH *HENs*

8.1 Motivation & Overview

It has been shown in the previous Chapter that the *multiple base cases* (*MBC*) methodology proposed by *Jones* (1991) is suitable for both targeting and design of direct batch *HENs*. However, two limitations have been identified, namely :

1. at the targeting stage, the mode of re-use of *HEXs* units across time slices is either *conventional*, *resequence*, or *repipe* (refer to Section 7.3); a mix of these three modes in a *HEN*, commonly encountered in practice, cannot be taken into account [1];
2. the *HEN* design methodology is heuristic and requires skills, since the designer has to simultaneously develop feasible *HENs* for each time slice and ensure the optimal re-use of the installed *HEX* area across time slices. Batch processes with more than ten time slices are frequent, and in these cases the *HEN* design may become too time consuming and the combinatorial issues too difficult to manage by hand.

This Chapter presents a methodology suitable for an automated synthesis of direct batch *HENs* which has been developed to circumvent the above two major limitations.

The problem of design & optimization of direct batch *HENs* is first stated in **Section 8.2**; the required data, the decision variables, the definition of the objective function and the simplifying assumptions made to tackle the problem are also described.

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1. In conjunction with the assumption of vertical heat transfer between composite curves, this may bias the minimum temperature approaches $\Delta T_{min\ l}$ obtained and fail to properly initialize the *HEN* design.

Section 8.3 analyses the practical constraints restricting the re-use of *HEX* matches across time slices by repipe or resequence. A categorization into thermo-physical, chemical, and schedule constraints allows a more systematic approach to the specification of these constraints.

Given an overall match structure, the derivation of all feasible slice-wise match structures is exemplified in **Section 8.4**, providing insight into the structural issues of the problem.

Section 8.5 summarizes the practical implications of decreasing the active area of a *HEX* for its re-use during a less area-demanding time slice; the problem of optimally re-using available *HEX* areas to minimize the utility costs incurred during a time slice is also introduced.

Based on the previous developments, an automated design & optimization solution approach based on genetic algorithms is proposed in **Section 8.6**. At the upper level, all structural issues (i.e. finding an overall match structure) are addressed, while the lower-level optimization aims at identifying the optimal areas to be given to the matches of the overall structures and the optimal active areas to be used during each time slice.

Finally, **Section 8.7** summarizes the key features as well as the present limitations of the proposed optimization approach and sketches proposals for further work.

Illustrative examples and further comments may be found in **Appendix H**.

8.2 Problem Statement

The design & optimization problem considered in this Chapter may be stated as follows.

Given :

- a batch process, defined by a list of I hot process streams and J cold process streams;
- the match-wise *HEX* type specifications, and the related *HEX* type cost function(s);
- a list of constraints on the *HEX* re-use opportunities;
- the desired number of process-to-process matches (M_{pp}) of the batch *HEN* to be designed (specified *a priori* by the designer);

- the available utilities;
- the economic framework and constraints of the project;

determine :

- the overall match structure (*OMS*) including M_{pp} matches;
- the heat exchange area $A_{ppO\ m}$ to be installed for each process-to-process match $X_{ppO\ m}$ of the *OMS*;
- the feasible and consistent [2] set of L slice-wise match structures (*SMS*) (i.e. match structures derived from the *OMS* by particularization to each time slice, taking the constraints on the *HEX* re-use into account);
- the active area $A_{pp\ l,m}$ (with $A_{pp\ l,m} \le A_{ppO\ m}$) to be used for each process-to-process match during each time slice l (i.e. of each *SMS*);

which minimize the specified economic criteria, e.g. the total batch costs (TBCs) [3]

Actually, it is often desirable to be provided with several good solutions instead of only one "best" solution. Combined with other requirements, this again substantiates an optimization approach based on genetic algorithms (*GA*s).

8.2.1 Required Data

1. **Specification of the batch process streams** :
   supply & target temperatures $T_{S\ p}$ & $T_{T\ p}$, heat capacity flowrate CP_p, start & stop times $t_{start\ p}$ & $t_{stop\ p}$, heat transfer film coefficient h_p.
2. **Match-wise HEX type specifications** :
   the default *HEX* type, and any particular *HEX* type required by a match $X_{ppO\ i,j}$ between hot process stream i and cold process stream j (as well as for matches with utilities).
3. **Utility streams** :
   inlet & outlet temperatures $T_{in\ u}$ & $T_{out\ u}$, heat transfer film coefficient h_u, specific cost c_u.

2. The meaning of "consistent" is made clear in Section 8.4 which addresses the particularization of the *OMS* to each time slice.

3. In common sense terms, the problem stated above searches for a direct batch *HEN* (i.e. a structure of M_{pp} matches and the associated heat exchange areas $A_{ppO\ m}$) as well as the optimum way of using the available matches and areas, which minimize the total batch costs.

4. **List of constraints on the HEX re-use opportunities** :
   a set of possible resequence and possible repipe opportunities [4].
5. **Economic framework of the project** :
   pay-off factor per batch a_B [5].
6. **Number of HEX matches** :
   the number of matches M_{pp} is specified a priori by the user, allowing for some control on the complexity of the *HEN* to be designed [6].

8.2.2 Scope & Assumptions

The problem is concerned with the grassroot design of direct batch *HENs*. It is assumed that :

- a preliminary analysis (according to the guidelines described in Section 3.6) has eliminated insignificant [7] time slices from consideration; the schedule of the remaining meaningful time slices is considered as fixed and binding [8];
- the process streams feature a constant heat capacity flowrate (i.e are single-segment streams) [9]; this assumption is required for a simple calculation of the operating temperatures of a *HEN* knowing the match areas (*Asbjornsen*, 1985; *Maréchal*, 1986);
- stream splitting is not allowed, meaning that the matches on a stream are serially arranged, resulting in a simple coding of the match structure [10];
- the utility heat rate required to meet the heat balance of process streams are supplied at the target temperature side of the process streams [11];

---

4. Considerations to define these actually feasible structural changes (accounting for the properties of streams, their schedule, and other constraints) are presented in Section 8.3.
5. This factor expresses the fraction of capital costs paid-off by each batch, and can be calculated from the number of batch per year N_{BPY}, the pay-off period POP and interest rate IR - refer to Section 3.3.
6. There is no preliminary calculation of a minimum number of matches to achieve a given level of heat recovery (moreover, it is not clear whether such a minimum number of matches would lead to the most cost-effective heat integration). The *a priori* specification of the desired number of *HEX* matches and hence the need to identify the optimum number of matches by external iteration on this parameter is an open issue which remains to be analysed. In fact, depending on the coding convention to be adopted for the overall match structure (refer to Sub-section 8.6.1), the specified number of matches may rather correspond to the upper bound on the number of matches of the direct batch *HEN*, since a sequence of several matches on the same pair of streams can actually be grouped together to make up a single match, hence the actual number of matches shall be smaller or equal to the specified number of matches M_{pp}.
7. Short and/or too schedule-sensitive time slices.
8. I.e. the identification of rescheduling opportunities is not addressed.
9. Streams undergoing phase changes or significant variations of the specific heat cannot be modelled as multi-segment streams, and should be modelled as several single-segment streams instead.

♦ the process-utility *HEXs* stay on the same process stream throughout the batch cycle time[12].

8.2.3 Top-down or Bottom-up Approach ?

With respect to the structural issues, the above problem statement implicitly assumes a top-down solution approach, in that the slice-wise match structures - i.e. the structure of active matches during each time slice - are derived from an overall match structure (overall *HEN*) including all matches. Alternatively, a bottom-up approach [13] could have been considered, in which the slice-wise structures would first be built (design of independent *HENs*), followed by a merging (reconciliation) step aiming at devising a superstructure embedding all slice-wise structures within a minimum number of matches, i.e. using the resequence and/or repipe opportunities as much as possible.

In the perspective of an automated synthesis, the top-down approach has been foreseen as more appropriate than the bottom-up one :

♦ from a conceptual point of view, starting from the overall structure level and particularizing to slice-wise structures seems more reasonable and is certainly more systematic than trying to identify a global structure from partial (i.e. slice-wise), not necessarily compatible structures. In addition, in the top-down approach, the total number of matches of the overall structure can be fixed by the designer, providing with a control of the *HEN* complexity and of the search domain;

♦ using the bottom-up approach, the number of matches of the resulting global *HEN* cannot be controlled at the onset, since it is very much dependant on the structural similarities and dissimilarities of the independently generated slice-wise structures [14].

10. Moreover, in order for the calculation technique of the operating temperatures of the *HEN* to be applied, fixed stream flowrates are required. Splitting a stream is still possible, as long as the distribution of mass flowrates (split fractions) in the branches is fixed and the splitting and mixing temperatures are fixed too (the optimization of split fractions is not addressed). A parallel arrangement of matches may also be approximated by a repeated serial sequence of matches on the stream which is a good candidate for splitting (at the expense of potentially requiring more *HEX* units.
11. The contributions of intermediate utilities, if any, are not optimized, i.e. possibly existing intermediate utilities should be made similar to process streams with fixed mass flowrates.
12. This is actually not a major limitation; it simply means that the optimal re-use of utility *HEX* units is not addressed.
13. The usual approach applied by heuristic methods.
14. E.g. if two slice-wise structures are similar and incorporate $M_{pp\ l}$ matches each, their "addition" towards obtaining the global structure will at the best be made of $M_{pp\ l}$ matches, while, if very dissimilar, the "addition" shall contain at worst $2 \times M_{pp\ l}$ matches.

The top-down approach provides a framework within which the problem is more clearly defined, and can be tackled in a more systematic manner.

8.2.4 *HEX* Re-use & Structural Evolution

In spite of its definite advantages, the top-down approach may also involve combinatorial difficulties associated to the derivation of the slice-wise matches structures. To illustrate the problem, consider **Figure 8-1** which represents a

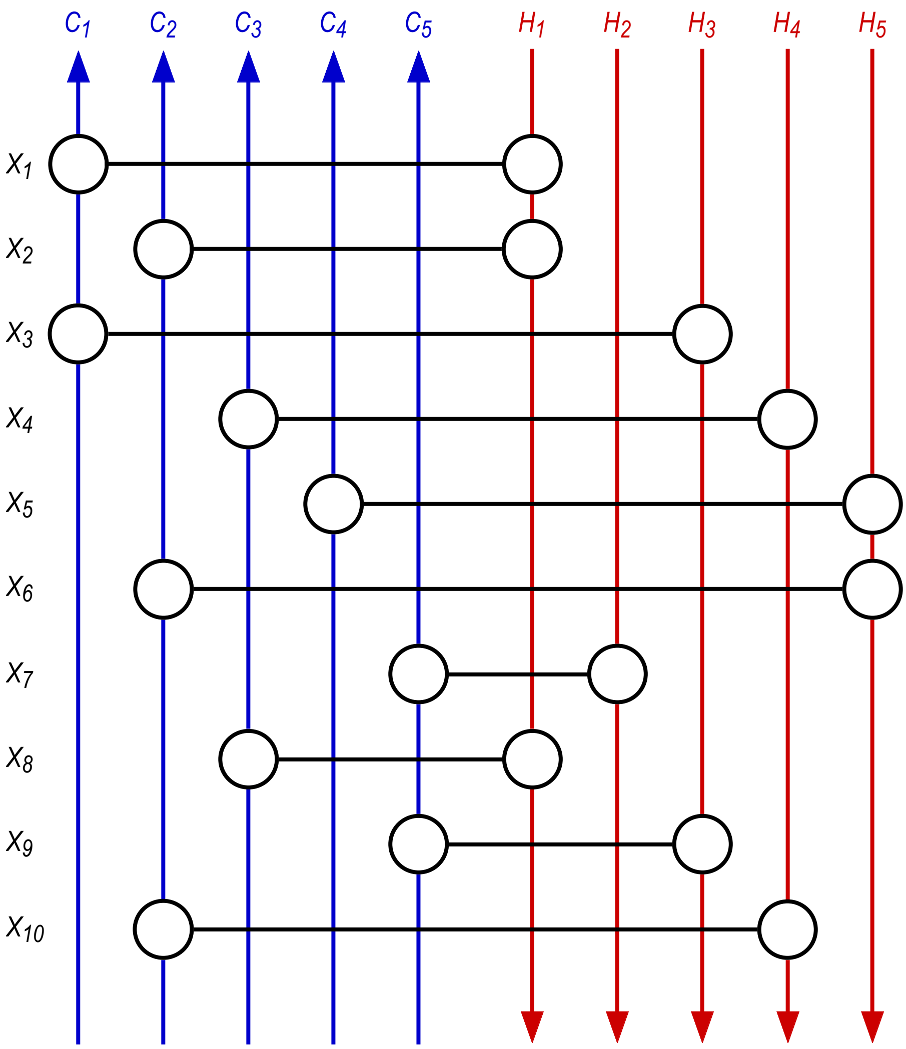


Figure 8-1 A possible overall match structure for example process *EP-2*.

possible overall match structure (*OMS*) for example process *EP-2* (described in Section A.2), including 10 matches [15]. If any match (*HEX* unit) must stay at the same place with respect to other matches (i.e. so-called conventional design - refer to Section 7.3), the slice-wise match structures are derived in a straightforward manner by simply leaving out any match which involves inactive streams during the considered time slice. There exists only one slice-wise match structure for each time slice.

If resequence and/or repipe modes of *HEX* re-use across time slices (refer to Section 7.3) are allowed for any match, the derivation of slice-wise match structures would imply hardly manageable combinatorial difficulties and a large number of possible match structures would exists for each time slice. To provide insight in these modes of *HEX* re-use, **Figure 8-2** illustrates the case of resequencing a pair

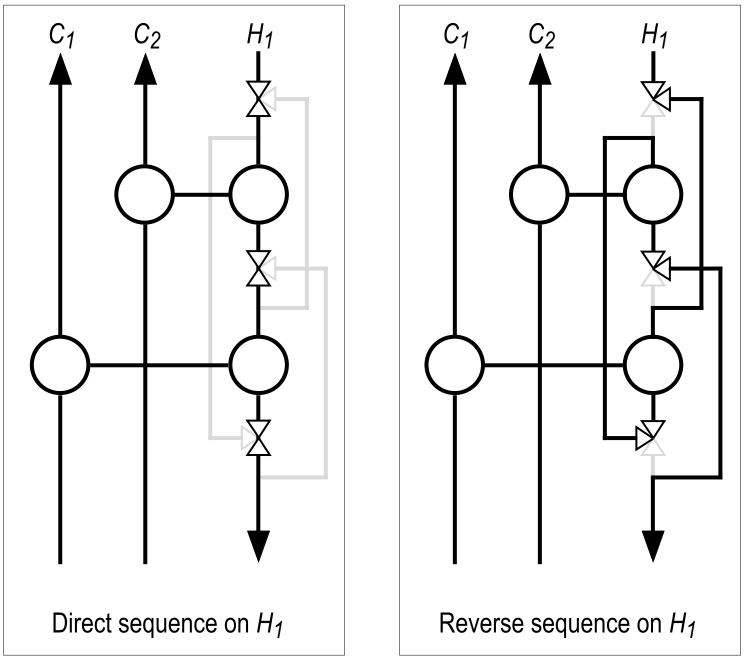


Figure 8-2 Resequencing a pair of *HEXs*.

of *HEXs* on a stream (H_1) and represents the related piping and valving [16]. **Figure 8-3** illustrates a case of repiping one *HEX* side only and represents the required piping and valving [17].

In real processes, the actual opportunities for resequence and/or repipe of *HEX* units across time slices are generally quite limited, so that the combinatorial size

15. To simplify notations, the matches are noted as X_m instead of $X_{ppO\ m}$, since all matches discussed in this context are process-to-process matches of the overall match structure.
16. At least three 3-way valves are needed; alternatively, six 2-way valves might be used.
17. At least six 2-way valves are needed for operation, while cleaning could require additional piping and valving. In the more general case of a repiping on both *HEX* sides, the number of required valves doubles.

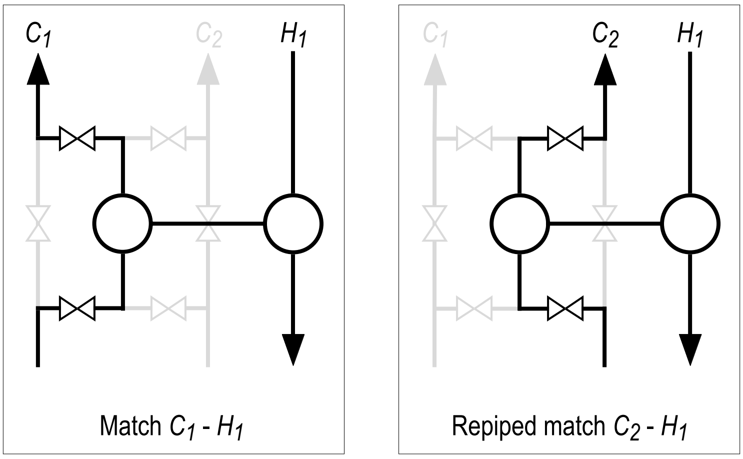


Figure 8-3 Repiping a *HEX* on one side.

involved in the derivation of slice-wise match structure is very significantly reduced and manageable. The practical constraints substantiating the above statement have been established and are summarized in the next Section.

8.3 Practical Constraints Restricting *HEX* Re-use Across Time Slices

Compared to the conventional re-use of *HEX* units alone, resequence and/or repipe provide with the potential benefit of additional area and/or *HEX* units savings, i.e. capital costs savings. However, as far as possible, an automated synthesis method should not spend time evaluating solutions which are infeasible in practice. Therefore a methodology is required to identify actually feasible repipe and resequence opportunities, and to specify (formalize) the resulting structural changes of the overall match structure.

The repipe opportunities have been found to be restricted by three types of constraints :

1. the compatibility of thermo-physical properties of the streams;
2. the chemical compatibility of the streams;
3. operational constraints resulting from the time schedule of the streams.

Constraint types 1. and 3. also restrict the opportunities for resequence; constraints of type 1. would only apply e.g. in case of significant changes the thermo-physical properties with temperature.

As will be seen, the above classification of constraints mainly provide the user with a framework for ultimately defining which structural changes are actually possible, but the related considerations are not "exact" science.

This Section describes the above types of constraints on the basis of the *EP-2* example process (refer to Section A.2).

8.3.1 Thermo-physical Compatibility

Different heat exchanger types (e.g. shell & tube, plate & frame, coaxial double tube, falling film evaporator, etc.) each have their specific application range and their recommended operating conditions.

For example, the suitability of plate & frame *HEXs* for high viscosity liquids or for high temperature gases is generally more restricted than that of shell & tube *HEXs*. Their maximum operating temperature is often imposed by gasket material, while their mechanical design principle restricts the maximum allowable operating pressure, as well as the pressure difference between the primary and secondary sides. In a repipe perspective (i.e. operating a *HEX* unit with another stream on one side - or between another pair of streams), such constraints have to be taken into account.

Constraints on operating conditions (which determine to a large extent the type of *HEX* to be used) can generally be formalized in terms of :

- the temperature span of a stream;
- the operating pressure;
- the phase (solid, liquid, gas).

The repipe of an *HEX* also requires that the pressure drop across the unit is not too different, that is, the pumping power remains acceptable. Detailed expressions of the pressure drop are complex and depend on the *HEX* type; however, among other factors, the following properties are of particular relevance :

- the viscosity of the stream;
- the density (or specific volume).

Based on the properties mentioned above (the list of which might not necessarily be exhaustive), the idea is to divide the streams into separate groups of "thermo-physical compatibility". Streams within a group of "thermo-physical compatibility" feature similar enough properties that they could potentially use the same *HEX* (at different times)[18] (refer to further comment in Sub-section H.1.1).

For example, the *EP-2* process streams listed in Table A-2 can be organized into the following "thermo-physical compatibility" groups [19]:

1. {H_1, H_2, H_5, C_1} for liquid, low viscosity, high density fluids;
2. {H_3, C_4} for liquid, high viscosity, middle density fluids;
3. {H_4, C_3} for gas of similar properties.

8.3.2 Chemical Compatibility & Cleaning

The preliminary check for "thermo-physical compatibility" allows to significantly restrict the number of cases for which the "chemical compatibility" has to be verified, since only streams belonging to the same "thermo-physical compatibility" group are concerned. The "chemical compatibility" accounts for at least the following aspects : the quality of the product, the safety, and the cleaning costs.

It is proposed to considered three categories of "chemical compatibility" :

1. total compatibility, between streams involving the very same fluid, or those which feature unimportant differences [20]. Total "chemical compatibility" means that cleaning is not required when switching between streams;
2. conditional compatibility, when a cleaning cycle is required either when switching from, e.g., stream 1 to stream 2, or during the reverse change (2 to 1), or in both cases. Any cleaning is associated with both capital costs (cleaning system including control, valving and piping. etc.) as well as operational costs (energy, cleaning agents, labour costs);

18. This concept of compatibility is not a binary property, i.e. there is no absolute criteria that allows unambiguous decision about the compatibility. The degree of similarity for which streams properties or operating conditions are to be considered as compatible is up to the designer; strict compatibility constraints will lead to safe designs, but with the potential drawback of not being cost optimal since the re-use of some *HEX* units might have been overlooked. The concept of compatibility is somewhat like a control parameter for trading-off safety against cost efficiency of the design.
19. Stream C_2 is likely not compatible with the first group of streams because of its high pressure, high temperature properties. Therefore C_2 shall not be a candidate for repiping a *HEX* designed for the first group of streams ... although a *HEX* designed for C_2 could potentially be re-used for streams with less constraining features, while the reverse would clearly not be possible. This feature demonstrates that the proposed approach based on the concept of groups of similar thermo-physical properties is actually a simplified method to specify the real opportunities to re-use *HEX* units. Stream C_5 generally requires a specially designed *HEX*, not to be re-used by other streams.
20. E.g. hot process water streams; milk and skimmed milk - both before or after pasteurization, to avoid biological cross contamination, etc.

3. incompatibility of streams, because either the cleaning would be too costly (or impossible), or various types of hazards could occur.

The common denominator of these three categories is the cost for changing from one stream to another one of the same "thermo-physical compatibility" group. Since actually the cleaning costs can hardly be calculated (or experience values are not available yet), the designer may distinguish between the following cases: • no cost; • low cost; • middle cost; • high cost; • very high cost.

The "no cost" option would be associated with "total compatibility", while "low cost", "middle cost", and "high cost" is meant to introduce ranking within "conditionnal compatibility". The "very high cost" option would practically exclude the *HEX* re-use and mean "incompatibility".

Unlike the "thermo-physical compatibility", which is a transitive property and leads to the definition of groups, the "chemical compatibility" allows to define costs associated to transitions (switching) between the members (streams) within a group. These costs can conveniently be organized into a matrix format, as illustrated below.

The chemical compatibility is established for the streams within each group of similar thermo-physical properties : for example, within the first group $\{H_1, H_2, H_5, C_1\}$, H_5 is supposed to include toxic release components which make cleaning for *HEX* re-use with H_1, H_2 or C_1 too expensive, or too risky. Cleaning costs for any transition between streams within the group are summarized in the following matrix format (**Figure 8-4**), where matrix elements shaded in grey represent infeasible transitions (or transitions which are not meaningful, like the elements on the diagonal) (refer to for comments pertaining to groups 2 and 3). As can be seen, the preliminary identification of groups of streams with similar thermo-physical properties allows to split the overall 10 x 10 matrix into smaller sub-matrices, reducing the number of stream transitions to be considered [21].

21. Note that if a transition is not feasible, the transition in the opposite direction has to be excluded from consideration too, for consistency reasons (e.g. in group 1, transitions from any stream to H_5, and in group 3, transition from C_3 to H_4).

Cleaning Costs		to stream …			
		H1	H2	H5	C1
from stream …	H1	0	0	CC_{H1H5}	CC_{H1C1}
	H2	0	0	CC_{H2H5}	CC_{H2C1}
	H5			0	
	C1	CC_{C1H1}	CC_{C1H2}	CC_{C1H5}	0

Group 1

Cleaning Costs		to stream …	
		H3	C4
from	H3	0	CC_{H3C4}
	C4	CC_{C4H3}	0

Group 2

Cleaning Costs		to stream …	
		H4	C3
from	H4	0	
	C3	CC_{C3H4}	0

Group 3

Figure 8-4 Chemical compatibility, expressed as cleaning costs for switching between streams (example process *EP-2*).

8.3.3 Time Schedule Constraints for Repipe

The original problem of designing flexible *HENs* for continuous processes using the *MBC* approach (*Jones*, 1991) did not require the consideration of time schedule constraints. The base cases (or operating modes) are supposed to be separated in time, or at least the *HENs* are operated over a long period compared to the switching time from one configuration to the next.

The cycle times of batch production processes are often in the range of hours, and the production volumes of high quality products are rather small. Changing the *HEN* configuration by repiping during operation of the related streams means disruption of the normal course, possible loss of valuable product [22], and often requires a cleaning cycle [23]. In conclusion, a safe strategy requires that repiping one *HEX* side be only possible at a time when no stream is flowing through this side, and provided that enough time (with a great probability) is available for the required cleaning cycle.

The feasible transitions represented on Figure 8-4 are further restricted by schedule constraints (refer to the schedule of streams of Figure A-3) :

1. **group 1** : focusing on the schedule of streams H_1, H_2 and C_1, it appears that repiping from C_1 to H_1 (or the opposite) is not feasible, since C_1 and H_1 overlap in time. However, H_1 and H_2 do not overlap in time (with a sufficient margin), as do C_1 and H_2, making the repipe feasible;

22. Unless a pumping/draining system is provided.
23. Except in the case of total compatibility of the related streams, or when switching between heat recovery streams.

2. **group 2** : repiping from H_3 to C_4 (as well as the opposite) is feasible since these streams do not overlap in time;
3. **group 3** : repiping from H_4 to C_3 is chemically not feasible. Moreover, from the point of view of the schedule constraints, this repiping would be difficult, since no time margin would be available for the cleaning process (although H_4 and C_3 do not overlap in time).

Figure 8-5 represents the feasible repipe opportunities, taking into account both the cleaning constraints and the schedule constraints. Elements shaded in light grey are infeasible transitions from the schedule point of view [24]

Cleaning Costs		to stream ... H1	H2	H5	C1
from stream ...	H1	0	0	CC_{H1H5}	CC_{H1C1}
	H2	0	0	CC_{H2H5}	CC_{H2C1}
	H5			0	
	C1	CC_{C1H1}	CC_{C1H2}	CC_{C1H5}	0

Group 1

Cleaning Costs		to stream ... H3	C4
from	H3	0	CC_{H3C4}
	C4	CC_{C4H3}	0

Group 2

Cleaning Costs		to stream ... H4	C3
from	H4	0	
	C3	CC_{C3H4}	0

Group 3

Figure 8-5 Feasible repipe opportunities (= non-shaded matrix elements), taking into account the cleaning and the schedule constraints (example process *EP*-2).

8.3.4 Time Schedule Constraints for Resequence

Resequencing does not require a cleaning cycle, nor does it imply losses of product, but changing the order of *HEX* units on a stream leads to transient conditions (on this stream and all streams which are matched "downstream") which might not be tolerated, depending on whether the temperature control of the related streams is critical (e.g. for reaction) or not (e.g. pre-heating of non-biological stream, or intermediate stream for in-vessel heating or cooling) [25].

24. Depending on the use of this matrix of feasible transitions, various additional costs (piping, valving, etc.) may be included.
25. Hence the feasibility of resequencing during operation is not only stream-dependent, but is a "downstream *HEN*" feature which has to be assessed. Since the opportunity for resequence is time slice dependent (because the propagation of transient conditions depends of the "downstream *HEN*" active at the time of resequence), the specifications of resequence opportunities would better be managed automatically on the basis of the presented considerations, and accounting for the overall match structure or slice-wise match structure being evaluated.

With respect to resequence, the following features are assumed for the example process :

- ♦ H_4 and H_5 are heat recovery opportunities and not process streams, hence they can be considered as insensitive to resequencing;
- ♦ C_5 does not experience significant temperature changes (evaporation); therefore resequence is not needed on C_5, while transient conditions resulting from resequencing on "upstream *HEN*" are tolerated;
- ♦ C_2 and H_1 are supposed to be "resequence insensitive" streams (i.e. their temperature control is not of critical importance, e.g. feed preheat or cooling);
- ♦ remaining streams (C_1, C_3, C_4 and H_2, H_3) are supposed to be highly temperature sensitive and do not tolerate resequence (either directly on the stream, or within the "upstream *HEN*").

8.4 Deriving Slice-wise Match Structures

The constraints on resequence and repipe opportunities described in the previous Section establish the fact that the number of feasible structural changes to a slice-wise match structure by repipe and/or resequence is generally quite restricted, so that each alternative structure may be considered and separately evaluated.

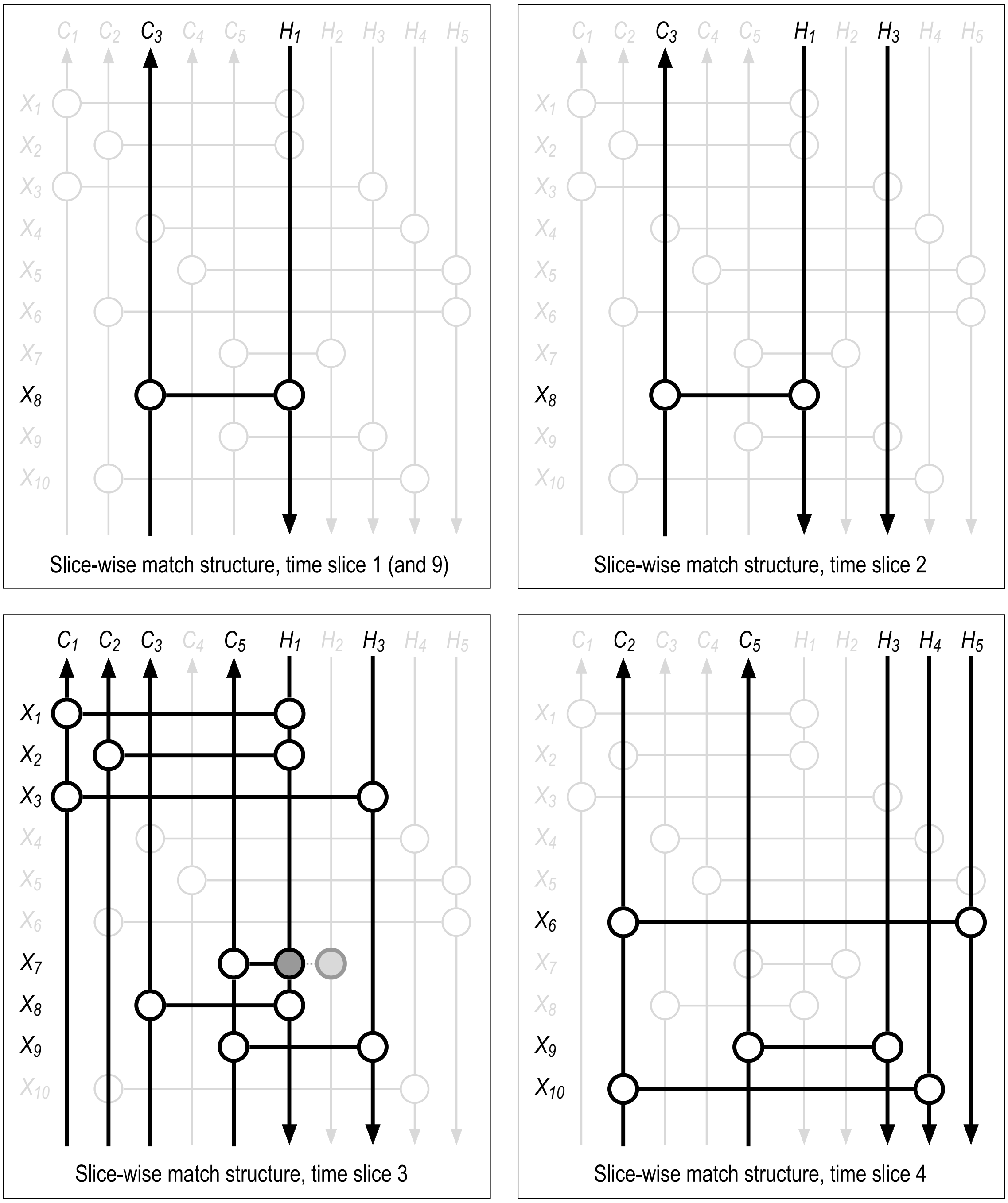
Given the overall match structure (*OMS*) of Figure 8-1, the schedule of the streams (refer to Figure A-3) and the feasible repipe opportunities (refer to Figure 8-5) and allow to derive the slice-wise match structures (*SMS*) represented in **Figures 8-6 and 8-7** [26]. In these Figures, shaded parts indicates matches which have been repiped and/or resequenced.

The derivation of all feasible slice-wise match structures for each time slice involves two steps :

1. first, the matches of the *OMS* which are not active during the considered time slice (i.e. those for which at least one stream does not exist) are simply ignored, resulting in the so-called *base case slice-wise match structure* [27];
2. second, for the same time slice, the structures which can be obtained by structural changes using feasible resequence and/or repipe opportunities are

26. Only one possible slice-wise structure is represented for each time slice; other slice-wise structures (if any) are described in the comments made for each time slice.

27. In other terms, the base case structure excludes any consideration of structural changes due to resequence and/or repipe opportunities.



Slice-wise match structure, time slice 1 (and 9)

Slice-wise match structure, time slice 2

Slice-wise match structure, time slice 3

Slice-wise match structure, time slice 4

Figure 8-6 Examples of slice-wise match structures (time slices 1 to 4, and 9).

exhaustively generated. To distinguish these slice-wise structures from the base case structure, they are called *modified slice-wise match structures*[28].

With respect to the generation of the modified slice-wise match structures (i.e. accounting for the repipe and resequence opportunities), detailed comments are

28. Depending on the constraints on resequence or repipe, there may be no modified slice-wise structure.

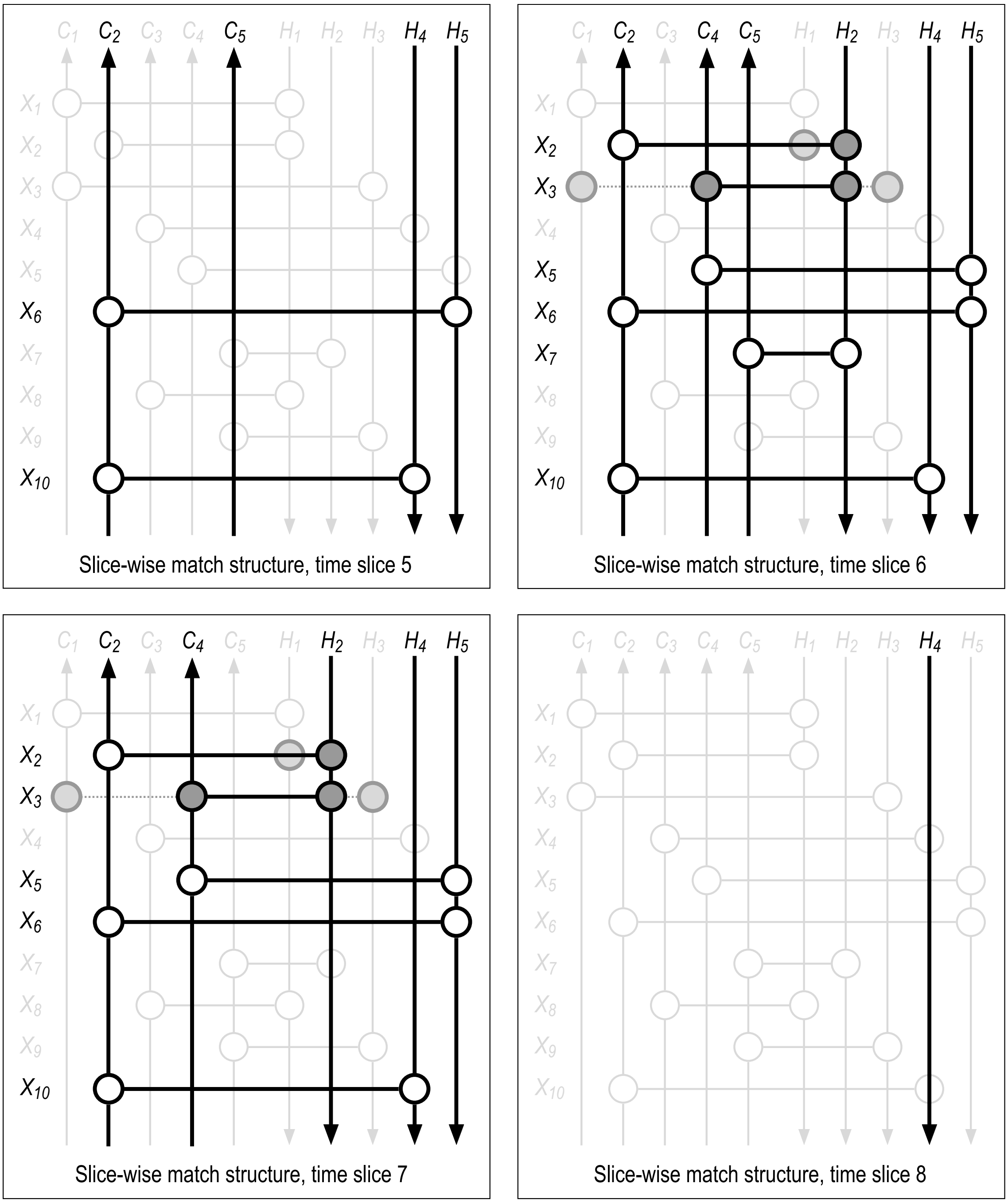


Figure 8-7 Examples of slice-wise match structures (time slices 5 to 8).

made in Section H.2 (the resequence and repipe opportunities are intentionally discussed in details in order to exemplify the issues).The aim of the present description of the approach consists in merely highlighting the essentially manageable nature of the structural optimization.

A systematic way of formalizing and managing these opportunities, in the perspective of a computer implementation of the generation of the modified slice-wise structures, is obviously needed. This requires a modelling of the resequence opportunities, in a way similar to the feasible repipe opportunities [29].

Slice-wise structures obtained by "permanent" (or "systematic") [30] repipe and resequence have been eliminated from the sets of slice-wise structures, in order to restrict the computational effort for the a given overall structure [31].

Summarizing the number of slice-wise match structures $N_{SMS\ l}$ for each time slice :

$N_{SMS\ 1} = 1$ $N_{SMS\ 2} = 1$ $N_{SMS\ 3} = 5$ $N_{SMS\ 4} = 2$ $N_{SMS\ 5} = 2$
$N_{SMS\ 6} = 32$ $N_{SMS\ 7} = 16$ $N_{SMS\ 8} = 1$ $N_{SMS\ 9} = 1$

Without accounting for identical or degenerated slice-wise structures, a total of $N_{SMS} = \sum_{l=1}^{9} N_{SMS\ l} = 61$ slice-wise structures have to be evaluated with respect to minimum (slice-wise) utility costs.

If structural changes from one time slice to the next were not restricted (i.e. if the time slices were fully independent of each other), the overall, batch-wise utility costs would be the sum of the minimum utility costs obtained for each time slice.

8.4.1 Consistent Sets of Slice-wise Structures

However, with respect to structural changes, the time slices are often not independent, due to the fact that repiping and/or resequencing can only occur during some time slices.

A *consistent set* (*CS*) of slice-wise match structures is defined as a series (sequence) of L slice-wise match structures (one for each time slice) in which any slice-wise match structure is feasible and compatible with all resequence and/or repipe decisions made during the previous time slices and which restores the *HEN* at the end of the batch cycle in an operation mode compatible with the one of the first time slice of the batch [32]. Different consistent sets of slice-wise match structures correspond to

29. But unlike repipe, resequence opportunities do not only depend on properties of the matched streams but also on those which are in the "downstream *HEN*". Further analysis work is definitely needed, and feedback from practice or simulation of resequencing should result in guidelines or systematic methods to focus consideration on a restricted number of modified slice-wise structures in case of excessively large numbers of modified structures. The feasibility of temperature driving forces have to be taken into account too.

30. By permanent or systematic, it is meant that the a match actually never operates in its originally position defined by the overall match structure, i.e. is always found, over a batch cycle, in other positions than the original one.

31. The eliminated slice-wise structures are actually embedded in other overall match structures.

different ways of operating an available overall *HEN*, while each of these sets meets a list of practical constraints. Each is characterized by its own potential to minimize the overall utility costs over a batch cycle; the consistent set with the highest potential (largest cost savings) has to be identified.

To illustrate the concept of consistent slice-wise structures, consider the case of *TS 6* and *TS 7* (refer to Figure 8-7) : repiping X_2 and/or X_3 from *TS 6* to *TS 7* is not feasible, hence consistent sets shall include slice-wise match structures for *TS 6* and *TS 7* in which the matches X_2 and X_3 feature similar positions with respect to repipe (but not necessarily with respect to resequence, which obeys other kinds of restriction). Again, systematic methods to formalize the consistency rules, and able to enumerate the consistent sets (1 .. N_{CS}), need to be developed [33].

8.5 Optimal Re-use of *HEX* Area to Minimize Utility Costs

The installed *HEX* areas $A_{ppO\ m}$ of the overall match structure have to be optimally used during each time slice to minimize the utility requirements [34]. Except for very simple slice-wise *HEX* match structures, finding the active areas $A_{pp\ l,m}$ (with $A_{pp\ l,m} \leq A_{ppO\ m}$) which minimize the utility requirements is not a straightforward task. A simple illustrative example is provided in Sub-section H.3.1.

The reduction of the active area of a match $A_{pp\ l,m}$ required for minimizing the utility costs is achieved by partial by-pass of the *HEX* unit. Although the principle is well known, a simple example is described Sub-section H.3.2. Recommendations for selecting on which side the by-pass should be applied are also provided.

8.6 Proposed *GA* Based Optimization Strategy

The design & optimization problem of direct batch *HENs* has been stated in Section 8.2. Both structural and parametric issues are involved. The use of a top-down approach to address the structural issues has been substantiated. Experience gained from the *GA* based optimization of indirect heat integration allows to be confident in the suitability of such an approach for the present problem as well,

32. In other terms, the actual operation of a *HEN* according to a consistent set of slice-wise match structures meets all schedule constraints with respect to resequence and repipe changes during a repeated batch cycle.
33. Note that the slice-wise match structures for *TS 3*, *TS 6* and *TS 7* include more streams and *HEX* units that will most likely be found in real batch processes. Therefore the number of possible slice-wise match structures for these time slices and the related combinatorial difficulties may in this case be overestimated.
34. In a multiple utility context, the total costs of utilities have to be minimized.

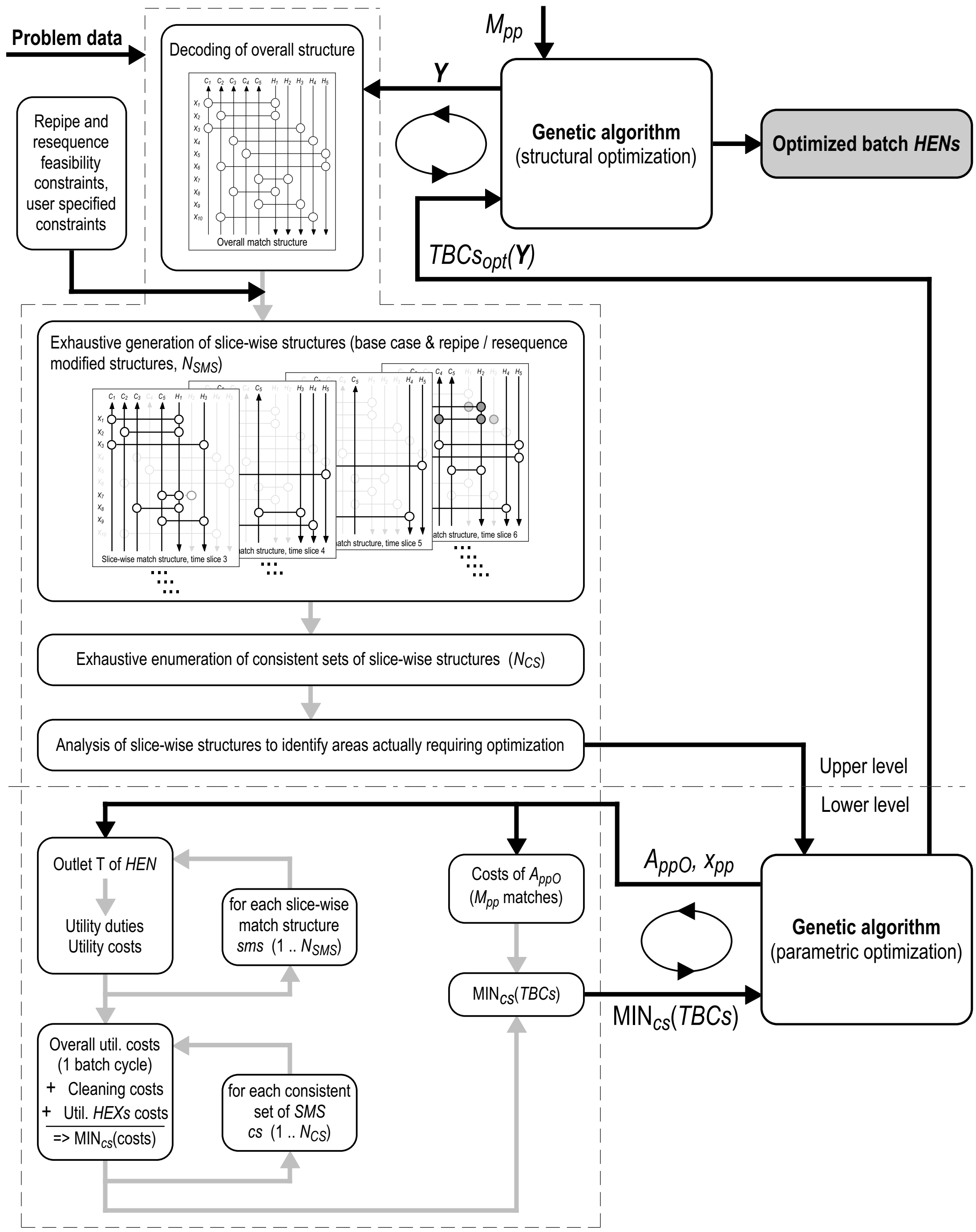


Figure 8-8 Proposed strategy based on genetic algorithms for the design & optimization of direct batch *HENs*.

provided that the optimization scheme includes two levels and the model ensures full segregation of structural and parametric issues.

The proposed *GA* based optimization strategy sketched on **Figure 8-8** meets these requirements, in that all structural decisions are made and optimized at the upper level, while the lower level addresses parametric issues solely.

8.6.1 Upper-level Optimization

At the upper level, a population of overall match structures (i.e. potential solutions including M_{pp} matches [35]) is postulated and optimized according to the *GA* evolutionary strategy. Several coding conventions may be envisaged for representing the overall match structure [36] [37].

Once decoded, each overall structure (one at a time) is particularized to each time slice first without structural changes (resulting in the base case slice-wise match structure), then with an exhaustive generation of allowed repipe and/or resequence structural changes (modified slice-wise match structures). The structural changes meet the practical constraints inherent to the problem, and any additional constraint the user may specify.

The slice-wise match structures are then organized into consistent sets of slice-wise match structures (N_{CS} sets), each representing a feasible structural operation mode of the overall match structure over a batch cycle [38].

In the perspective of the lower-level optimization, the slice-wise structures are analysed in order to identify match structures or match sub-structures for which the problem of finding the best operation of the available areas can be solved in a straightforward, deterministic way (e.g independent matches). The optimum active

35. The optimum direct batch *HENs* shall actually be searched among *HENs* including a number of units less than or equal to M_{pp} (refer to footnote in Section 8.2).

36. Several existing coding conventions have been reviewed (*Androulakis* & *Venkatasubramanian*, 1991; *Lewin* et al., 1998; *Wang* et al.,1997). The first cited seems suitable, but different issues remain to be analysed, e.g. with respect to the definition of the crossover operator, and to an ordering/re-organisation convention of the string so as to avoid the same structure to be coded in a variety of strings. For example, assuming that each match is described by a couple of number, the first referring to hot process streams and the second to cold process streams, the overall structure of Figure 8-1 can be coded as {1-1, 1-2, 3-1, 4-3, 5-4, 5-2, 2-5, 1-3, 3-5, 4-2}; but since several matches of the overall structure can be moved (since independent of each other), {1-1, 1-2, 2-5, 3-1, 3-5, 4-3, 1-3, 4-2, 5-4, 5-2} actually describes the same structure. The coding convention should also facilitate the identification of infeasible matches (e.g. thermodynamically infeasible matches or owing to non-overlapping time schedules) in order to prevent them from being generated, or easily identified and ignored. But *HEXs* featuring heat transfer in the reverse direction should actually not be a problem for the calculation of the temperatures of the *HEN*.

37. In any case, the coding shall be significantly more compact than the binary variable representation used in mathematical programming approaches.

38. The organization into consistent sets could alternatively be performed while generating the slice-wise match structures - this is still an open issue.

area of these matches do not require optimization and therefore the number of decision variables of the lower-level optimization is decreased.

8.6.2 Lower-level Optimization

At the lower level, the problem consists in finding the areas to be installed ($A_{ppO\ m}$) and the best operational use of these areas during each time slice which minimize the utility costs (while also accounting for the costs of the required utility *HEXs* and the cleaning costs possibly incurred by the repipe stream change-over).

The decision variables managed by the *GA* are :

- the areas $A_{ppO\ m}$ of the M_{pp} matches (vector A_{ppO} on Figure 8-8);
- the area fractions $x_{pp\ l,m}$ (with $0 \leq x_{pp\ l,m} \leq 1$) of these areas to be used for each slice-wise match structure [39] (vector x_{pp} on Figure 8-8).

First, for each slice-wise *HEN* [40] requiring optimization, given the active areas $A_{pp\ l,m}$ (defined as $A_{pp\ l,m} = x_{pp\ l,m} \cdot A_{ppO\ m}$) of the matches, the temperatures of the *HEN* are obtained by matrix inversion (*Asbjornsen*, 1985; *Maréchal*, 1986) and the utility duties and costs to meet the target temperature of process streams are calculated. Depending on the active areas used, utility cooling on cold streams and/or utility heating on hot streams may be required, representing costs penalties for making the *HEN* operation feasible.

Second, the overall utility costs (operational costs) are calculated for each consistent set of slice-wise structures, and the consistent set featuring the lowest "operational" costs (accounting for the utility costs - both operational and capital costs - and the possible required cleaning costs) is identified.

Finally, the *TBCs* (objective function) are calculated and returned to the *GA* (refer to next Sub-section).

The areas and the area fractions for the considered overall match structure are repeatedly improved by the *GA* evolutionary strategy, until a convergence criteria is met. At this point, the best area parameters are assumed to be identified for the given overall structure, and this information is returned to the upper-level

39. A $x_{pp\ l,m}$ variable is needed for each active match (and which actually requires optimization) of each slice-wise match structure, according to the preliminary analysis performed at the upper level.

40. At this level, this is no more solely a structure, but an actual *HEN* since the area (duty, etc.) of matches is also provided.

optimization. The evaluation of the next overall match structure (next individual) can be started.

Note that the lower-level optimization does not require any ΔT_{min} specification for the matches, allowing the full exploration of the related energy-capital costs trade-offs.

8.6.3 Objective Function

The total batch costs (*TBCs*) account, at a batch level, for the operational costs (utility consumption costs, and *HEX* cleaning costs in case of repiped *HEX* across time slices) and the capital costs (M_{pp} process-to-process *HEX* areas, M_{pu} utility *HEXs*, valves for *HEX* resequencing, repiping and cleaning) [41]:

$$TBCs = a_B \cdot \left(\sum_{m=1}^{M_{pp}} CF_{xt\,m}(A_{ppO\,m}) + \sum_{m=1}^{M_{pu}} CF_{xt\,m}(A_{puO\,m}) + V \cdot C_v \right) + \sum_{l=1}^{L} \Delta t_l \cdot \left(c_{cu} \cdot \sum_{i=1}^{I} \dot{Q}_{cu\,i,l} + c_{hu} \cdot \sum_{j=1}^{J} \dot{Q}_{hu\,j,l} \right) + \sum_{repipe} CC_{pa \Rightarrow pb} \tag{8-1}$$

where:

- a_B is the pay-off factor per batch(refer to Section 3.3);
- $CF_{xt\,m}(A_{ppO\,m})$ gives the capital cost of the area $A_{ppO\,m}$ of process-to-process match m of the overall match structure (cost function $CF_{xt\,m}$ for *HEX* type $xt\,m$ specified for this match);
- $CF_{xt\,m}(A_{puO\,m})$ gives the capital cost of the area $A_{puO\,m}$ of process-utility match m of the overall match structure (cost function $CF_{xt\,m}$ for *HEX* type $xt\,m$ specified for this match);
- $V \cdot C_v$ is the capital cost of V valves of unit cost C_v;
- Δt_l is the duration of time slice l ($l : 1 .. L$);
- c_{cu} and c_{hu} are the unit cost of cold utility and the unit cost of hot utility, respectively;
- $\dot{Q}_{cu\,i,l}$ and $\dot{Q}_{hu\,j,l}$ are the cold utility duty required on hot stream i during time slice l, and the hot utility duty required on cold stream j during time slice l, respectively;

41. From a practical standpoint, the piping costs should also be accounted in the *TBCs*, otherwise the actually cost-optimal *HENs* may be overlooked by the optimization.

- $CC_{pa => pb}$ represents the cleaning costs needed for repiping one side of an *HEX* from process stream a to process stream b; the cleaning costs should include operational costs (cleaning agents, energy, labour, etc.) as well as the amortization of the required cleaning-in-place system, valves, etc. The summation concerns all individual repipe changes which occur during a batch cycle and which require adequate cleaning.

8.7 Summary & Further Work

Key issues for the design of optimum direct batch *HENs* have been identified and analysed.

The analysis of the constraints restricting the structural changes (by repipe and/or resequence of the *HEX* matches) during a batch cycle results in a methodology to classify and specify the different types of constraints (thermo-physical compatibility, chemical compatibility, schedule related constraints). These constraints are expected to sufficiently restrict the number of possible slice-wise match structures for the exhaustive evaluation and comparison of the various ways of operating a *HEN* over a batch cycle to be performed. This allows a top-down approach, in which an overall match structure is first postulated and then derived into slice-wise match structures, to be applied [42].

The insight into the problem of cost-optimum re-use of a given *HEN* across time slices has allowed the proposal of a practice-oriented design & optimization strategy based on genetic algorithms. The optimization scheme includes two levels and ensures the full segregation of decision variables into structural and parametric variables : the upper level is concerned with the search for an optimal match structure (the number of matches being specified *a priori* by the user), while at the lower level, the optimization of the match areas to be installed and of the optimal operation of these matches across time slices is addressed.

The proposed approach needs to be implemented and tested to verify that it meets the goal stated for the optimization of direct batch *HENs*; the confidence in the capability of the *GA* to address this type of problem also arises from the experience gained from the *GA* optimization of indirect heat recovery schemes (refer to Chapters 5 and 6 of Part II). By extension, the approach may also be applied to the design of flexible continuous *HENs* addressed by the *MBC* methodology of *Jones* (1991) [43].

42. Compared to the bottom-up approach applied by heuristic design method, the top-down approach provides with a framework within which the problem is more clearly defined, and can be tackled in a more systematic manner.

While the *GA* technique is well suited for the optimization of the *HEN* structure, the *GA* based parametric optimization remains open to questions, since a mathematical model for this problem has not been written yet. In spite of the required computing time, the proposed *GA* solution strategy definitely presents the following advantages :

- a single overall, or a match-wise ΔT_{min}, does not need to be specified, allowing in principle for the extensive exploration of the energy-capital costs trade-off of each match (a feature required for this type of problem);
- the robustness of the *GA* makes the approach essentially insensitive to the type of non-linearities which may be present (or introduced later) in the model (e.g. *if ... then ... else* decisions for *HEX* costs functions defined on several size ranges);
- at both the upper and the lower levels, a significant part of the calculations can be achieved in parallel; this feature provides with a useful room for manoeuvre to keep control of the computing time;
- the approach delivers several good *HENs*, instead of the "single best";
- each lower-level optimization returns feasible and optimized solutions for the considered overall match structure.

For completeness, the following potential limitations of the approach are to be mentioned :

- the combinatorial complexity associated with the repipe and/or resequence opportunities could in some instances [44] become hardly manageable, so that guidelines or heuristics rules are needed to restrict the number of slice-wise match structures to be evaluated. But the method can easily incorporate such rules inside the optimization, which is not the case of mathematical based approaches;
- even when resorting to parallel computing, the need to cut down the computing time may limit the size [45] of the processes which can efficiently be considered. The number of time slices, the number of active streams within each time slice,

43. And, of course, to the design of a continuous *HEN* featuring only one time slice (or base case), provided that no stream split exists.
44. The possible number of modified slice-wise match structures significantly depends on the overall match structure evaluated.
45. In this context, the size (or complexity) of a process is not only related to the number of streams and the number of matches to place, but also significantly depends on the time dimension of the process (number of time slices, schedule of the streams). If the simultaneity of the streams is high, a significant proportion of the matches will be operated during each time slice, resulting in both a large number of active area fractions to be optimized and a potentially large number of modified slice-wise match structures to consider.

and the number of matches are foreseen to be key figures, but experience is lacking with respect to their implication for the required *CPU*-time issues;

- the proposed approach should be adapted to support stream splitting.

The proposed approach comes with sound foundations, but further work remains to be done :

- ♦ constraints on repipe and resequence opportunities : the concepts and guidelines developed in this work should be validated in actual process conditions and be improved;
- ♦ derivation of the modified slice-wise structures : a systematic way to derive these match structures must be developed. Furthermore, a method for the analysis of the structures is needed to identify unpromising structures. This is also a challenging aspect of the internal representation of the match structures within the calculation model;
- ♦ coding convention to be used by the *GA* : the suitable coding convention for the overall match structure depends on the type of *GA* to be used for the structural optimization and on the definition of the crossover operator. The generation of meaningful structures and the capability to preserve beneficial matches are also concerned.

As already highlighted, one of the main drawbacks of the direct heat integration is the sensitivity to inevitable variations of schedule. This important aspect is not addressed by the proposed *GA* based optimization; a sensitivity analysis to schedule variations has to be performed *a posteriori* for the various *HEN* solutions provided, and hopefully some *HEN* reasonably immune to schedule variations might be identified. It could be possible to take these issues into account during the optimization process by specifying forbidden matches, provided that a methodology is developed to identify the critical matches with respect to schedule variations.

In order for the *GA* synthesis approach to be robust and generally suitable for batch processes, the proposed method should be extended to address mixed direct-indirect heat recovery networks. Such an extension obviously requires further analysis work.

Part IV

CONCLUSIONS

Chapter 9

CONCLUSIONS

This work has addressed the indirect heat integration (i.e. resorting to intermediate heat storage) and the direct heat integration (i.e. heat exchanges between coexisting process streams) of batch processes. Tools and methods for the targeting of these two limiting cases of heat integration are proposed, and are completed by the development and the application of an automatic design & optimization framework using the *Struggle* genetic algorithm (*GA*). Only grassroot design problems are addressed.

Further work towards mixed direct-indirect heat integration is suggested in Appendix I.

9.1 Main Contributions Achieved for Indirect Heat Integration

- On the basis of the so-called vertical model assumption, a graphical procedure has been developed to determine the minimum number of heat storage units (*HSUs*) and their assignment ranges as a function of the amount of heat recovery (*HR*). It combines the time average model (*TAM*) energy composites with the discrete effects of the supply temperature of the process streams.
  The main benefit of the graphical procedure is to provide insight into the links between the set of streams to be heat integrated, the heat recovery, the minimum number of HSUs, and the constraints set on the operating temperature of HSUs. It allows the screening of opportunities to avoid intermediate HSUs by cascading process streams, as revealed by a slice-wise instead of a stream-wise analysis of the supply temperature.
- The vertical model assumption also allows a straightforward calculation of first order approximations of indirect heat recovery schemes (*IHRSs*) suitable for targeting purposes. The total batch costs (*TBCs*) versus heat recovery (*HR*) diagram has been proposed to present the corresponding indirect heat recovery

schemes (*IHRS*) solutions.

The validity of this targeting approach has been established on a simple example process; a deviation of a few percents has been observed with respect to the best solutions obtained by GA optimization. The sub-optimality of the delivered solutions arises from the vertical model itself, which cannot properly explore the HSU capacity - HEX area costs trade-off (an optimal exploitation of this trade-off effect results in significantly lower HSU capacities at the expense of slightly larger heat transfer area - but the actual effect depends on the considered process).

- A *GA* based *IHRS* synthesis framework has been developed and extensively tested. It includes practice-relevant *IHRS* models for closed (standard) as well as for *open heat storage systems* [1]. Their application on a brewery process which had already been subject to a detailed analysis by another author results in the following essential conclusions.

  Optimization runs and more theoretical analysis work have provided understanding of the observed shortcomings (low heat recovery, insufficient preservation of population diversity, slow convergence). The developed improvements of the optimization strategy (preliminary phase of HR maximization, account of structural (discrete) variables in the distance function, two-levels optimization strategy) efficiently solve these problems. It is now established that Struggle ensures a robust and efficient parametric optimization, provided that a two-levels optimization scheme is applied, in which the upper level addresses the optimization of all structural variables (segregation of discrete and continuous variables). This condition results from the difficulty to mix discontinuous (structural) variables and continuous (parametric) variables in the distance function, unless the number of possible structures is much smaller than the population size.

  With these improvements, the delivered solutions for closed storage IHRSs are as good as state-of-the-art solutions developed using a combinatorial method, followed by a post-optimization requiring designer's interaction. The capability of a passive technique presently used to help the GA explore opportunities to avoid connections to intermediate HSUs is actually too limited; a closer control on the match structure and the full segregation of variables are achieved by the proposed extended IHRS model. The practical relevance of the models may easily be further increased by taking into account additional factors such as the piping costs, heuristic based or if ... then ... else decisions, etc., without detrimental effect on the GA optimization.

  Optimization results demonstrate that the open storage IHRS model is a vital alternative for the indirect heat integration of processes found in the food & beverage industries which include significant process water streams; compared to closed storage IHRSs, both a significant decrease of the TBCs and a large increase of the HR may be obtained.

1. In such a *IHRS* model, the storage fluid is a process fluid (most generally process water) which enters the storage system, is heated (or cooled) and leaves the *HSUs* whenever these process streams are required.

It has further been verified that, in order for the solutions to be realistic, the brewery process must be optimized over a period of one week instead of over one batch cycle time. Considering the significant differences observed (in all respects) between these two cases, short-cut calculation methods to extrapolate to one week operation solutions obtained on a batch cycle time basis are not suitable.

- Within the *IHRS* models, systematic procedures for the minimization of the utility consumption required to restore the mass balance of *HSUs* have been developed. An analogy between mass imbalances and the *Grand Composite Curve* has been drawn and resulted in a systematic procedure to calculate the optimal *HSU* mass rebalance contributions to be achieved by mixing of storage fluid. Moreover, for the open storage IHRS model, another procedure provides a near-optimal scheduling of the *HSU* mass rebalance contributions to achieve feasible operation at lowest utility costs.
  The procedures take all possible cases (configurations) into account and work successfully whatever the actual number of HSUs is.

- In addition to the brewery process analysed in this work, a preliminary heat integration study of grassroot multi-purpose batch plants in the pharma industry has been achieved. Possibilities and limitations of the proposed *IHRS* models have been identified.
  This analysis indicates that the fixed-temperature/variable mass HSUs do not provide advantages over a mixed temperature HSU in case of a significant proportion of non-flowing streams. Tight composites, long batch periods, low spacial and temporal energy intensities, expensive heat transfer materials, and the trade-off between heat recovery and the cooling/heating rates and times are other features of these processes. The piping costs of the heat recovery networks (depending on the layout of the plant) and the costs of additional controls valves, may not be neglected.

- The presently excessive *CPU*-time needed to achieve an optimization in the whole structural solution domain is due to the interpreted nature of the *Matlab* code of the models.
  A compilation of the code or recoding in C++ will allow speed-up factors large enough to achieve the same optimization in a couple of hours. A targeting stage using the methods developed in this work also helps to restrict to promising search domains.

More details on the methodological aspects of the developed tools & methods may be found in Section 4.6 (targeting) and Section 5.6 (*GA* based synthesis framework), while extended conclusions on their validity and practical relevance are given in Section 6.5.

9.2 Main Contributions Achieved for Direct Heat Integration

The major issues involved in direct batch *HENs* have been analysed, allowing a two-levels *GA* based synthesis approach meeting the required segregation of decision variables to be developed. The upper level is concerned with the search for an optimal match structure (the upper bound on the number of matches being specified *a priori* by the user), while at the lower level, the optimization of the match areas to be installed and of the optimal operation (i.e. factor of active area) of these matches across time slices is achieved.

- Key practical constraints (thermo-physical compatibility, chemical compatibility, schedule related constraints) restricting the structural changes by repipe or resequence of *HEX* units across time slices have been identified and a structured approach to specify these constraints has been proposed.
  These constraints are expected to sufficiently restrict the number of possible slice-wise match structures [2] *for the exhaustive evaluation and comparison of the various ways of operating a HEN over a batch cycle to be performed. This allows a top-down approach, in which an overall match structure is first postulated and then derived into slice-wise match structures, to be applied* [3].
- The problem of optimal operation of an existing *HEN* across time slices has been stated.
  A GA driven parametric optimization of the fractions of active area uses an existing procedure involving matrix inversion for calculating the temperature of a HEN given its structure and the HEX areas. Apart from the known advantages of GA based optimization (e.g. robustness, multi-solutions), the proposed approach allows an extensive exploration of the energy-capital costs trade-offs of each match, since a single overall, or a match-wise ΔT_{min} *does not need to be specified* [4].
- The developed approach has two types of limitations :
  1. streams splitting is not accounted for yet (the calculation method resorting to matrix inversion required fixed heat capacity flowrates);
  2. combinatorial difficulties and/or excessive CPU-time may be encountered in case of insufficiently restricted resequence or repipe opportunities

2. I.e. the particularization of the overall match structure to a given time slice, for which all matches featuring at least one inactive stream are left out.
3. Compared to the bottom-up approach applied by heuristic design method, the top-down approach provides a framework within which the problem is more clearly defined, and can be tackled in a more systematic manner.
4. This feature, which appears to be essential for optimally re-using excess *HEX* area across time slices, is generally not present in existing HEN synthesis methods.

More details on the proposed *GA* based synthesis of direct batch *HENs* and on further work needed may be found in Section 8.7.

Part V

APPENDICES

Appendix A

CASE STUDIES DATA

A.1 Example Process *EP-1*

Example process *EP-1* is a simple imaginary process originally set up for testing the capabilities of the *multiple base cases* (*MBC*) methodology (*Jones*, 1991) to target and design direct heat exchanger networks for batch processes (refer to Chapter 7). Therefore *EP-1* is not provided with a process flowsheet.

The data relevant to *EP-1* are summarized in **Table A-1**. The schedule of the process streams is sketched on **Figure A-1**. For the targeting and design of direct

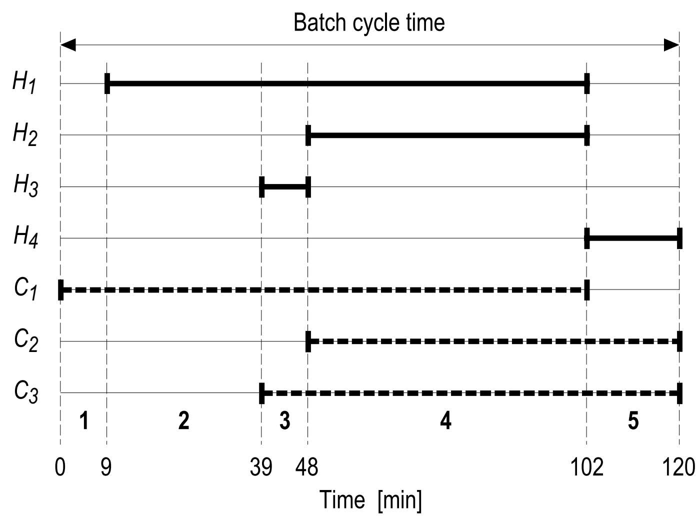


Figure A-1 Schedule of the *EP-1* process streams and corresponding time slices (one batch cycle time).

batch *HENs* (Chapter 7), unlike all other cases, the two hot utilities HU_1 and HU_2

Stream Name	T supply [°C]	T target [°C]	CP [kW/°C]	Heat Rate [kW]	Heat [kWh/bat.]	t start [min]	t stop [min]	h [W/m²°C]
C1	25	100	1	-75	-127.5	0	102	1000
C2	130	180	3	-150	-180	48	120	1000
C3	80	105	5	-125	-168.75	39	120	1000
H1	135	15	1.1	132	204.6	9	102	1000
H2	100	95	20	100	90	48	102	1000
H3	165	125	3.5	140	21	39	48	1000
H4	165	125	3.5	140	42	102	120	1000

Utility Name	T in [°C]	T out [°C]	t start [min]	t stop [min]	h [W/m²°C]	Unit Cost [CHF/kWh]
HU	191	190	0	120	1000	0.08
CU	10	11	0	120	1000	0.005
HU1	191	190	0	48	1000	0.08
HU2	116	115	48	120	1000	0.08

Storage Fluid	T SF min [°C]	T SF max [°C]	Spec. Heat [kJ/kg°C]	Density [kg/m³]
Water	2	135	4.185	1000

Cycle Time [min]	Nb. Batch/Year [batch/year]	Pay-off Period [year]	Interest Rate [–]	Annuity Factor [–/year]
0 –> 120	2000	5	0.1	0.2638

HEX cost : $C_X = C_{OX} + C_{rX} \cdot \left(\frac{A}{A_r}\right)^{m_X}$

HSU cost : $C_S = C_{OS} + C_{rS} \cdot \left(\frac{V}{V_r}\right)^{m_S}$

C_{OX} [CHF]	C_{rX} [CHF]	A_r [m²]	m_X [–]
0	40000	100	0.71

C_{OS} [CHF]	C_{rS} [CHF]	V_r [m³]	m_S [–]
0	150000	100	0.71

Table A-1 Data of the example process *EP-1*.

have been considered instead of *HU*, as indicated in Table A-1. Nevertheless, the time slice composites of **Figure A-2** are drawn with *HU* only.

The following additional features and comments apply :

- the set of process streams defined in Table A-1 is actually not representing a batch, but the streams present in the period of analysis (i.e. a batch cycle time);
- hot streams H_3 and H_4 are supposed to be associated with the same equipment (possible since H_3 and H_4 do not overlap in time). In other words, a heat exchanger on H_3 can be re-used on H_4. Furthermore, H_3 and H_4 actually

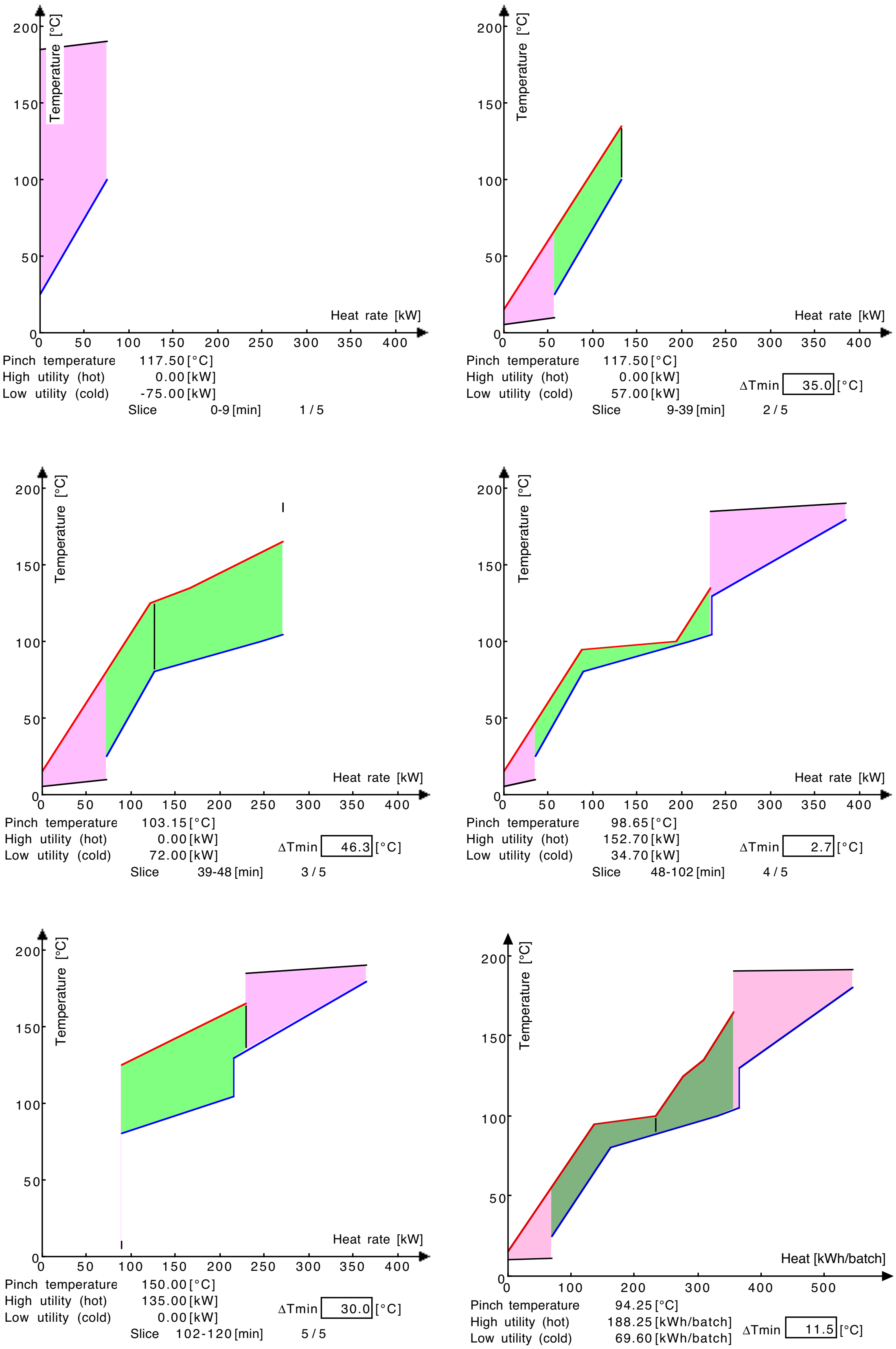


Figure A-2 Time slice and *TAM* composite curves of example process *EP-1*.

feature the same properties so that they can be considered as a single stream present during several time periods;

- the streams and their schedule have been selected so that the process includes time slices of significantly different durations, and time slice composite curves which features large differences with respect to their heat balance and their pinch temperature (see Figure A-2). These features have been identified as a prerequisite for checking e.g. the variability of the optimal slice-wise pinches $\Delta T_{min\ l}$, the effect of the re-use of *HEX* units across time slices, and the opportunity for an indirect heat integration.

A.2 Example Process *EP-2*

Process *EP-2* is an imaginary process used for illustrating the concepts proposed in Chapter 8 and the guidelines described in Appendix B. **Table A-2** provides the list

Stream Name	Fluid & Properties	t start 1) [min]	t stop 1) [min]	Location
H1	fluid A, liquid, low viscosity, high density	640	300	**1**
H2	fluid A, liquid, low viscosity, high density	420	620	**1**
H3	fluid B, liquid, high viscosity, middle density	90	340	2
H4	contaminated waste fluid C, gas (heat recovery)	300	640	3
H5	contaminated waste fluid A, liquid (heat recovery)	300	540	4
C1	fluid D, liquid, low viscosity, high density	150	300	5
C2	fluid D, liquid, high pressure, high temperature	150	620	6
C3	fluid C, gas	640	300	7
C4	fluid B + water, liquid, high viscosity, middle density	420	620	8
C5	fluid F in evaporation	150	540	9

Notes: 1) Batch cycle: 0 - 720 minutes

Table A-2 Stream data of example process *EP-2*.

of streams and **Figure A-3** sketches their schedule. Temperature and heat capacity flowrate informations are not included since they are actually not required for the illustration purpose.

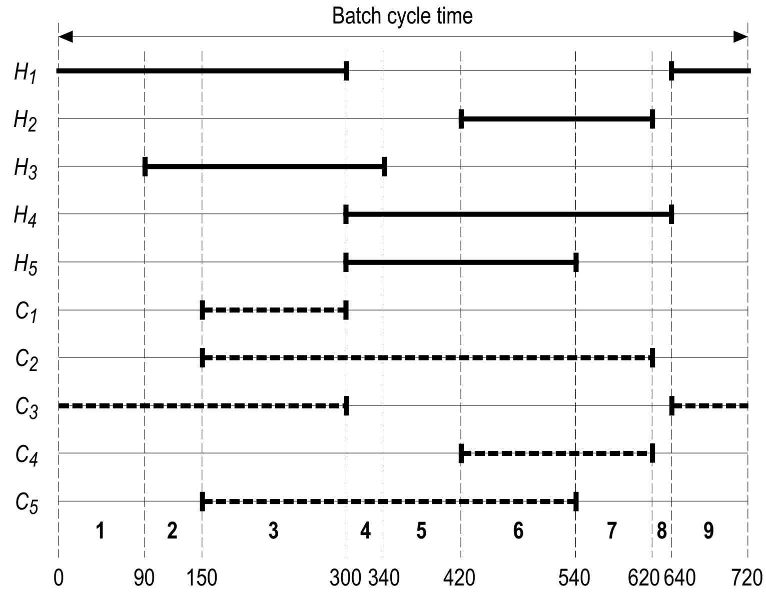


Figure A-3 Schedule of the *EP-2* process streams (one batch cycle).

A.3 Process *EP-3*

Process *EP-3* is a brewing process studied and reported by *Mikkelsen* (1998). The actual flowsheet of the process is not provided; however, from the thermal processes standpoint, the brewing is quite standard so that the brewing process at the *Brasserie du Cardinal* described later in Section A.4 may be considered as a reliable alternative source of supplementary information regarding this issue.

The data relevant to *EP-3* are summarized in **Table A-3**. In repeated operation, the schedule of the process streams within a repetition period is sketched on **Figure A-4**. The following additional features and comments apply here :

- hot streams H_{10}, H_{11} and H_{12} are heat recovery opportunities (wort vapours released during wort boiling) and not process streams, meaning that their final temperature can take any value within the range $[T_{Target}, T_{Supply}]$;
- H_{12} features the same schedule as H_{11} and actually represents the condensate cooling, H_{11} corresponding to the condensation. These two streams may be modelled as a single stream $H_{11/12}$ (this is done e.g. for the open storage system optimization reported in Sub-section 6.3.2) unless one would like to be able to separately decide to use H_{11} and/or H_{12};
- the boiling of the wort (refer to Section A.4) is not included in the list of cold streams since the required temperature level cannot be met by indirect heat

Stream Name	T supply [°C]	T target [°C]	M [kg]	c p [kJ/kg°C]	Heat Rate [kW]	Heat [kWh/bat.]	t start [min]	t stop [min]	h [W/m²°C]
C1	8	51	30000	3.5	-1254	-1254	0	60	4000
C2	51	70	30000	3.5	-2217	-554	60	75	4000
C3	70	100	30000	3.5	-1750	-875	90	120	4000
C4	8	37	38000	3.8	-2326	-1163	75	105	4000
C5	61	67	67200	3.7	-2486	-414	120	130	4000
C6	67	76	67200	3.7	-3730	-622	190	200	4000
C7	8	76	64000	4.186	-5060	-5060	345	405	4000
C8	74	100	117200	3.9	-3301	-3301	345	405	4000
C13	30	70	151200	4.186	-2110	-7032	0	200	4000
H9	98	11	105200	3.9	4958	9915	540	660	4000
H10	101	100	800	2257	1505	502	120	140	4000
H11	101	100	12000	2257	5016	7523	405	495	4000
H12	100	30	12000	4.186	651	977	405	495	4000

Utility Name	T in [°C]	T out [°C]	CP [kW/°C]	h [W/m²°C]	Unit Cost [DKK/kWh]
HU	175	174	–	4000	0.09
CU	1	2	–	4000	0.0612

Storage Fluid	T SF min [°C]	T SF max [°C]	Spec. Heat [kJ/kg°C]	Density [kg/m³]
Water	2	100	4.186	1000

Cycle Time [min]	Nb. Batch/Year [batch/year]	Pay-off Period [year]	Interest Rate [–]	Annuity Factor [–/year]
200	1500	10	0.05	0.1295

HEX cost : $C_X = C_{OX} + C_{OX\ circ} \cdot N_{circ} + C_{rX} \cdot \left(\frac{A}{A_r}\right)^{m_X}$

A [m²]	C_{OX} [DKK]	$C_{OX\ circ}$ [DKK]	C_{rX} [DKK]	A_r [m²]	m_X [–]
Cost function used by Mikkelsen :					
< 20	75600	0	10224	1	1
≥ 20	180000	0	4968	1	1
Cost function used in this work :					
< 20	65600	10000	10224	1	1
≥ 20	170000	10000	4968	1	1

HSU cost : $C_S = C_{OS} + C_{rS} \cdot \left(\frac{V}{V_r}\right)^{m_S}$

V [m³]	C_{OS} [DKK]	C_{rS} [DKK]	V_r [m³]	m_S [–]
< 100	0	22800	1	0.78
≥ 100	0	63000	1	0.5593

Table A-3 Data of the simple brewery process *EP-3* (*Mikkelsen*, 1998).

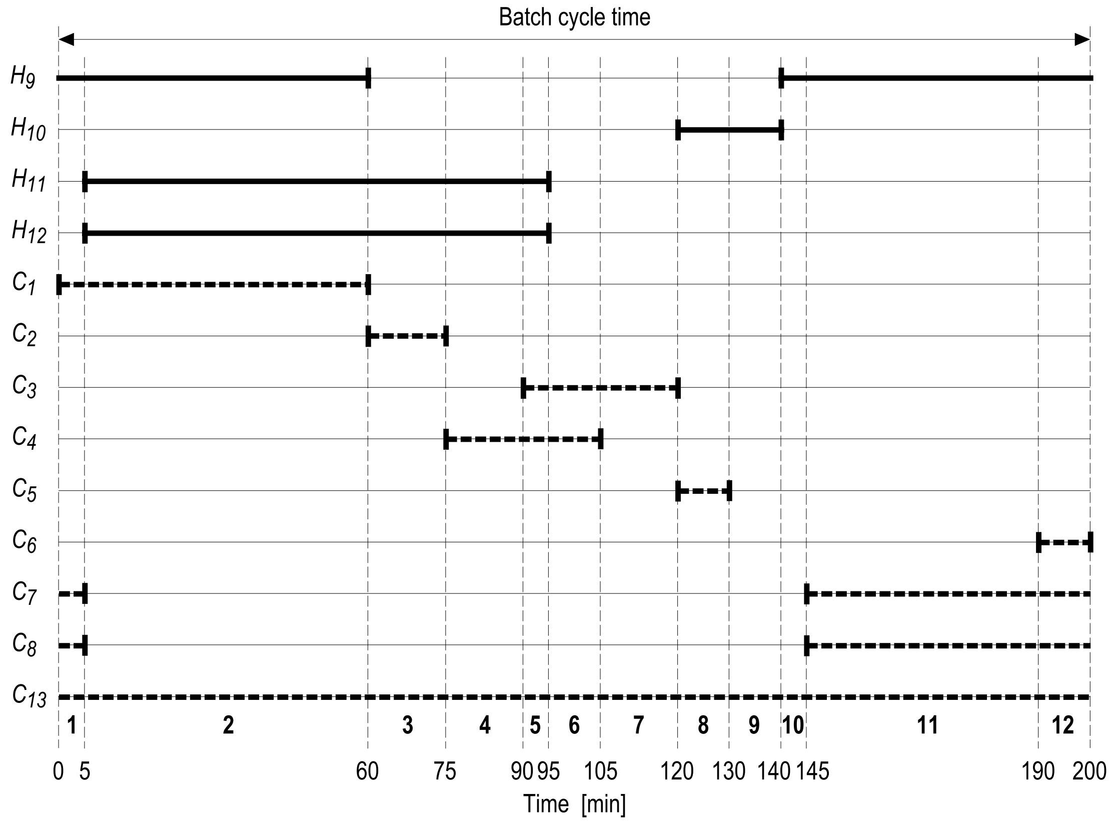


Figure A-4 Schedule of the *EP-3* process streams and corresponding time slices (one batch cycle).

integration anyway (it would make sense if hot utility would be accumulated, e.g. as superheated water, instead of being directly supplied, or in case of mechanical vapour recompression);

- the *TAM* composites curves (average heat rate over a batch cycle) including all 13 streams are represented on **Figure A-5** for an arbitrary pinch $\Delta T_{min} = 10\ °C$;
- several cold streams (e.g. C_2, C_3, C_5 and C_6) are actually non-flowing streams (in-vessel heating) with a prescribed temperature-time profile and should not be assumed to be like flowing streams (see Section A.4). For the closed storage system including 3 *HSUs*, this turns out *a posteriori* not to be an issue since even with this most optimistic assumption, the supply temperatures of these streams are already enough constraining to be excluded from the optimum heat integration solution (see Sub-section 6.3.1). However, the open storage *IHRS* solution described in Sub-section 6.3.2 integrates C_2 and a more rigorous modelization should be adopted (e.g. time discretization allowed by the improved *IHRS* model, refer to Sub-section 3.2.1);

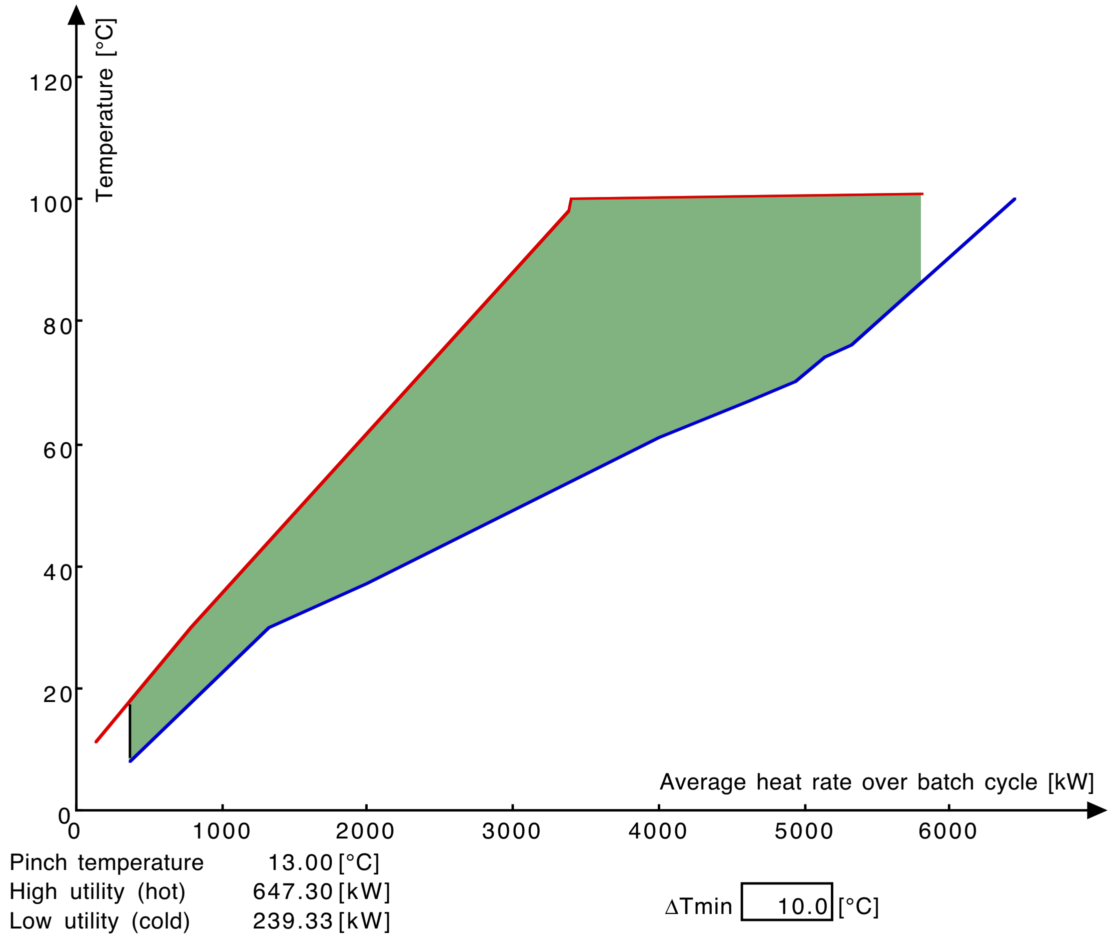


Figure A-5 *TAM* composites of brewery process *EP-3* (all 13 streams included).

- the *HEX* cost functions used in the *GA* optimization models include a fixed cost per circuit unit (inlet-outlet headers) to account for the total area being split in several units with connections to intermediate *HSUs* (refer to Sub-section 5.3.2); for a *HEX* made up of one single unit, the capital cost returned by both costs functions is identical.

A.4 Process *EP-4*

Process *EP-4* represents the brewing process of a lager beer at the *Brasserie du Cardinal* (*Krummenacher*, 1992, 1995); hot water needs outside the brewhouse are also included.

The flowsheet of the brewing process and the state of the main equipment units (Gantt Chart) for one brewing batch (i.e. one brew) are depicted on **Figure A-6**. The numerical data relevant to *EP-4* are summarized in **Table A-4**.

Brewing process streams 160 min batch cycle time	Stream Name	T supply [°C]	T target [°C]	M [kg]	c p [kJ/kg°C]	Heat Rate [kW]	Heat [kWh/bat.]	t start [min]	t stop [min]	h [W/m²°C]
Brewing water heating	C1	15	58.0	34500	4.185	-2112	-1725	12	61	5000
Mash boiler 1st temp. rise	C2	53	61.0	16500	3.7	-1163	-136	67	74	2000
Mash boiler 2nd temp. rise	C3	61	74.5	16500	3.7	-916	-229	86	101	2000
Mash boiler 3rd temp. rise	C4	74.5	98.0	16500	3.7	-1196	-399	118	138	2000
Mash tank 1st temp. rise	C5	53	62.0	33000	3.7	-1145	-305	67	83	2000
Mash tank 2nd temp. rise	C6	62	68.0	33000	3.7	-814	-204	118	133	2000
Sparging water heating	C7	15	76.0	37500	4.185	-1922	-2659	325	408	5000
Wort pre-heating to boil	C8	72	97.5	71500	4.1	-4153	-2076	423	453	3000
Wort boiling (average)	C9	104	105.0	5005	2250	-2157	-3128	463	550	3000
Wort cooling to fermentation	H1	95	7.5	65495	4.1	4303	6527	587	678	3000
Wort vapor condens. &	H2/1	96	95.0	793	2250	2975	496	463	473	3000
sub-cooling (atmos. boil.)	H2/2	95	10.0	793	4.1	461	77	463	473	3000
Wort vapor condens. &	H3/1	103	102.0	919	2250	1914	574	487	505	3000
sub-cooling (press. boil.)	H3/2	102	10.0	919	4.1	321	96	487	505	3000
Wort vapor condens. & sub-	H4/1	96	95.0	3293	2250	2744	2058	505	550	3000
cooling (pres. rel. & atm. boil.)	H4/2	95	10.0	3293	4.1	425	319	505	550	3000

Streams outside brewhouse 5 days a week (Mon-Fri)	Stream Name	T supply [°C]	T target [°C]	M [kg]	c p [kJ/kg°C]	Heat Rate [kW]	Heat [kWh/bat.]	t start [min]	t stop [min]	h [W/m²°C]
Average streams for a 160 min batch cycle model (assuming 30 batches/week)										
Flash-past. post-heating (KEG)	C10b	65	70.0	28060	4.1	-60	-160	0	160	3000
Flash-past. post-heating (bottles)	C11b	65	70.0	20740	4.1	-44	-118	0	160	3000
KEG washing water	C12b	15	80.0	9000	4.185	-255	-680	0	160	5000
Bottling facility washing water	C13b	15	80.0	13500	4.185	-383	-1020	0	160	5000
General hot tap water needs	C14b	15	65.0	4500	4.185	-98	-262	0	160	5000
Average streams for a "macro batch cycle" over 1 week (Mon-Fri 6h-18h) : the five time periods mentioned below apply to each of the 5 streams										
Flash-past. post-heating (KEG)	C10w	65	70.0	841800	4.1	-80	-959	360	1080	3000
Flash-past. post-heating (bottles)	C11w	65	70.0	622200	4.1	-59	-709	1800	2520	3000
KEG washing water	C12w	15	80.0	270000	4.185	-340	-4080	3240	3960	5000
Bottling facility washing water	C13w	15	80.0	405000	4.185	-510	-6121	4680	5400	5000
General hot tap water needs	C14w	15	65.0	135000	4.185	-131	-1569	6120	6840	5000

Table A-4 Stream data of the brewery process *EP-4*.

The main steps of the brewing process may be summarized as follows :

1. brewing water (heated up to 58 °C - stream C_1) and crushed malt are mixed together, forming the so-called mash, and transferred to the mash tank. The resulting mash temperature is about 53 °C;

2. 1/3rd of the mash is transferred to the mash boiler to undergo there a specific temperature-time profile (streams C_2, C_3, C_4), while the remaining 2/3rd in the mash tank are subject to the thermal processes given by streams C_5 and C_6. Mashing ends up with the remixing in the mask tank. These stage-wise thermal processes develop complex bio-chemical reactions to solubilize starch and decompose it into simpler fermentable sugars;

3. the mash is transferred to the lauter tub to separate the spent grains from the liquid, resulting in the wort. After lautering, sparging with water at 76 °C (stream C_7) takes place to dissolve the remaining sugars still present in spent grains;

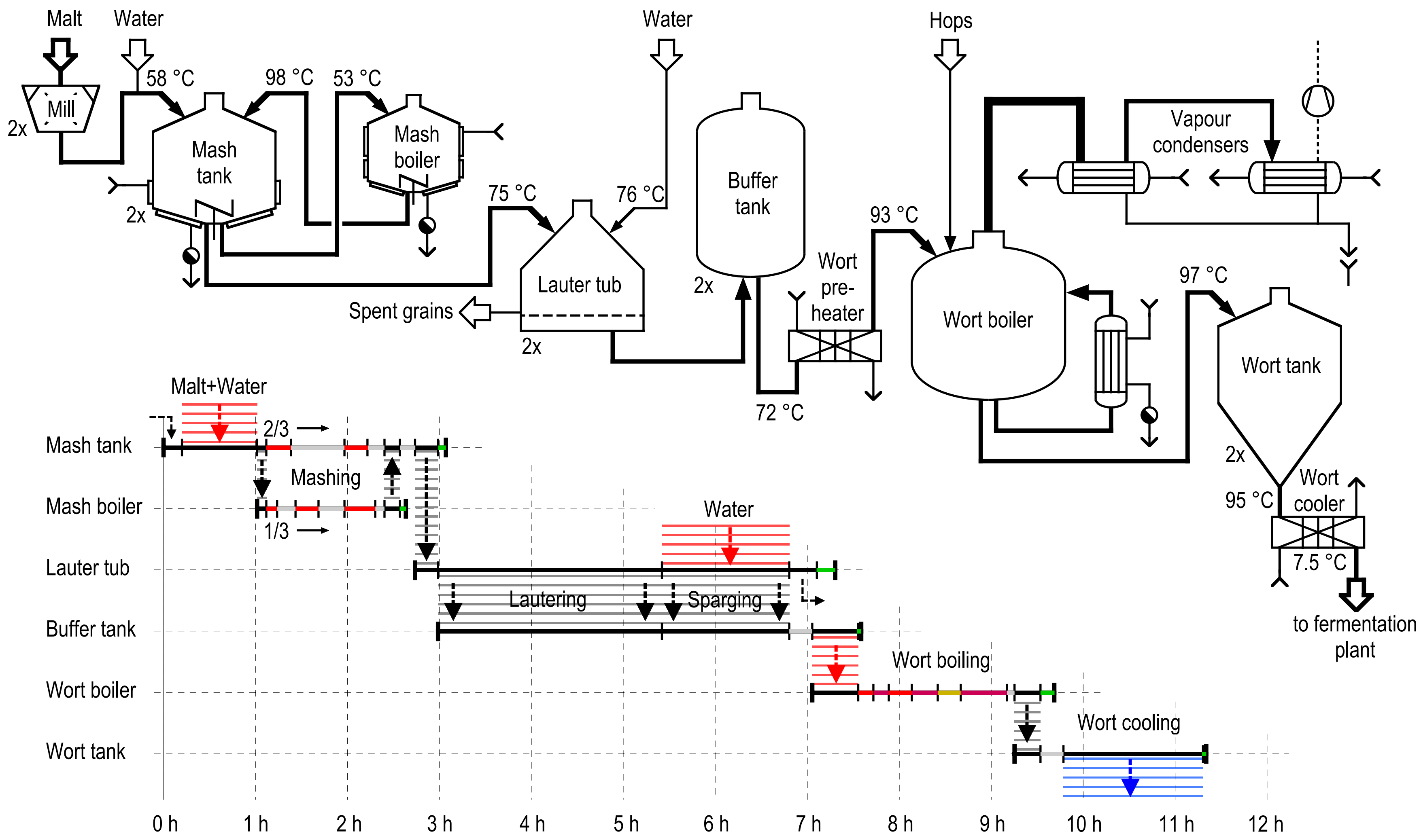


Figure A-6 Flowsheet and Gantt chart of the brewing process *EP-4* (*Brasserie du Cardinal*).

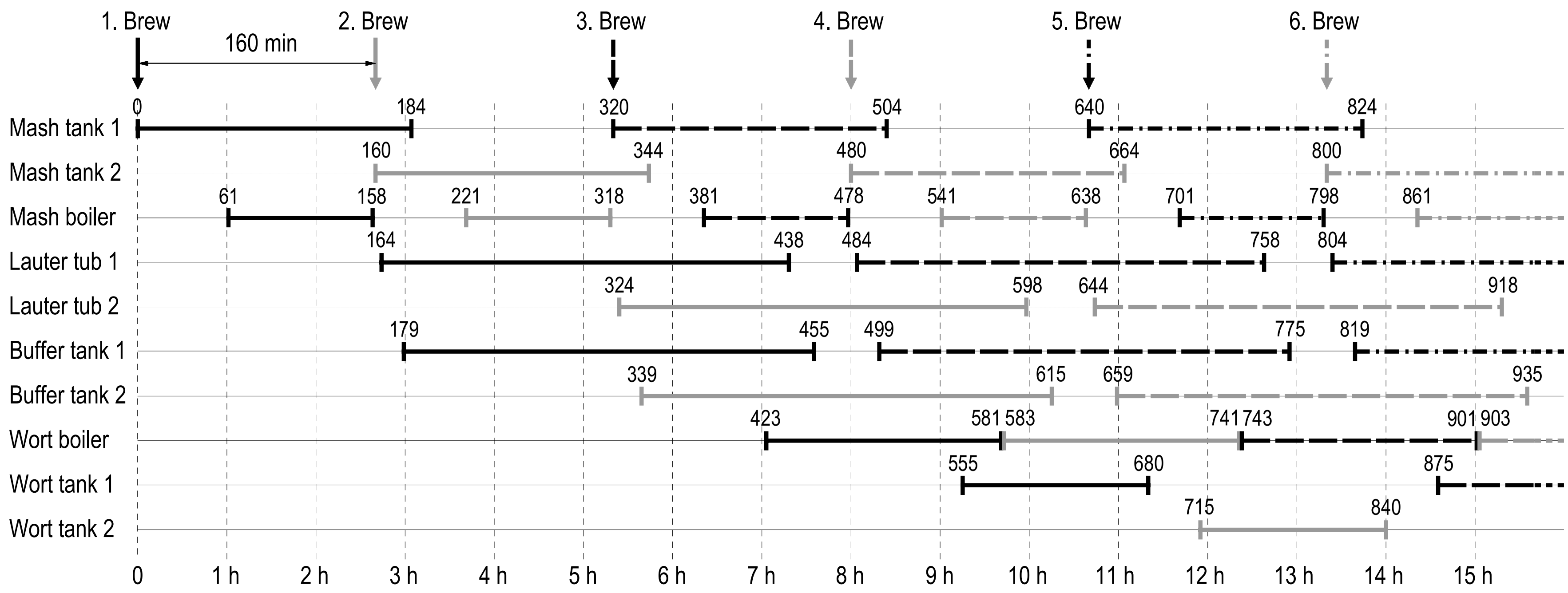


Figure A-7 Gantt chart of brewing process *EP-4* in repeated operation with standard 160 *min* batch cycle.

4. from the buffer tank, the wort is heated up to atmospheric boiling temperature (stream C_8) before being partially evaporated in the wort boiler. About 7 % of the wort are evaporated during boiling, which actually comprises several steps (1. boiling at atmospheric pressure; 2. heating up to pressure boiling; 3. boiling under pressure; 4. pressure release; 5. atmospheric boiling until a specified sugar content is reached). These steps can be modelled by a single average stream C_9 in the context of indirect heat integration because hot utility is required anyway. The high energetic content of wort vapours may be recovered by condensation and cooling (streams H_2, H_3, H_4);

5. the wort is transferred to the wort tank to allow to settle for a while, before being cooled down to 7.5 °C to be prepared for fermentation (stream H_1).

The processing time of one brew takes more than 11 *hours*, but the occupancy of each of the major pieces of equipment is much shorter (see Gantt chart on Figure A-6).

The mash tank, the lauter tub, the buffer tank and the wort tank are actually doubled and work out-of-phase, so that a new batch may be started every 160 *minutes* (batch cycle time) as represented on **Figure A-7**. The single wort boiler becomes the time bottleneck. The equipment units are better used and the production capacity of the brewhouse is increased.

The *TAM* composites of the brewing process, including also streams C_{10} to C_{14}, but excluding C_9, are plotted on **Figure A-8**. The composites curves are similar (in

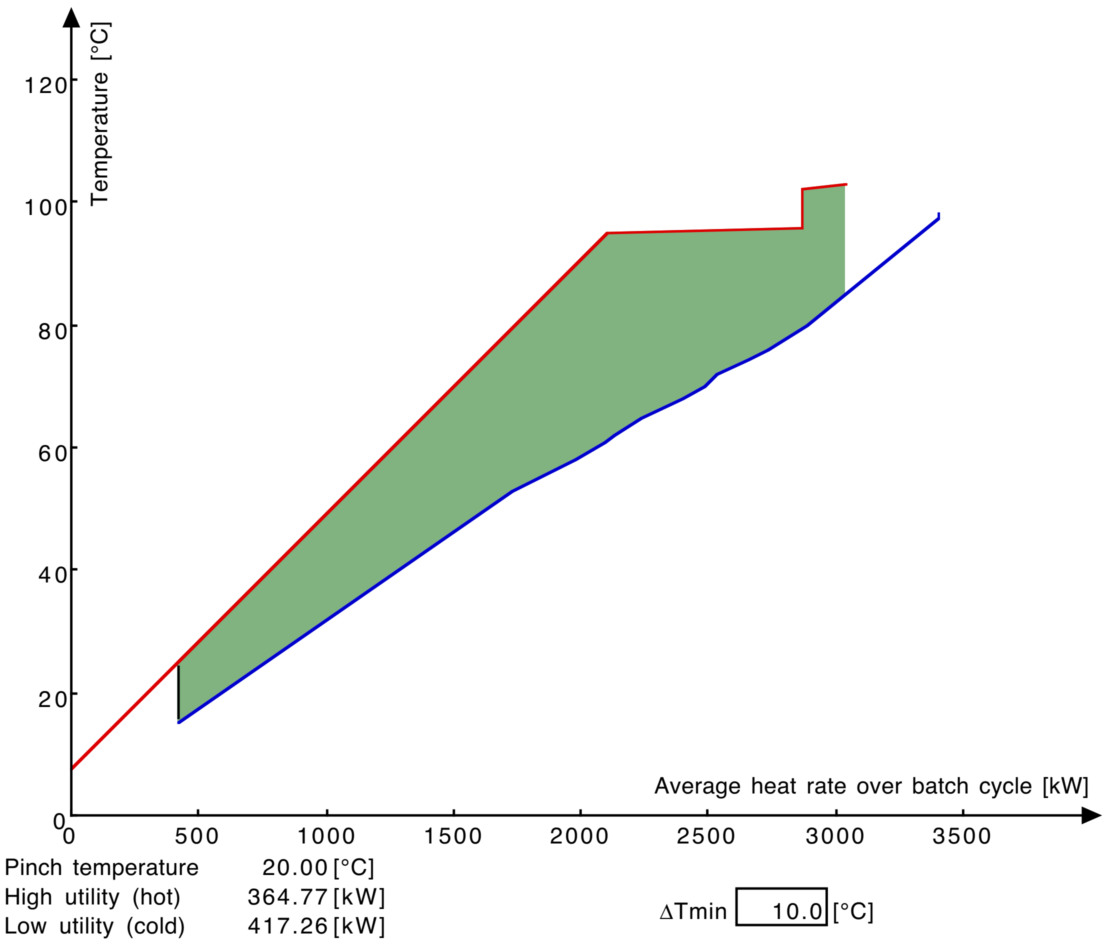


Figure A-8 *TAM* composites curves of *EP-4*.

shape) to that of *EP-3*, and demonstrate that large temperature driving forces are available for the indirect heat integration.

The following additional comments should be considered :

- among cold process streams, C_1, C_7, and C_{10} to C_{14} correspond to heating of process water (process water streams) and amount to a large part of the heating needs potentially supplied by indirect heat integration. According to the stream data extraction rules, non-isothermal mixing of brewing water (stream C_1) and malt should be avoided. However, mixing malt and water first, followed by heating of the mixture, excludes the possibility of preparing brewing water by direct mixing of storage water, the latter solution being probably more interesting (but this statement should be verified);
- streams H_2 to H_4 are non-flowing streams (in-vessel heating) which should not be replaced by corresponding flowing streams, owing to the fact that the temperature-time profiles are needed to develop and control the complex bio-chemical reactions which take place. However, before considering a detailed modelization, it is recommended to first assume that these streams are flowing streams and verify after optimization of this best case, whether these streams are part of the integrated streams or not. If they must be integrated, a more detailed modelization is needed to confirm or invalidate this preliminary result;
- fouling of the wort boiling *HEX* causes significant variations of the schedule : the duration of boiling progressively increases (as a result from the decreased heat rate), and cleaning of the *HEX* has to be carried out after 6 brews, delaying the start of every 7th brew by 30 *minutes* (with respect to the standard cycle time of 160 *minutes*). In addition, unavoidable batch-to-batch variations exist, e.g. because the boiling phase only stops when a specified sugar content has been reached;
- furthermore, considering the start-up and shut-down phases [1] of the brewing, as well as the separate and non-synchronous operation of the kegging and bottling facilities [2], the actual repetition period is one week rather than one batch cycle (160 *min*), or even 6 batch cycles (990 *min*) accounting for fouling. To get realistic optimum *IHRSs* (in particular with respect to the size of *HSUs*), the design/optimization should be performed on one week;
- the significant schedule fluctuations preclude direct heat exchanges between process streams, unless the storage capacity of processing or buffer tanks [3] may be used during idling phases to accumulate process water in anticipation of its

1. The start-up and shut-down phases represent more than 22 *hours* out of about 100 *hours* for a production of 30 brews per week.
2. Unlike brewing, operated with 3 shifts (i.e. 24 h / 24), the bottling and kegging facilities are operated with 1 or 2 shifts, monday to friday.
3. E.g. the mash tanks, which include more than 2 *hours* idling period.

later use. Another possibility consists in increasing the cycle time to 190 *min* for all brews, to avoid the disruption of the cycle time due to the cleaning phase. But the production capacity decreases, and the labour costs and the specific energy consumption most likely increase.

Appendix B

GUIDELINES FOR PROCESS SIMPLIFICATION

Guidelines for reducing the number of time slices to be considered for direct heat integration have been summarized in Sub-section 3.6.4. This Appendix recalls these guidelines, provides examples and presents simple quantitative criteria to identify streams which could be neglected with respect to the definition of time slices.

B.1 General Guidelines

To simplify the schedule of batch processes, consider the following guidelines :

1. eliminate "artificial", meaningless time slices generated by streams not relevant to the process-to-process heat integration (e.g. owing to infeasible temperature driving forces), or by soft streams;
2. identify highly schedule sensitive time slices and suppress them;
3. neglect streams of small duration and/or small heat content;
4. consider simple rescheduling opportunities allowed by existing equipment units (synchronization of streams using available storage capacities of process vessels), as long as the rescheduling is compatible with process requirements.

B.2 Meaningless Time Slices

Meaningless time slices may be identified using the following criteria :

- the obvious preliminary condition is to define the period of analysis (batch cycle) so that either its start or its stop time coincides with the start or stop time of a process stream. In this way, the number of time slices is decreased by one (e.g. consider the schedule of *EP-2* process streams sketched on Figure A-3, where time slices 1 and 9 are actually strictly identical and could be grouped together by selecting another "time window");

- process streams which cannot take part in the process-to-process heat exchanges owing to temperature infeasibilities [1] (irrespective of the time schedule) must be removed from the list of streams defining the time slices;
- if only direct heat exchanges are considered, the above condition applies on a time slice basis as well; the temperature feasibility condition must systematically be checked for each stream responsible for the definition of a time slice. The time slice may be left out if the temperature feasibility condition is not met. For example, considering the schedule of *EP-2* process streams again, it can be seen that stream H_3 is responsible for the definition of time slice 2 and 4; if the supply temperature of H_3 is lower than that of C_3 and/or C_5, time slice 2 and/or 4 may be left out;
- an obvious particular case of the above condition states that any time slice featuring only streams of the same type (hot or cold) is not of interest to the can be ignored for the *HEN* design problem (it simply adds a constant to the total annual costs). This is the case of time slice 8 from the *EP-2* example process;
- the above temperature feasibility condition are even more restrictive for heat recovery streams, whose heat integration is only useful when heat is delivered above the slice-wise pinch (or cooling needed below the slice-wise pinch);
- critical process streams for which the engineer knows at the onset that they need to be supplied by utilities (e.g. for controlability/quality reasons) are also eliminated from the heat integration problem, hence from the definition of the time slices.

B.3 Short Time Slices

Schedule sensitive time slices are mainly concerned with time slices whose "short duration" (relatively to other time slices) is not due to corresponding short duration streams, but rather because a stream appears slightly before another one ceases to exist (or reversely). Assuming a significantly shrunk time scale of *EP-2* for the consistency of the discussion (refer to Figure A-3), time slices 4 and 8 are examples of this kind of "short duration" time slices :

1. I.e any hot process stream whose supply temperature is lower than the lowest supply temperature of cold streams, and any cold process stream whose supply temperature is higher than the highest supply temperature of hot streams.

- time slice 4 is generated by the slightly delayed stop time of stream H_3. From the point of view of H_3, the stop time of H_1, C_1 and C_3, and the start time of H_4 and H_5 are advanced. However, since H_3 is the only stream which time deviates from the other ones, this stream is obviously responsible for the existence of time slice 4, and not the other streams responsible for the early end of time slice 3. In case of schedule variation, stream H_3 could possibly stop earlier (down to the stop time of C_1 and C_3, making the slice 4 to disappear. One could, more likely, also argue that the schedule of any stream among H_1, H_4, H_5, C_1 and C_3 might change, which would introduce a new time slice. Regarding time slice 4, if the effective heat recovery opportunity offered by H_3 during this slice is small (either because of a small duration or of a relatively small heat rate, or because of unfavourable temperature level for heat recovery), one would neglect the part of H_3 during this slice by assuming it is satisfied by cold utility, i.e. time slice 4 would be neglected. The schedule variation of the other streams around the end of time slice 3 is most likely, and this should be solved by utility and utility *HEX* (if not already needed for other slices).
- time slice 8 is defined by streams H_1, H_2, H_4, C_2, C_3 and C_4. Stream H_4 is the only stream present during this slice 8, hence it has to be matched with the cold utility, and the time slice eliminated from the heat integration analysis.

Three problems likely associated with such times slices can be mentioned :

- the high sensitivity to schedule variations which make the calculated heat recovery potential unlikely;
- relatively significant transient effects;
- a low potential heat recovery potential, or more generally low potential costs savings.

Criteria to decide whether a time slice has to be taken into account or can be neglected are therefore needed.

B.4 Quantitative Criteria

Two simple criteria are proposed :

1. a time slice **l** which absolute duration is smaller than a threshold duration should be neglected :

$$\Delta t_{\mathbf{l}} \leq \Delta t_{min} \qquad \textbf{(B-1)}$$

this constraint of minimum duration takes primarily the controllability/ transients effects into account; the threshold duration Δt_{min} value depends on plant and process parameters;

2. for a time slice which satisfies the condition of minimum absolute duration (i.e. $\Delta t_{\mathbf{l}} > \Delta t_{min}$), it remains to be verified that the heat recovery potential associated with the stream(s) which generates it is not too small relatively to other times slices. Various criteria can be formulated, e.g. :

- the relative duration of the time slice, i.e. the ratio of its duration over the batch cycle time, which is very easily calculated. With respect to the contribution to the heat recovery, this criteria implicitly assumes that the rate of heat recovery is almost independent of the time slice, i.e. uniform over the batch cycle;
- a more detailed estimation of the benefit to cost ratio associated with the stream(s) responsible for the definition of this slice; it accounts for the ability of this slice (more precisely the stream(s) which defines it) to significantly contribute to the objective function. Such a criteria may be more robust, but (if it is to be used before *MBC* supertargeting) is still plagued with fundamental limitations (such as the by-default constant ΔT_{min} assumption and the inability to account for the re-use of *HEX* units and the related capital savings).

A simple criteria is proposed, which is based on the criteria first mentioned (i.e. the relative duration of the time slice) but modified to account for the relative contribution to overall heat recovery :

$$RB_{\mathbf{p},\mathbf{l}} = \left.\frac{\Delta t_{\mathbf{l}}}{\sum_{l} \Delta t_{l}} \cdot \frac{\Delta HR_{\mathbf{p},\mathbf{l}}}{\sum_{l} HR_{l}}\right|_{\Delta Tmin_{l} = Cte} \tag{B-2}$$

where:

- $RB_{\mathbf{p},\mathbf{l}}$ is the relative benefit of considering the contribution of process stream $\mathbf{p}$, responsible for the definition of time slice $\mathbf{l}$, in the heat integration;
- $\Delta t_{\mathbf{l}}$ is the duration of time slice $\mathbf{l}$;
- $\sum_{l} \Delta t_{l}$ is the period of analysis, i.e. the batch cycle time;
- $\Delta HR_{\mathbf{p},\mathbf{l}}$ is the contribution of process stream $\mathbf{p}$, during time slice $\mathbf{l}$, to the heat recovery. $\Delta HR_{\mathbf{p},\mathbf{l}} = \Delta HR_{\mathbf{l}} - \Delta HR_{p \neq \mathbf{p},\mathbf{l}}$ where $\Delta HR_{\mathbf{l}}$ is the heat recovery contribution of time slice $\mathbf{l}$ with all process streams included, for a given ΔT_{min}, while $\Delta HR_{p \neq \mathbf{p},\mathbf{l}}$ is the heat recovery contribution of time slice $\mathbf{l}$ with all process streams except stream $\mathbf{p}$;

- $\sum_{l} HR_l$ is the overall heat recovery, with all process streams included, for the period of analysis. The heat recovery of each time slice is obtained with a single ΔT_{min} (e.g. ΔT_{min}=10 °C). A high sensitivity of $RB_{\mathbf{p},\mathbf{l}}$ to the actual ΔT_{min} might indicate a poor confidence in the proposed criteria.

The criteria for "neglecting" time slice $\mathbf{l}$ defined by process stream $\mathbf{p}$ is expressed by:

$$\frac{RB_{\mathbf{p},\mathbf{l}}}{\sum_{l} RB_l} \leq \varepsilon_{RB} \tag{B-3}$$

where:

- $RB_{\mathbf{p},\mathbf{l}}$ is defined by Equation B-2 above;
- $\sum_{l} RB_l$ is the overall relative benefit of all time slices; individual RB_l are calculated using Equation B-2, but with $\Delta HR_{\mathbf{l}}$ instead of $\Delta HR_{\mathbf{p},\mathbf{l}}$ (i.e. the relative benefit of all process streams in the time slice $\mathbf{l}$);
- ε_{RB} is the relative benefit threshold value (e.g. set at some value in the range 0.02-0.1).

If not a single, but several streams are responsible for the definition of the time slice $\mathbf{l}$, the relative benefit defined by Equation B-2 is evaluated globally for these streams.

Streams of small duration (third category) can also be analysed with the same Equations B-2 and B-3.

B.5 Comments

It is important to clarify what is meant by "neglecting" a time slice on the basis of Equations B-2 and B-3. Neglecting does not mean ignoring what actually happens during this time period, in particular the heat recovery allowed by the streams $p \neq \mathbf{p}$ that exist during this slice and do not define this slice (e.g. streams H_4, H_5, C_2 and C_5 during time slice 4 of the *EP-2* process - Figure A-3). It simply means that stream H_3, which stop time defines time slice 4, should be supplied by the cold utility from time 300 *min* to 340 *min*, and since H_3 does no more define the time 340 *min* as a time when the stream population (for heat recovery) changes, the original time slice

4 disappears and a new, longer time slice from time 300 *min* to time 420 *min* is now defined.

The relative benefit expressed by Equation B-2 accounts for the heat recovery (the contribution which decrease the total costs) and the time needed to recover this heat : the longer the best, since the area (and hence the capital costs) are minimized. It is implicitly assumed that the capital costs associated with heat recovery are uniform, which is generally not the case (because of different temperature driving forces, of *HEX* re-use, etc.) [2].

Although guidelines can be specified, the preliminary simplification of the process schedule requires judgement and there isn't a single right way to make this simplification. Not only small time slices and the streams responsible for these have to be identified, but also potential new time slices due to schedule variations should be anticipated. Note also that in-vessel streams featuring large temperature variations may need to be time segmented and increase the number of time slices.

Depending on the remaining complexity/number of time slices left after a first simplification, a more severe threshold value ε_{RB} might be required.

Another reason to bring back the process schedule to a limited number of "essential" time slices should be mentioned: if small time slices are kept in the specification of the *GA* based synthesis of direct batch *HENs*, this specification is constraining and potentially prevents resequence and/or repipe to take place for "essential" time slices. Eliminating these small time slices can help to find better re-use of *HEX* units. Then, the population of "optimal" solutions provided by the *GA* should be analysed with respect to their additional ability to integrate the previously excluded streams by re-using otherwise unused *HEX* units. Hopefully some solutions will allow this; in the opposite case, the user may decide to include the stream in the heat integration and launch another design/optimization run.

2. If the heat transfer film coefficient features large variations between process streams, it could be introduced as a correction factor in Equations B-2 and B-3.

Appendix C

SYSTEMATIC PROCEDURES FOR OPTIMAL MIXING OF STORAGE FLUID

This Appendix complements Sub-section 5.3.5. and provides a detailed description of the proposed systematic procedures for the optimal mixing of heat storage fluid.

Figure C-1 sketches a case including four *HSUs* and illustrates the problem. To

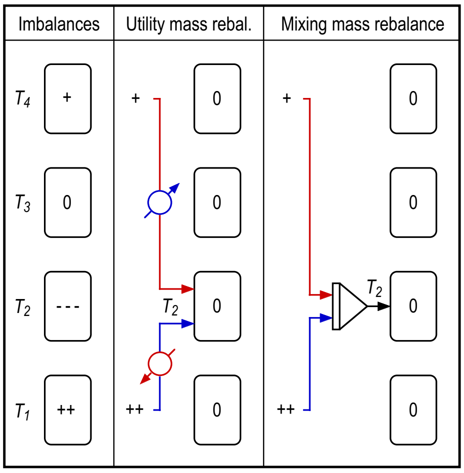


Figure C-1 A 4-*HSUs* system featuring mass imbalances over a cycle : imbalance state prior to any correction (left); restoring the mass balance using utilities (centre); restoring the mass balance by resorting to mixing (right).

keep things simple, the temperatures of *HSUs* are equally distributed (i.e. the temperature difference between two adjacent *HSUs* is equal whatever the *SSs*). This assumption allows to restrict the considerations to mass imbalances only, instead of considering the heat imbalances. On Figure C-1, "+" denotes a unit of mass in excess, "–" represents a unitary default of mass, and 0 a perfect mass balance. The overall mass balance is satisfied in any case because of the mass conservation principle in a closed system, resulting in the $K-1$ independent equality (refer to Sub-section 3.4.3).

Instead of resorting to both utility heating and cooling (central column of Figure C-1), mixing of storage fluid in excess can be applied and achieves, in this particular case, a perfect mass balance (right column of Figure C-1).

The above considerations motivated the development of a systematic procedure to calculate the minimum rebalancing utility requirements, and the corresponding mixing contributions [1].

It is first demonstrated that any overall mixing contributions can be decomposed into a set of elementary and independent mixing steps, each of which implies only mixing of mass from the two surrounding *HSUs*. This helps getting insight into the mixing issues and is a prerequisite towards the development of a mass flowrate rebalance strategy for open storage systems (refer to Section 5.4).

C.1 Decomposition into a Set of Elementary Mixing Steps

Referring to Figure C-1, the overall mass transferred by mixing can be decomposed in a straightforward manner into two elementary mixing steps, as represented on **Figure C-2**. Another example is illustrated by **Figure C-3**; again, to simplify, the

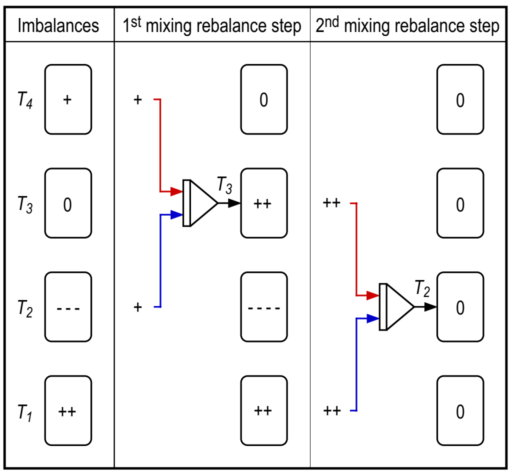


Figure C-2 Decomposition of the global mixing of Figure C-1 into two elementary mixing steps (example 1).

1. The extent to which this systematic procedure embeds the heuristic calculation method proposed by *Mikkelsen* (1998) has not been analysed.

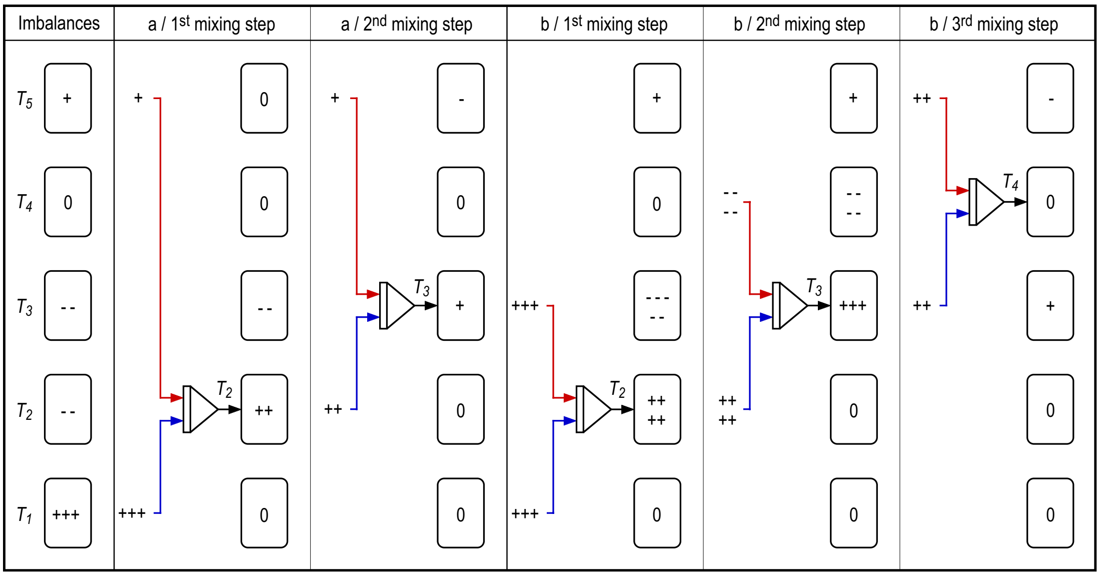


Figure C-3 Decomposition into a set of elementary mixing steps (example 2).

HSU temperatures are assumed to be equally distributed. The decomposition into elementary mixing steps is worth the following comments [2]:

- starting at either end of the range of *HSUs* concerned by mixing, the decomposition is always possible; the mass flows can be calculated one after the other by mixing law to meet the temperature constraint of the *HSU*, and/or to match the global mixing mass transfer between *HSUs*.
- compared to the original global mixing, the elementary mixing steps provide with additional degrees of freedom with respect to scheduling (each step may be scheduled independently). The mixing steps may be organized sequentially (in whatever order) or simultaneously (this last case corresponding to the global mixing), the final state being equivalent.

C.2 Systematic Procedure for Optimal Mixing

Observing that mixing can reduce mass balancing utility requirements as long as both utility cooling and utility heating are required, while cooling is needed at a higher temperature than heating, optimum mixing (i.e. for minimum utility) is clearly related to a pinch problem. An excess of mass which requires cooling is like a hot stream. Actually, the mass balance state of a *HSU* cannot be analysed for itself

2. In any case, the temperature of the mixed fluid must match the temperature of the *HSU* it flows into.

(in isolation), but has to account for the mass balance of the other *HSUs*, what is called the *cumulated mass balance*.

These considerations lead to the use of the *Grand Composite Curve* (*GCC*) representation. A simple system including four *HSUs* represented on **Figure C-4**

Imbalances [Δm]	MBB_k [Δm]	$CMBB_k$ [Δm]	GCC_k [ΔQ/Δm]	$GCCWP_k$ [ΔQ/Δm]	$CMBUB_k$ [Δm]	$MBUB_k$ [Δm]	M_{M_k} [Δm]	1st mixing rebalance step [Δm]		2nd mixing rebalance step [Δm]	M_{BU_k}
+++ 100°C	3	3	0	0	$^{13}/_{5}$	$^{13}/_{5}$	$^{-2}/_{5}$		3	$^{2}/_{5}$	$^{13}/_{5}$
- 75°C	-1	2	75	65	0	$^{-13}/_{5}$	$^{-8}/_{5}$	$^{8}/_{3}$	$^{-11}/_{3}$	75°C	$^{-13}/_{5}$
--- 60°C	-3	-1	105	65	0	0	3	60°C	$^{2}/_{3}$	$^{2}/_{3}$	0
+ 20°C	1	0	65	65	0	0	-1	1	0		0

Figure C-4 Illustration of the proposed systematic procedure to calculate the optimum mixing mass contributions in order to minimize mass balancing utility requirements (refer to explanations in text).

illustrates the procedure. The initial mass imbalances of the *HSUs* (before any rebalancing measure) is given in Δm mass units; the temperatures of the *HSUs* are chosen so as to simplify the calculations (but are not equally distributed any more !). From the individual mass imbalances (denoted MBB), the *cumulated mass before balance* - called $CMBB$ - is calculated from the highest temperature *HSU* towards the lowest temperature *HSU*. By definition, $CMBB_k$ of HSU_k is given by :

$$CMBB_k = \sum_{n=k}^{K} MBB_n = CMBB_{k+1} + MBB_k \quad \textbf{(C-1)}$$

$CMBB_k$ represents, for HSU_k, the total amount of mass which should be cascaded to the lower temperature HSU_{k-1} (i.e. cascaded downwards). Obviously, $CMBB_1 = 0$ considering the closed nature of the heat storage system.

$CMBB_k > 0$ representing the mass to cool from T_k down to T_{k-1}, it can be associated a cooling requirement equal to [3]:

3. In order to simplify the calculations related to Figures C-4 and C-5, it has been assumed $c_{pSF} = Cte = 1$.

$$GCC_k = GCC_{k+1} + CMBB_{k+1} \cdot c_{pSF}(T_{k+1} - T_k) \qquad \text{with} \qquad GCC_K \equiv 0$$

$$\text{or} \qquad GCC_k = \sum_{n=k+1}^{K} CMBB_n \cdot c_{pSF}(T_n - T_{n-1}) \tag{C-2}$$

Figure C-5 represents, in solid line, GCC_k as tabulated in Figure C-4. It clearly

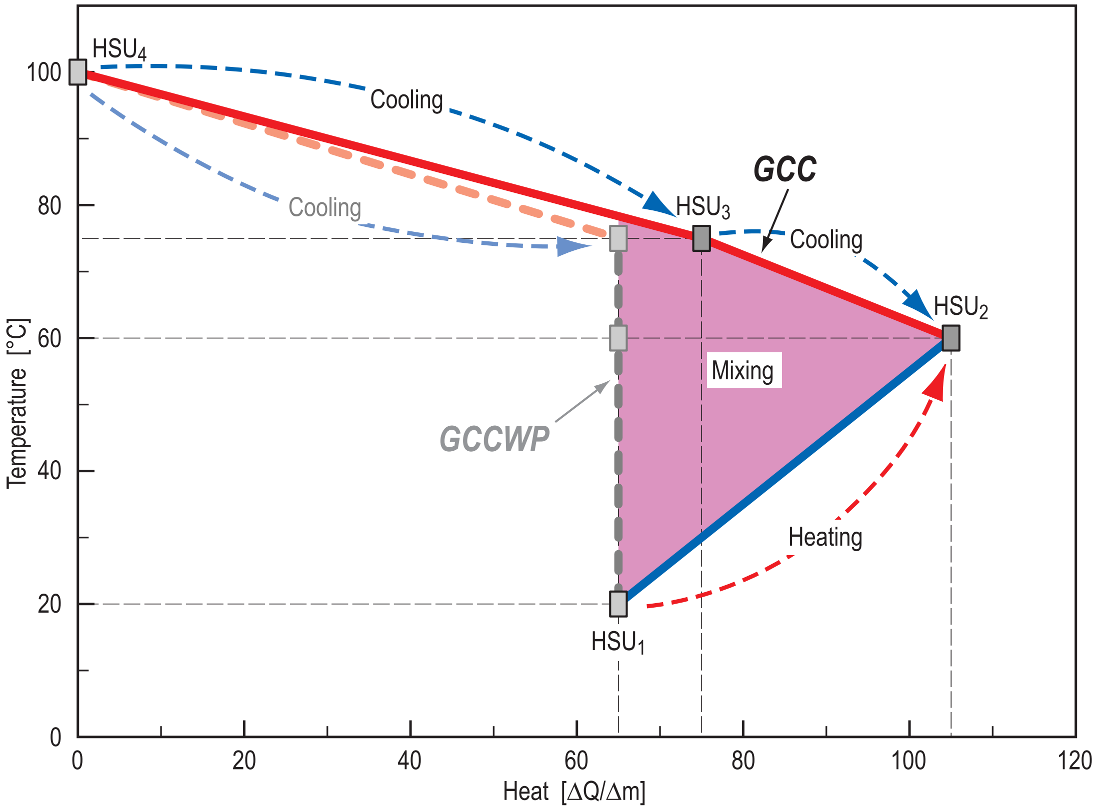


Figure C-5 *Grand Composite Curve* representation of the mass imbalances of the system represented in Figure C-4 (refer to additional comments in text).

appears that HSU_2 is located in a so-called pocket, known to be an energetically self-balanced zone. HSU_3 is also located in a pocket.

From a mixing point of view, the meaning is somewhat different. HSU_2 can be perfectly balanced by mixing of storage fluid coming from HSU_4, HSU_3 and HSU_1; it is balanced because the two *HSUs* surrounding HSU_2 are both located in the pocket. This is not the case of HSU_3: after mixing, the remaining utility requirement corresponds to the cooling of the remaining excess mass in HSU_4 from T_4 down to T_3.

These graphical interpretations are actually not strictly needed; the calculation procedure continues by determining a GCC *without pockets*, denoted $GCCWP$, as represented in doted line on Figure C-5. Back-calculating the cumulated mass imbalances corresponding to $GCCWP_k$ yields $CMBUB_k$, the *cumulated mass before utility balance* (after optimal mixing) defined as :

$$CMBUB_k = (GCCWP_{k-1} - GCCWP_k) / [c_{pSF}(T_k - T_{k-1})] \tag{C-3}$$

From $CMBUB_k$, the *mass before utility balance* (after optimal mixing) is back-calculated by :

$$MBUB_k = CMBUB_k - CMBUB_{k+1} \tag{C-4}$$

The detour through $MBB \rightarrow CMBB \rightarrow GCC \rightarrow GCCWP \rightarrow CMBUB \rightarrow MBUB$ [4] allows to calculate the overall mixing mass contributions $M_{M\,k}$:

$$M_{M\,k} = MBUB_k - MBB_k = M_{BU\,k} - MBB_k \tag{C-5}$$

where:

- $M_{M\,k} > 0$ corresponds to a mixing mass flow coming into HSU_k;
- $M_{BU\,k} \equiv MBUB_k > 0$ represents a balancing utility mass flow coming into HSU_k.

The overall mixing mass contributions $M_{M\,k}$, as well as the decomposition into two elementary mixing steps, are reported on Figure C-4.

The developed procedure is general and applies to any number of *HSUs*. The global mixing mass contributions and the decomposition into elementary mixing steps are easily calculated. The optimum mixing mass contributions are graphically illustrated by changing the GCC into the $GCCWP$ (refer to Figure C-5).

Remember that the procedure has been developed for *IHRS* problems featuring only one hot utility (supplying heat above the hottest *HSU*), and only one cold utility (sinking heat below the coldest *HSU*). In case of intermediate temperature utilities (other than the *HSUs*) or power units, the procedure most likely needs to be revised and modified.

4. The notations MBB, $CMBB$, GCC, $GCCWP$, $CMBUB$, $MBUB$ are preferred to e.g. M_{BB}, CM_{BB} to highlight that these are calculation concepts rather than actual masses.

Appendix D

OPTIMIZATION RELATED ISSUES

The *GA* based optimization and the main features of the *Struggle GA* have been described in Section 3.7. This Appendix complements Section 5.5 by providing a more detailed description of the problematic aspects specifically related to the use of the *Struggle GA* and the remedial actions taken.

The limited capability for developing individuals featuring a high level of heat recovery is considered first (**Section D.1**), followed by observed difficulties to keep diversity in the population which have been traced back to the definition of the distance function (**Section D.2**). These resulted in the necessity to implement a two-levels optimization scheme (**Section D.3**), and in further improvements of the scheme by including the actual (low-level) structure of the *IHRS* (using the $k_{max\ i}$ and $k_{min\ j}$ variables) into the distance function obtained (**Section D.4**). Finally, the mathematical model of the *IHRS* synthesis problem is presented (**Section D.5**).

Practical results obtained using the current state of implementation of the *GA* optimization scheme are presented in Chapter 6, while some guidelines pertaining to selection of the optimization parameters may be found in Appendix F.

D.1 Limited Search Capability for Large Heat Recovery

Early optimization trials with the simple *IHRS* model of *EP-1* were scarcely able to explore solutions featuring high levels of heat recovery (*HR*) and were stuck to sub-optimal solutions (i.e. at inferior levels of heat recovery). Note that the *TBCs* versus *HR* lower bound curve of *IHRS* problems often shows quite flat optimum region(s) which may extend over a large range of *HR* (see examples in Chapter 6). These trials aimed at minimizing the *TBCs*, while solutions previously obtained with the heuristic method were used as upper bound target values. This limited search capability seemed inconsistent with the advocated robustness of *GAs*.

This problem has been traced back to a mismatch of the replacement strategy of *Struggle* with the penalty induced by the *HSU* mass imbalances; although a detailed understanding of the whole process is definitely not straightforward, the following considerations qualitatively explain this statement :

- devising cost optimum *IHRSs* requires that the whole set of x variables be accurately adjusted, and in particular the set of $x_{i,k}$ and $x_{j,k}$ variables, which control the supply and sink of storage fluid in each *HSU*. Any mass imbalance of the *HSUs* has to be compensated by utility supply (after mixing opportunities have been exhausted, if any), i.e. is associated with a cost penalty [1]. The necessity to resort to utilities instead of ensuring the mass balances solely with the contributions of process streams has been explained in Sub-section 5.2.5. The penalty induced by any imbalance of the mass supply with respect to the mass sink makes the solutions (individuals) more expensive and decreases the actual heat recovery; this corresponds to the individual's position being pushed in the upward-left direction on the *TBCs vs HR* diagram.
- finding the optimum set of x variables requires progressive improvements by exploitation of good characteristics of individuals in the population [2] (the probability that a generated individual spontaneously features perfect mass balances is very low indeed, not to say zero). If the *TBCs* are used as the objective function from the very beginning, the population evolves slowly from left to right towards the optimum (on a *TBCs vs HR* diagram), but almost ceases to improve once the local derivative (still <0) of the *TBCs* with respect to the *HR* is small. Individuals with a actually larger *HR* do not develop in the population: the cost penalty resulting from imperfect *HSU* balances of any offspring gives it a low probability to replace its existing nearest competitor, or if it does, the population loses diversity, leading to a decreased capacity of significant improvement. Loss of diversity and cost penalty certainly combine in this process. Increasing the mutation rate does not help, because of the unavoidable mass imbalances of the *HSUs*.
- individuals featuring a potentially large *HR* but temporarily not able to compete with existing good individuals are prematurely rejected (i.e. not kept in population) before they can improve and achieve their full capability. The replacement strategy of *Struggle*, judging an individual as good or bad just after being generated, is detrimental in this respect.

1. The required utility to restore mass balance conditions can be viewed as the penalty to make the *IHRS* actually feasible.
2. The dependence of $T_{i,k}$ and $T_{j,k}$ on x_k could also add to the probability of mass imbalances, but the actual effect is difficult to assess.

To develop individuals with large *HR*, more chances should be given, at least during a first phase, to such individuals. Two strategies have been developed to bypass this shortcoming :

1. during a first phase, the *HR* is maximized (actually $OF = -HR$ is minimized) to allow for large *HR* individuals to develop in the population [3]. After this first phase, $OF = TBCs$, as usually. To avoid the risk of early disappearance of large *HR* individuals by a too abrupt change, intermediate steps minimizing a blend of *TBCs* and *HR* may be used.
2. the *TBCs* are minimized from the very beginning, but during a first phase, the specific cost of the mass balancing utilities (i.e. the cost to make the *IHRS* feasible) is significantly reduced if the individual features a raw *HR* larger then the current best *HR*. This temporarily provides large *HR* individuals with better chances to survive (i.e. to be kept by *Struggle*); in other terms, larger infeasibilities are tolerated for large *HR* individuals. After this first phase, the actual specific cost of utilities is used.

In both strategies, it is necessary, during the first phase, to add a constant value to the *OF* to ensure that individuals generated during the first phase (which associated *OF* value has actually been manipulated) be quickly replaced by better offsprings.

Both strategies aim at providing large *HR* individuals more chances to develop, and have been demonstrated to perform well on the *EP-3* brewery process (refer to Chapter 6). However, the second one (reduced mass balancing utility cost strategy) does not develop individuals featuring a *HR* larger than that corresponding to the $TBCs_{min}$ (the global optimum). In practice, this turns out to be a drawback since the user is also interested in getting an idea of what happens in the region around the optimum.

D.2 Loss of Structural Diversity

Using a single-level scheme and the distance function as defined in Sub-section 5.2.8, optimization runs could not identify the known best *IHRS* solution for the simplified brewing process *EP-3* [4]. Unlike expectations, structural diversity was not present in the final population, and the temperatures of *HSUs* showed little individual-to-individual variations.

3. The number of generations to assign to this first phase depends in particular on the number of *HSUs* and the number of process streams and should be determined by trial.
4. Instead, a *IHRS* structure quite similar (but yet different) to the one of the known best solution was returned.

The distance function (based the on cut-off temperatures of process streams exclusively) mixes various distance contributions together and is unable to make a clear distinction between structural and parametric differences (or the distinction is insufficient for a proper replacement strategy). The structural diversity is not kept and the individuals of the population tend to feature similar properties, in particular similar temperatures of *HSUs*. To attempt to correct this problem, the structural dimension of the similarity measure between individuals has been introduced by accounting for the set of binary *DVs* in the distance function, and selecting a weight large enough to prevail over the parametric contributions to the distance. In this way, individuals of different structures are spread apart in the distance space, excluding possible overlap in the parametric distance ranges of different structures. In other words, the structural difference is given a "macroscopic" contribution, and the parametric differences result in "microscopic" contribution to the distance.

The use of this new distance definition for the single-level optimization scheme clearly demonstrated, as expected, that the structural diversity is preserved, but the *GA* failed to address the parametric optimization. With at best one individual per structure and no chance for increasing this number [5], the improvement of the *OF* of a structure by crossover of structurally different individuals is very inefficient indeed ! Improving the parametric features of an individual requires a blend crossover of structurally similar individuals: the probability of mating two such individuals quickly decreases as the number of possible structures becomes of the order, or exceeds, the population size N_{Pop}. Increasing the number of generations to compensate for this decrease is illusory and globally inefficient. The only reasonable solution is a two-levels optimization scheme, unless the structural dimension can be restricted to a few structures [6] by a preliminary analysis.

D.3 Two-levels Optimization Scheme

The two-levels optimization scheme is depicted in **Figure D-1** :

- the upper level addresses the optimization of the structure (defined by the set of streams to be (potentially) integrated - vector Y of binary variables) [7];
- at the lower level, the parametric optimization (vector X of continuous x variables) of a given structure is performed. A preliminary phase of *HR*

5. If an offspring has the same structure but a worse OF, the existing individual is kept; in the opposite case, it is replaced by the offspring; in both cases, only one individual remains.
6. Given by $2^{n_{biv}}$ where n_{biv} is the number of binary *DVs* to be optimized.
7. Refer to comments of Sub-section 5.3.6.

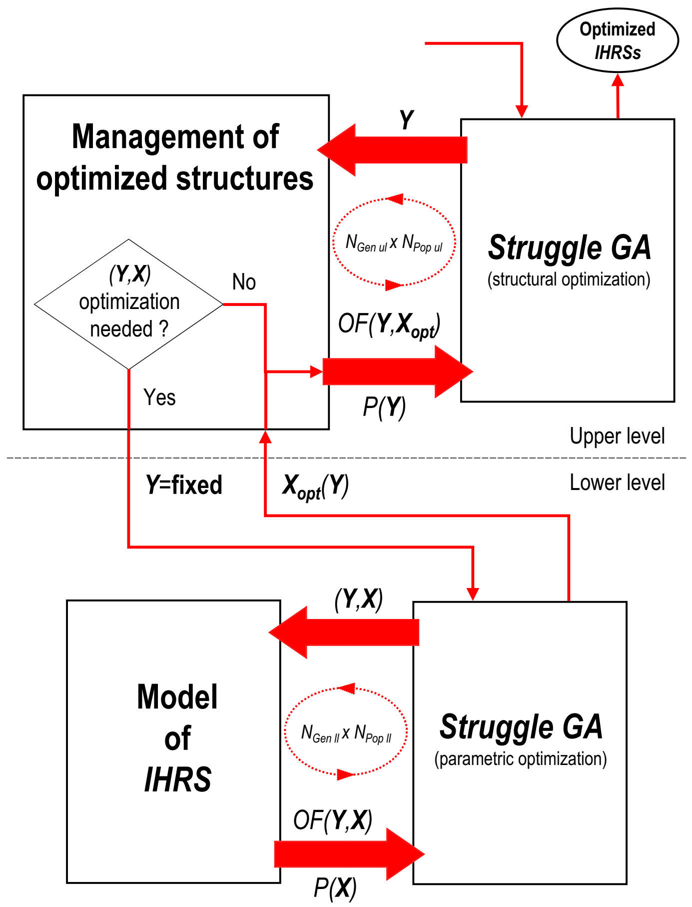


Figure D-1 Two-levels optimization scheme.

maximization is applied anyway. The distance function is based on the cut-off temperatures, as mentioned in Sub-section 5.2.8.

A detailed optimization of each structure is scarcely possible because of *CPU*-time limitations, at least for the present implementation. Techniques to bypass, or prematurely leave, the lower level optimization of unpromising structures have been introduced; the optimum *IHRS* of any optimized structure is stored for further reference. On the average, one *OF* evaluation typically takes 0.75 second on a PC/ *Windows NT* / 333 *MHz* processor frequency; the prototype nature of the *Matlab* model provides with a very significant scope for improvement (code optimization & compilation, or direct coding in *C*++). In combination with more up-to-date processor frequencies, speed-up factors up to 1000 can reasonably be expected.

D.4 Accounting for Low-level Structures

Using the two-levels optimization, further analysis of the population of low-level individuals revealed a poor diversity with respect to the temperatures of the *HSUs* (these temperatures are responsible for the actual structure defined by k_{max} and k_{min} - refer to Sub-section 5.2.6). Again, this problem results from the distance being defined, at the lower level, by the cut-off temperatures exclusively. The contribution to the distance arising from differences in k_{max} and/or k_{min} (due to different temperatures of *HSUs*) is too small and cannot be distinguished from differences in the heat contributions of streams.

The preliminary phase of *HR* maximization makes the temperatures of the *HSUs* converge towards values beneficial for the *HR*. This concentration effect cannot be undone during the minimization of the *TBCs*, and the solutions may be trapped in a local sub-optimum, since the k_{max} & k_{min} structure maximizing the *HR* is not necessarily the one leading to the global optimum, as suggested by the results obtained for *EP-1* in case of 3 *HSUs* represented on Figure 4-14).

The distance function at the low level (Equation 5-11) has been modified to a combination of a structural distance and a parametric distance :

$$D(X_a, X_b) = \sqrt[2]{(D_K(X_a, X_b))^2 + (D_T(X_a, X_b))^2} \tag{D-1}$$

where:

- $D_K(X_a, X_b) = w_k \cdot \sqrt[2]{\sum_{i,k}[q_i(k_{max\ i\ a} - k_{max\ i\ b})]^2 + \sum_{j,k}[q_j(k_{min\ j\ a} - k_{min\ j\ b})]^2}$
- $D_T(X_a, X_b) = \sqrt[2]{\sum_{i,k}[q_i(T_{i,k\ a} - T_{i,k\ b})]^2 + \sum_{j,k}[q_j(T_{j,k\ a} - T_{j,k\ b})]^2}$

The weight w_k has been selected so that a single difference in k_{max} or k_{min} results in a larger distance contribution than that arising from reasonable differences in the cut-off temperatures.

The number of ($k_{max\ i}$, $k_{min\ j}$) sets of values for a single upper-level structure defined by the binary *DVs* may be large and results in the detrimental effects pointed out at the end of Section D.2 (low probability of mating two individuals featuring identical ($k_{max\ i}$, $k_{min\ j}$), low convergence) [8]. Non-promising ranges of temperatures of *HSUs* could be identified by a preliminary analysis and be eliminated from the search domain.

The need to account for ($k_{max\ i}$, $k_{min\ j}$) at the lower level (given an upper-level structure) results in an hybrid solution where structural issues are not limited to the upper level, but extend to the lower level as well. Shifting the interface between the two levels to restrict the lower level to parametric optimization is unfortunately not possible with the present approach.

At the upper level, the structural effect of T_k must be accounted, i.e. a range of temperature be selected for each T_k, while the actual value of T_k within this range should be optimized at the lower level. This segregation is achieved by the extended *IHRS* model proposed in Appendix E.

D.5 Mathematical Model

The mathematical model of a closed storage *IHRS* can hardly be written in a simple compact form. The main equations are listed below, but without explanations of the meaning of the involved terms; references to corresponding parts of the text are provided for convenience.

Minimize :

$$
\begin{aligned}
TBCs = {} & a_B \cdot \sum_{i=1}^{I} x_{bi} \sum_{k=1}^{K-1} \left(C_{OX} + C_{rX} \left(\frac{A_{i,k}}{A_r} \right)^{m_X} \right) \\
& + a_B \cdot \sum_{j=1}^{J} x_{bj} \sum_{k=1}^{K-1} \left(C_{OX} + C_{rX} \left(\frac{A_{j,k}}{A_r} \right)^{m_X} \right) \\
& + a_B \cdot \sum_{k=1}^{K} \left(C_{OS} + C_{rS} \left(\frac{V_k}{V_r} \right)^{m_S} \right) \\
& + \sum_{i=1}^{I} c_{CU} \cdot M_i \cdot c_{pi} \cdot [x_{bi}(T_{i,\,\mathrm{k=1}} - T_{Si}) + T_{Si} - T_{Ti}] \\
& + \sum_{j=1}^{J} c_{HU} \cdot M_j \cdot c_{pj} \cdot [T_{Tj} - T_{Sj} - x_{bj}(T_{j,\,\mathrm{k=K}} - T_{Sj})] \\
& + \sum_{k=2}^{K} c_{HU} \cdot M_{BU\ k} \cdot c_{pSF} \cdot [T_k - T_{k-1}] + c_{CU} \cdot (-M_{BU\ k}) \cdot c_{pSF} \cdot [T_k - T_{k-1}]
\end{aligned}
\qquad \textbf{(D-2)}
$$

8. From a methodological standpoint, accounting for ($k_{max\ i}$, $k_{min\ j}$) is correct; but experimental evidence that it allows to identify better *IHRSs* is still lacking, due to present *CPU*-time constraints.

where:

- x_{bi} and x_{bj} are the binary decision variables ($I + J$ *DVs*) deciding which process streams should be part of the heat integration (refer to Sub-section 5.3.6);
- $T_{i,k}$ and $T_{j,k}$ are the continuous decision variables ($(K-1) \cdot (I+J)$ *DVs*). Note that $A_{i,k}$, $A_{j,k}$ and V_k are function of these temperature variables, as expressed below;
- $A_{i,k} = \left(\frac{1}{h_i} + \frac{1}{h_{SF}}\right) \cdot \frac{\dot{Q}_{i,k}}{\Delta T_{LM\ i,k}}$
- $\dot{Q}_{i,k} = \dot{M}_i \cdot c_{pi} \cdot (T_{i,k+1} - T_{i,k})$
- $\Delta T_{LM\ i,k} = \frac{(T_{i,k+1} - T_{k+1}) - (T_{i,k} - T_k)}{\ln\left(\frac{T_{i,k+1} - T_{k+1}}{T_{i,k} - T_k}\right)}$
- corresponding expressions for cold streams ($A_{j,k}$, $\dot{Q}_{k,j}$, $\Delta T_{LM\ k,j}$) may be found by analogy;
- $V_k = \frac{Max_l[M^*_{k,l}] - Min_l[M^*_{k,l}]}{\rho_{SF}}$ (refer to Sub-sections 3.4.3 & 3.4.4);
- $$M^*_{k,l} = M^*_{k,l-1} + \Delta t_l \cdot \left[\left[\sum_j a_{l,j} \cdot \dot{M}_{k,j} - \sum_i a_{l,i} \cdot \dot{M}_{k,i} - \frac{MBB_k}{\Delta t_{BC}}\right] - \left[\sum_j a_{l,j} \cdot \dot{M}_{k-1,j} - \sum_i a_{l,i} \cdot \dot{M}_{k-1,i} - \frac{MBB_{k-1}}{\Delta t_{BC}}\right]\right]$$
- the last term of $TBCs$ represents the costs for mass rebalancing resorting to utilities; if a preliminary optimal mixing strategy (refer to Appendix C) is used, $M_{BU\ k} = M_{M\ k} + MBB_k$. If $M_{BU\ k} > 0$, only the first part (hot utility) applies, while if $M_{BU\ k} < 0$, only the second part (involving cold utility) applies.

subject to :

$$T_k > T_{k-1} \qquad (k : 2 \ .. \ K) \qquad \textbf{(D-3)}$$

$$T_{k=1} \geq T_{HSUmin} \qquad \textbf{(D-4)}$$

$$T_{k=K} \leq T_{HSUmax} \qquad \textbf{(D-5)}$$

$$T_{i,k} \leq T_{i,k+1} \qquad (k : 1 \ .. \ K-1) \qquad \textbf{(D-6)}$$

$$T_{i,k=K-1} \leq T_{S\ i} \qquad \textbf{(D-7)}$$

$$T_{i,k=1} \geq T_{T\ i} \qquad \textbf{(D-8)}$$

$$T_{j,\,k+1} \geq T_{j,\,k} \qquad (k\ :\ 1\ ..\ K-1) \qquad \textbf{(D-9)}$$

$$T_{j,\,k=\mathrm{K}} \leq T_{T\ j} \qquad \textbf{(D-10)}$$

$$T_{j,\,k=2} \geq T_{S\ j} \qquad \textbf{(D-11)}$$

$$T_{i,\,k} > T_k \qquad (k\ :\ 1\ ..\ K-1) \qquad \textbf{(D-12)}$$

$$T_{j,\,k} < T_k \qquad (k\ :\ 1\ ..\ K-1) \qquad \textbf{(D-13)}$$

Comments

1. Inequality constraints D-3 to D-13 are automatically met thanks to the definition of the dimensionless continuous decisions variables x_k, $x_{i,\,k}$, $x_{j,\,k}$ (refer to Sub-sections 5.2.3, 5.2.4 and 5.3.1, and to Figure 5-1).
2. In Equation D-2, the first term of $TBCs$ corresponds to "batch-ised" capital cost of hot process - storage stream heat exchangers, the second to "batch-ised" capital cost of storage - cold process stream heat exchangers, the third the "batch-ised" capital cost of heat storage units, the fourth the cost of cold utilities on hot process streams, the fifth the cost of hot utilities on cold process streams, and the last term the cost of mass balancing utilities.
3. The cost function to be used for each *HEX* unit is actually type and size dependent (refer to Sub-section 5.3.2).
4. The cost function of *HSUs* to be used generally depends on the capacity of each *HSU* (several capacity ranges).
5. The specific cost of utilities may depend on the actual operating temperature of the utility (e.g. for chillers and heat pumps).
6. The mass balancing utilities make *IHRSs* feasible in any case; the associated costs correspond to the penalty associated with deviations from the mass balance constraints when considering the contributions of process streams solely (refer to Sub-sections 3.4.3 and 5.2.5).

Appendix E

PROPOSED EXTENDED *IHRS* MODEL

The proposals for methodological improvements described below [1] build on the shortcomings which progressively arose from the implemented models by better understanding of the possibilities and limitations of the *Struggle GA* for the *IHRS* optimization problem. Two models are proposed below which use a modified set of *DVs* and provide a direct control over the structure of matches [2]. The first model represents a straightforward extension of the implemented models described in Chapter 5, and does not deserve a special attention; the second model (**Section E.2**) further extends the first one to include the potentially beneficial supply of utility on a storage stream before returning to a *HSU* [3]. General aspects of the models are described first (**Section E.1**).

E.1 General Aspects

Both models use a two-levels optimization scheme. All structural decisions are made at the upper level, for the reasons mentioned in Section 5.5.

The need to account for the structural influence of the *HSU* temperatures at the upper level results in the decisions in which temperature ranges to allocate the *HSUs*. The temperature ranges are defined using the following procedure [4] :

1. collect all supply temperatures of the process streams $T_{S\,i}$ and $T_{S\,j}$, as well as that of the hot and cold utilities (to allow for the possibility of storing utilities);

---

1. Only closed storage systems have been considered; their applicability for open storage systems remains to be analysed.
2. These models have not been implemented yet, since they require significant modifications in the existing modules and reprogramming straight away in e.g. *C++* to take up the challenge of the computing time (i.e. bypass the computing time bottleneck due to the *Matlab* interpreter) which is a major issue owing to the large structural dimensions involved.
3. A technique first proposed by *Mikkelsen* (1998) which allows to make an infeasible match feasible.

2. correct these temperatures by a minimum temperature difference $T_{S\,i} - \varepsilon_T$ and $T_{S\,j} + \varepsilon_T$; do the same for utility streams [5];
3. eliminate from the list multiple identical temperature values;
4. if the feasible operating temperature range of the storage fluid is more restrictive, restrict the list of temperatures accordingly.

As a result from the above procedure, the number of possible ranges for *HSU* temperatures, TR, is obtained ($TR \leq I + J + 1$), as well as the bound of each temperature range (e.g. temperature range 1 from T_{r1} to T_{r2}, etc.).

At the upper level, the structure of an *IHRS* is described by two sets of discontinuous variables :

- variables deciding in which temperature range each *HSU* operates [6];
- variables deciding the existence of process-storage stream matches.

E.1.1 Upper-level HSU Variables

With respect to the *HSU* variables, two main options exist [7]:

1. for a fixed number K of *HSUs* (decided by the user), K integer values within $[1, TR]$ must be generated and manipulated by the *GA*. It is not reasonable to allocate more than two *HSUs* in a single temperature range. To solve the problem of variable bounds and their propagation, dimensionless y_k variables should be used : y_k determine the temperature ranges in the same way x_k determine the operating temperatures T_k, resulting in similar dependence links at the structural level;
2. another coding for the same fixed number K of *HSUs* consists in generating and manipulating a set of K integer variables y_k, each of which $1 \leq y_k \leq TR$. This coding allows several *HSUs* in a single temperature range. However, by random generation or by crossover, the values of these variables are generally not sorted

4. *CombatTES* (*Mikkelsen*, 1998) uses a similar procedure.
5. Although it does not ensure that an internal pinch might not be more limiting, in particular with multi-segment utilities - but this is a side problem here.
6. The actual temperatures within the allocated ranges are decided and optimized at the lower level.
7. If the computing time is not an issue, problems with a variable number of *HSUs* could be tackled. In this case, a binary variable could be associated to each temperature range, specifying whether a *HSU* exists in this range or not. This solution would only allow for one *HSU* per range, and would result in a large number of variables describing the matches (one for each stream and range) but only those which correspond to an allocated temperature range would be meaningful.

so that *Struggle* needs to be modified to sort the variables before applying the crossover operator and the distance function [8] [9].

E.1.2 Upper-level Match Variables

The need for the possibility of intermediate connections to *HSUs* and the pitfalls encountered in the *RMFD* technique (refer to Sub-section 5.3.4) bred the explicit control over the connections to the *HSUs*.

To define the matches with process stream i while providing control over the connections, a binary variable $y_{i,k}$ is associated with each *HSU*: $y_{i,k} = 1$ means a connection to HSU_k exists (whether the storage fluid is extracted or supplied or both depends on the existence of connections to *HSUs* above or below or both). Building the superstructure of process-storage stream matches corresponding to the postulated $y_{i,k}$ is straightforward, as illustrated on the left of **Figure E-1** for matches with stream H_i. Obviously, at least two connections should be provided for a match to actually exist with stream i.

With I hot process streams and J cold process streams, $K(I+J)$ binary variables are needed to define the structure of the *IHRS* by specifying connections to *HSUs*. Since the connections are actually decided at the same level (i.e. simultaneously) as does the allocation of the *HSUs* over the temperature ranges, the connection information cannot account for the temperature feasibility conditions defined in Sub-section 5.2.6, and some of the specified connections may not result in feasible matches. Infeasible matches may be treated in two ways (refer to Figure E-1) :

1. by ignoring the match and the infeasible connection (in the same way $x_{i,k}$ are ignored for $k > k_{max-1}$ in the implemented models) [10];
2. by making infeasible matches feasible, resorting to utility applied on the storage stream. The cost penalty arising from the amount of utility required to make the individual feasible is a true measure of its infeasibility [11]. The set of $y_{i,k}$ and $y_{j,k}$ binary variables is discriminant.

---

8. If these variables are included in the definition of the distance function.
9. This sorting technique could be used for the generation of temperatures T_k as well, instead of the x_k !
10. This is simple and has been proved to work, but maybe misleading for the *GA* because the set of $y_{i,k}$ and $y_{j,k}$ binary variables are not discriminant. To help the *GA* to avoid infeasible connections, a fixed penalty can be added. In this way, the upper level optimization should converge towards *IHRSs* including feasible connections exclusively
11. Whether this is an advantage over a fixed penalty, or not, is not clear, because the *GA* does not consider the derivative of the *OF*; however, this is not merely an optimization technique but represents in some cases a heat integration opportunity.

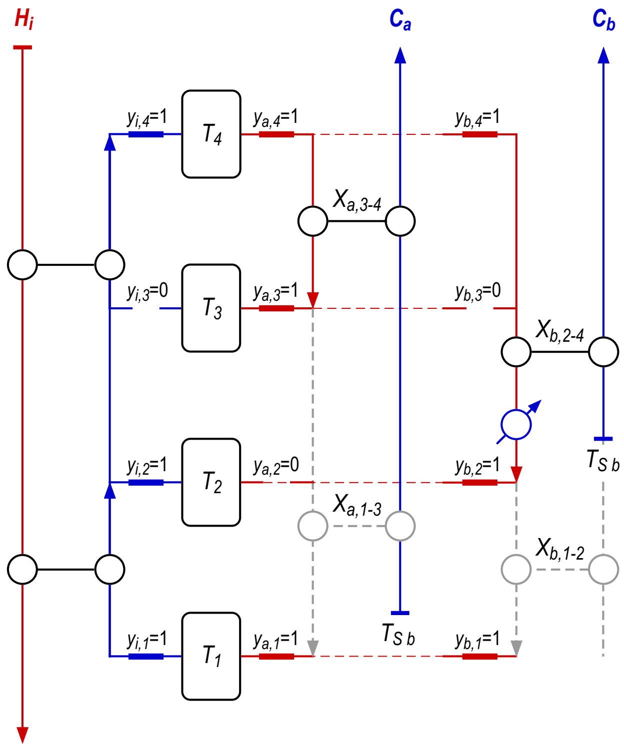


Figure E-1 Connections to *HSUs* and definition of matches by means of binary variables $y_{i,k}$ (hot stream H_i); infeasible matches (on cold streams C_a and C_b) may be ignored (matches $X_{a,1\text{-}3}$ and $X_{b,1\text{-}2}$), or be made feasible by supply of utility on the storage stream before returning to the *HSU* (match $X_{b,2\text{-}4}$).

E.1.3 Management of Decision Variables

To summarize, at the upper level, the K integer variables y_k define the allocation of the *HSUs* to the temperature ranges, while binary variables $y_{i,k}$ and $y_{j,k}$ postulate the connections to *HSUs*. The definition of the *TR* temperature ranges ensures that whatever the actual operating temperature of a *HSU* within a given range, the feasibility of a process-storage stream match only depends on y_k; in other words, the structure of feasible matches is fully determined at the upper level once y_k, $y_{i,k}$ and $y_{j,k}$ are specified. The bounds on the temperature of *HSUs* are also known.

At the lower level, the continuous *DVs* of the given structure to be optimized are :

- the *HSU* temperatures T_k (each within specified fixed bounds);
- the cut-off temperature (or heat contribution) of each feasible match f included in the *IHRS* structure determined at the upper level, and specified as $x_{i,f}$, $x_{j,f}$.

As it is presently done for the implemented models, results obtained from the lower-level optimizations should be stored for further reference, to avoid launching the lower-level optimization of an already optimized structure a second time.

The separation of the *DVs* into a set of structural *DVs* optimized at the upper level, and a set of parametric *DVs* managed at the lower level is very beneficial for the definition of the distance function. At the upper level, it remains to be analysed whether y_k, $y_{i,k}$ and $y_{j,k}$ variables should be mixed in the distance function, and if yes, how the relative weights should be defined.

E.2 Consideration of Infeasible Matches

Cold process streams C_a and C_b (refer to Figure E-1) include infeasible matches $X_{a,\,1\text{-}3}$, $X_{b,\,1\text{-}2}$ and $X_{a,\,2\text{-}4}$. As mentioned above, infeasible matches may be simply ignored (e.g. $X_{a,\,1\text{-}3}$ on stream C_a), leading to *IHRSs* which are similar to those obtained in this work, but providing with a better control over the connections to intermediate *HSUs*. In the case of C_a, the optimization should try $y_{a,\,2} = 1$ instead of $y_{a,\,1} = 1$.

The other approach, i.e. making an infeasible match feasible, is illustrated on stream C_b : because $T_{S\,b} > T_2$, match $X_{b,\,2\text{-}4}$ is not feasible (the return temperature of the storage fluid into HSU_2 is too high), unless a utility cooler is inserted downwards on the storage stream as represented [12].

The motivation to make infeasible matches feasible is not solely a numerical trick. In some instances, it may provide more cost-effective *IHRSs* by allowing the heat integration of a stream featuring a significant heating or cooling contribution, which should otherwise be left out (because an additional *HSU* at a suitable temperature is not available).

Such instances are not represented on Figure E-1, which only aims at illustrating the technique. However, in the case of C_b, if match $X_{b,\,2\text{-}4}$ should be left out, a significant heating contribution from the *HSUs* would be wasted. Setting $y_{b,\,3} = 1$ would be a first option to place a feasible match $X_{b,\,3\text{-}4}$; but even in this case, it might be sensible to make $X_{b,\,2\text{-}3}$ feasible by the cooler [13]. For the *HSU* temperature assignment problem, the introduction of an external cooler or heater relaxes the

12. A similar technique (i.e. introduction of a utility heater) could be applied for infeasible matches on hot process streams as well.

strict condition of temperature feasibility, and allows to increase the amount of *HR* beyond the limits imposed by the constraining number of *HSUs*.

Any infeasible match made feasible by a utility heat exchanger actually includes a trade-off effect between the extra amount of utility supplied [14] and the decrease of the area of the process-storage stream match [15].

To address the optimization of this additional degree of freedom, a variable $q_{i,x}$ has to be introduced for each infeasible match to be made feasible : $q_{i,x}$ expresses e.g. the supplied heat rate over the minimum heat rate [16]. Although it is expected that these additional *DVs* can be managed without problem at the lower level, the technique should be restricted to cases likely to be beneficial.

With this respect, it clearly appears (refer to Figure E-1) that making $X_{b,\,1\text{-}2}$ feasible is not reasonable from a heat integration (and economical) standpoint; individuals with $y_{b,\,3} = 1$ should be rejected by optimization. It can hence be stated that infeasible process-storage stream matches with *HSUs* whose temperature range does not overlap that of the process stream have to remain infeasible [17].

In addition, given a number of *HSUs*, the analysis of the set of streams and the application of the methodology proposed in Chapter 4 help in identifying the critical process streams which could benefit from the technique. This analysis can be performed either at the onset, or after a preliminary simplified optimization run, to get a rough idea of the operating region of optimum *IHRSs*.

13. This can be understood as some kind of a "heat pump" effect, in that a (hopefully) small external utility cooling (or heating, resp.) contribution enables the integration of a process cooling (heating, resp.) contribution. The larger the ratio of the process contribution over the external contribution, the more likely the economical benefit ... provided that changes to the operating temperatures of *HSUs* cannot allow to do without, for the same amount of *HR* and the same set of process streams.
14. Compared to the minimum utility supply needed to ensure a feasible match, i.e. for the storage fluid to reach temperature $T_{S\,b} + \varepsilon_T$ at the outlet of match $X_{b,\,2\text{-}4}$.
15. Actually, the trade-off is more complex since the capacity of the *HSUs* is also influenced by the modified mass flowrate of the related storage stream.
16. Or any other dimensionless relationship.
17. Reversely, the supply temperature of the stream has to be within the temperature range of the *HSUs* connected by the match for the latter to be a candidate to become feasible.

Appendix F

EXAMPLE & GUIDELINES FOR *GA* OPTIMIZATION

A two-levels *GA* optimization process is commented below. Owing to the fact that the lower level still includes both structural and parametric variables, a poor convergence (i.e. a slow improvement of the population as a function of the number of generations) is obtained for the upper as well as for the lower-level optimizations. In spite of its untypical behaviour, this *GA* optimization example is used to provide an illustration of the developed graphical interface.

Guidelines relevant to the current implementation of the two-levels *GA* optimization scheme are also presented.

F.1 *GA* Optimization Process

The behaviour of a two-levels *GA* optimization process (refer to Figure 5-10) [1] is represented on **Figure F-1** [2]:

- the upper graph (*TBCs vs HR* diagram) plots the smallest *TBCs* of all evaluated individuals as a function of the *HR*; the overall lowest *TBCs*, the achieved *HR*, as well as the corresponding set of potentially integrated streams are also displayed;
- the middle graph represents the improvement, as a function of the upper-level generation, of the *TBCs* of the best structure (•), and of the mean *TBCs* of the structures in the population (+);

---

1. *Mdl* = closed storage system / *OS* = two / DF_{ul} = *BDV*; DF_{ll} = *CoT*& k_{max} & k_{min} / $N_{Pop\ ul}$ = 20; $N_{Pop\ ll}$ = 100 / $N_{Gen\ ul}$ = 20, $N_{Gen\ ll}$ = 100 / Sty_{ll} = *HR* max during 40 generations / selected streams C_8 H_9; other streams to be optimized (1024 alternate sets) / 3 *HSUs*.
2. Figure F-1 represents the final state after the optimization has been completed. During a lower-level optimization, the *TBCs* vs *HR* characteristic of the currently considered set of streams is also drawn (using a different colour) on the *TBCs* vs *HR* graph.

- the lower graph relates to the lower-level optimization of a given structure (here potentially C_1, C_3, C_4, C_6, C_8, C_{13}, H_9, H_{10}); the stochastic evolution (i.e. increase and decrease) of the *TBCs* during the first 40 generations results from the *HR* being maximized, before the *TBCs* actually become the objective function to be minimized. The large weight on k_{max}&k_{min} used in the distance function allows the existence and preservation of individuals featuring different match structures, and explains the significant difference observed on this graph between the best (•) and the mean (+) *TBCs* of the population.

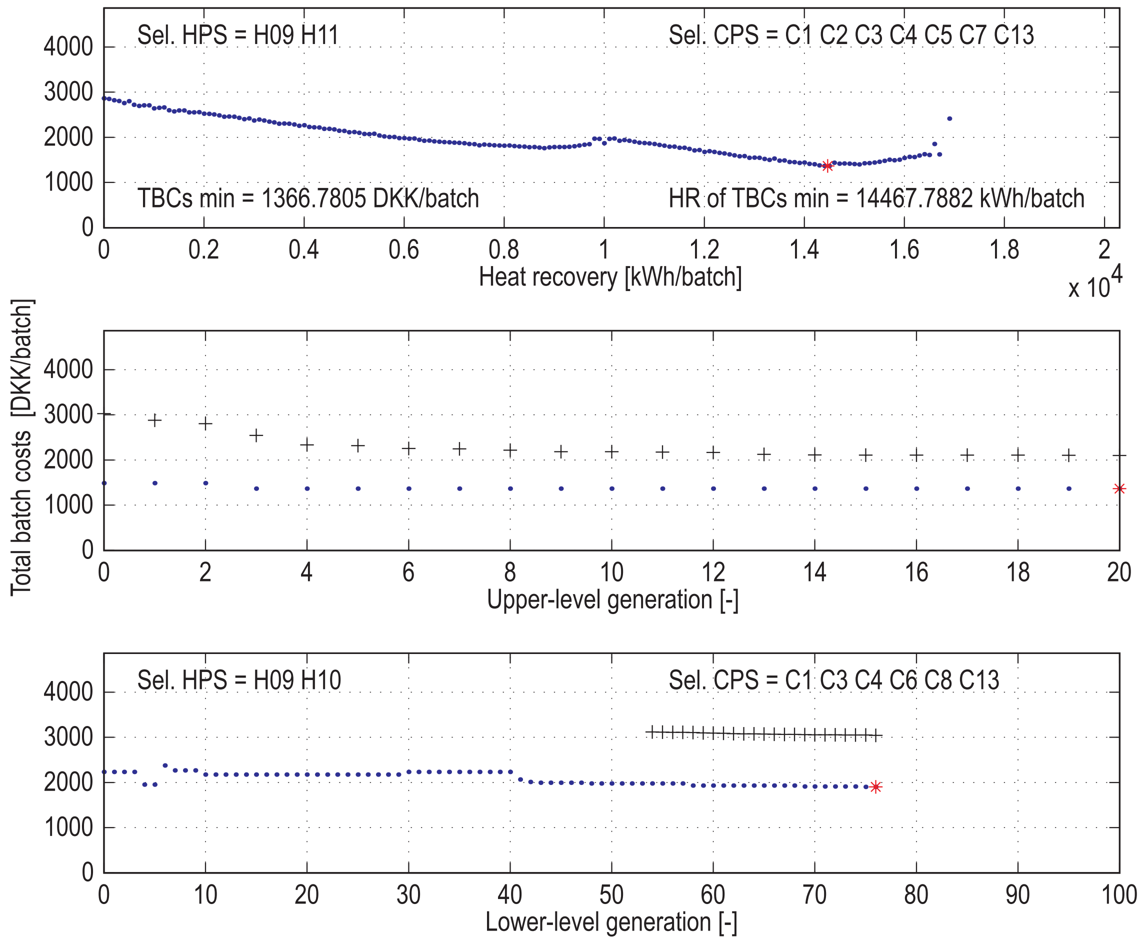


Figure F-1 Typical evolution of a two-levels *GA* optimization.

A local optimum is clearly seen on the *TBCs* vs *HR* diagram at about 9000 *kWh*/batch, followed by an increase of *TBCs* for *HR* up to about 9900 *kWh*/batch, before entering another zone where the "global" optimum is identified. The local optimum is likely obtained when H_9 and H_{10} are the only two hot streams selected (the integration of H_{11} is needed to increase the *HR* beyond the above values). The numerical results file further indicate that the set of streams actually integrated in the "global" optimum *IHRS* includes C_1, C_4, C_7, C_{13}, H_9, H_{11}. This is the set of the global optimum described in Sub-section 6.3.1, while the "lowest" *TBCs* is still significantly higher (by 7 %), due to the much smaller number of generated individuals featuring this structure and hence a further potential for fine adjustment (in particular by increasing the *HR*). Considering this small number of generated individuals (compared to that of other structures reported in the result file), the identification of the actual best structure during this optimization run is somewhat surprising, and should not be interpreted as a proof for the efficiency of this still hybrid optimization scheme. In case of very close optimum *TBCs* values (corresponding to different structures) but statistically different proportions of individuals, the above rough optimization run may fail to identify the true optimum structure (refer to Section F.2).

The small improvement of the *TBCs* shown on the upper-level optimization graph from generation 5 to 20 could unduly prove the inability of the *GA* to efficiently optimize structural variables. In the present case, owing to the hybrid lower-level optimization, the actual set of integrated streams C_1, C_4, C_7, C_{13}, H_9, H_{11} is embedded in several upper-level sets of selected streams, resulting is a higher probability to come to this set during the early generations. Further, one may simply be lucky to find this set during the first generations. Finally, to reduce the computing time in the current implementation, once a low-level structure defined by k_{max}&k_{min} has been optimized (i.e. a sufficient number of individuals of that structure be generated), the best value for this structure is registered and used as the best one for any later instance of that structure in later lower-level optimizations.

As shown on the lower graph, the lower-level optimization is left after the 76th generation and does not continue until the 100th. This is so because it became clear, according to the implemented checks, that the considered set of streams cannot, at best, compete with the currently known best solution. This prevents the *GA* from spending valuable computing time for optimizing unpromising structures.

F.2 Guidelines

In the above example, small values have been set for the number of individuals ($N_{Pop\ ul} = 20$; $N_{Pop\ ll} = 100$) and the number of generations ($N_{Gen\ ul} = 20$; $N_{Gen\ ll} = 100$) because of *CPU*-time constraints. For a preliminary screening of the set of streams to be integrated using the present implementation [3], it cannot be

3. In which the lower-level optimization includes both structural and parametric issues. This hybrid method, implemented for a short term use to quickly get results, shall be replaced by the model proposed in Appendix E.

stated, unfortunately, that the approximate *TBCs* values obtained using a restricted number of generations shall all feature the same quality (precision) whatever the match structure.

The first reason lies in the partially stochastic character of the search method (the search for good solutions of one structure might be more "lucky" than an other). Furthermore, the individuals are generally not equally distributed among the different structures represented in this population (i.e. the number of individuals of a structure may be larger or smaller with respect to another structure). These unequal proportions originate in the fact that the match structures are associated with ranges of *HSU* temperatures of significantly different extensions. With the uniform distribution of the value of *DVs* within their definition range, the larger the *HSU* temperature range of a structure, the more numerous the individuals of that structure in the population. The probability to mate two parents featuring the same structure - and hence the rate of improvement of that structure over generations - is proportional to the number of individuals featuring this structure.

The following simple guidelines pertain to the present implementation of the single and two-levels optimization schemes :

1. achieve short preliminary optimization runs to determine the typical time for one *OF* evaluation. This set an upper bound to the possible number of individuals and generations to get a result in a prescribed *CPU*-time;
2. perform optimization runs considering neither the binary *DVs* (selecting streams) nor k_{max}&k_{min} (describing the matches) in the distance function to obtain upper bound solutions. It helps getting a rough idea of the location of the optimum, the important streams, and the number of generations needed to reach a reasonable convergence level;
3. the number of stream sets and/or match structures to evaluate is a key issue. Whenever possible or needed, restrict the search domain based on insight into the problem (refer to Chapter 4) and common sense : identify reasonable temperature ranges of *HSUs*, select streams considering their heat contribution and the degree to which their supply temperature constrains the temperatures of *HSUs*, and select for optimization those which are uncertain;
4. experience with respect to the convergence of the upper-level optimization is still lacking [4]. Given $N_{set\ max}$ the maximum number of alternate set of streams to be evaluated, the capability of the *GA* to identify the set leading to the lowest

4. *Struggle* has been originally developed for the optimization of problems involving continuous variables only, and its efficiency for integer (discontinuous) variable problems is not known.

TBCs within a significantly smaller number of evaluation ($N_{set\ eval} < N_{set\ max}$) has not been established. Whether a small number of generations and a large population is better than a small population evolving over a large number of generations is not clear;

5. at the lower level, if the structural $k_{max}\&k_{min}$ are not taken into account in the distance function, setting $N_{Pop\ ll} \approx 2..3 \cdot RIV$, with RIV the number of continuous decision variables to be optimized, works well. If $k_{max}\&k_{min}$ are taken into account in the distance function, the above rule of thumb no longer applies and the maximum number of match structures $N_{struct\ max}$ should be assessed so as to select $N_{Pop\ ll} > 2 \cdot N_{struct\ max}$ for the reasons discussed in Appendix D. With this respect, the number of generations $N_{Gen\ ll}$ should be proportional (or even over-proportional) to the number of streams included in the set selected at the upper level, because the larger the number of streams, the larger the number of possible match structures.

Appendix G

DERIVATION OF THE CONSTRAINTS

This Appendix describes the constraints of the linear programming formulation for the area target in resequence design considered in Chapter 7. These developments are taken from *Jones* (1991).

In order for the optimization to be formulated as a *LP* problem, the constraints on heat rates should be converted into constraints on areas. The original constraints on variables $\dot{\boldsymbol{Q}}_{\boldsymbol{i},\,\boldsymbol{j},\,\boldsymbol{n},\boldsymbol{l}}$ (the heat rate of match i-j in each enthalpy interval n of time slice l) are :

- for hot streams: $I_{n,\,l}$ stream enthalpy balances :

$$\sum_{j} \dot{\boldsymbol{Q}}_{\boldsymbol{i},\,\boldsymbol{j},\,\boldsymbol{n},\boldsymbol{l}} = \Delta \dot{H}_{i,n,l} \tag{G-1}$$

where:

- $\Delta \dot{H}_{i,n,l}$ is the enthalpy change of hot process stream i in enthalpy interval n during time slice l, as defined by the composite curves;
- $I_{n,\,l}$ designates the number of hot process streams contributing to enthalpy interval n during time slice l $(0 \le I_{n,\,l} \le I)$.

- for cold streams: $J_{n,\,l}$ stream enthalpy balances :

$$\sum_{i} \dot{\boldsymbol{Q}}_{\boldsymbol{i},\,\boldsymbol{j},\,\boldsymbol{n},\boldsymbol{l}} = \Delta \dot{H}_{j,n,l} \tag{G-2}$$

where:

- $\Delta \dot{H}_{j,n,l}$ is the enthalpy change of cold process stream j in enthalpy interval n during time slice l, as defined by the composite curves;

- $J_{n,l}$ designates the number of cold process streams contributing to enthalpy interval n during time slice l $(0 \le J_{n,l} \le J)$.

♦ $I_{n,l}$ x $J_{n,l}$ boundary values on the heat rate of matches $\dot{\boldsymbol{Q}}_{\boldsymbol{i,\,j,\,n,l}}$:

$$\dot{Q}_{MIN\ i,\,j,\,n,l} \le \dot{\boldsymbol{Q}}_{\boldsymbol{i,\,j,\,n,l}} \le \dot{Q}_{MAX\ i,\,j,\,n,l} \tag{G-3}$$

where:

- $\dot{Q}_{MAX\ i,\,j,\,n,\,l} = MIN(\Delta\dot{H}_{i,n,l};\Delta\dot{H}_{j,n,l})$ is the maximum heat rate that can be transferred from hot stream i to cold stream j in enthalpy interval n during time slice l;
- $\dot{Q}_{MIN\ \mathbf{i},\,\mathbf{j},\,n,l} = MAX\left(0;\Delta\dot{H}_{\mathbf{i},n,l} - \sum_{j \ne \mathbf{j}} \Delta\dot{H}_{j,n,l}\right)$ or, alternatively

  $\dot{Q}_{MIN\ \mathbf{i},\,\mathbf{j},\,n,l} = MAX\left(0;\Delta\dot{H}_{\mathbf{j},n,l} - \sum_{i \ne \mathbf{i}} \Delta\dot{H}_{i,n,l}\right)$ defines the minimum heat rate that must be transferred from hot stream $\mathbf{i}$ to cold stream $\mathbf{j}$ in enthalpy interval n during time slice l; subscripts $\mathbf{i}$ and $\mathbf{j}$ indicate particular values, to distinguish them from summation indices i and j.

Noting that :

- all matches within the enthalpy interval n of time slice l experience the very same temperature driving force $\Delta T_{LM\ n,\,l}$;
- $\dfrac{\dot{Q}_{i,\,j,\,n,l}}{\Delta T_{LM\ n,\,l}} \equiv A_{i,j,n,l} \cdot \left(\dfrac{1}{h_i} + \dfrac{1}{h_j}\right)$;
- $(1/h_i + 1/h_j)$ does not depend on the enthalpy interval n, allowing for a summing up over the enthalpy intervals to provide slice-wise area contributions $A_{i,j,l}$, reducing the total number of decision variables and constraints;

the original constraints given by Equations G-1 to G-3 are transformed into the following set of constraints for the new decision variables $\boldsymbol{A_{i,j,l}}$, (i.e. the heat transfer area of match i-j during time slice l, defined as $\boldsymbol{A_{i,j,l}} \equiv \sum_n A_{i,j,n,l}$) :

♦ I_l constraints with respect to hot streams :

$$\sum_j U_{\boldsymbol{i},\,j,\,l} \cdot \boldsymbol{A_{i,j,l}} = \sum_n \frac{\Delta\dot{H}_{i,n,l}}{\Delta T_{LM\ n,\,l}} \tag{G-4}$$

♦ J_l constraints with respect to cold streams :

$$\sum_i U_{i,\,\boldsymbol{j},\,l} \cdot \boldsymbol{A_{i,j,l}} = \sum_n \frac{\Delta\dot{H}_{j,n,l}}{\Delta T_{LM\ n,\,l}} \tag{G-5}$$

- I_l x J_l boundary values on the area of matches $\boldsymbol{A_{i,j,l}}$:

$$A_{MIN\ i,\ j,l} \le \boldsymbol{A_{i,j,l}} \le A_{MAX\ i,\ j,l} \tag{G-6}$$

where:

- $1/U_{i,\ j} = 1/h_i + 1/h_j$ is the overall heat transfer coefficient between hot stream i and cold stream j;
- $\Delta\dot{H}_{i,n,l}$ ($\Delta\dot{H}_{j,n,l}$) is the enthalpy change of hot stream i (the enthalpy change of cold stream j, respectively) in enthalpy interval n during time slice l;
- $\Delta T_{LM\ n,\ l}$ is the logarithmic mean temperature difference of enthalpy interval n in time slice l;
- $A_{MAX\ i,\ j,l} = \sum\limits_n \frac{MIN(\Delta\dot{H}_{i,n,l};\Delta\dot{H}_{j,n,l})}{\Delta T_{LM\ n,\ l}}$ is the maximum area that can be installed between hot stream i and cold stream j during time slice l;
- $A_{MIN\ \mathbf{i},\ \mathbf{j},\ l} = \sum\limits_n \frac{MAX\left(0;\Delta\dot{H}_{\mathbf{i},n,l} - \sum\limits_{j \ne \mathbf{j}} \Delta\dot{H}_{j,n,l}\right)}{\Delta T_{LM\ n,\ l}}$ or alternatively

  $A_{MIN\ \mathbf{i},\ \mathbf{j},\ l} = \sum\limits_n \frac{MAX\left(0;\Delta\dot{H}_{\mathbf{j},n,l} - \sum\limits_{i \ne \mathbf{i}} \Delta\dot{H}_{i,n,l}\right)}{\Delta T_{LM\ n,\ l}}$ defines the minimum area that must be installed between hot stream $\mathbf{i}$ and cold stream $\mathbf{j}$ during time slice l; subscripts $\mathbf{i}$ and $\mathbf{j}$ indicate particular values, to distinguish them from the summation indices i and j.

Constraints given by Equations G-4 and G-5 indicate how decision variables $\boldsymbol{A_{i,j,l}}$ can be shifted between streams, while these must stay within boundaries defined by Equations G-6.

All coefficients of the three sets of equations are fully defined by the stream data and the slice-wise pinch $\Delta T_{min\ l}$, according to the vertical model.

The balance nature of Equations G-4 and G-5 makes the set of $I_l + J_l$ over-determined; the actual number of independent equations is $I_l + J_l - 1$.

Appendix H

SYNTHESIS OF DIRECT BATCH *HENs* - EXAMPLES

This Appendix provides illustrative examples and further comments the methodology for the synthesis of direct batch *HENs* proposed in Chapter 8.

H.1 Practical Constraints Restricting *HEX* Re-use Across Time Slices

H.1.1 Additional Comments on Thermo-physical Compatibility

Identifying the "thermo-physical compatibility" groups isn't an obvious task; experience and insight are needed. Stream properties have to be compared, and suitable *HEX* types should be identified, since the operating range and the related compatibility conditions depend on the type of *HEX*.

Note the following simple practical rules and comments :

- compatibility groups featuring less than two streams are not of interest;
- a compatibility group can include both hot and cold streams;
- according to the assumptions mentioned in Sub-section 8.2.2, streams including phase changes have to be split into several single-segment streams.

H.1.2 Additional Comments on Chemical Compatibility & Cleaning

Various heuristics could be developed to simplify the number of transitions to consider, since some of these might never take place. A severe restriction to the feasibility of some transitions originates from the batch schedule, as described in Sub-section 8.3.4. Although these schedule constraints are described separately to make a clear distinction between various types of "compatibility", in practice however, these constraints should be accounted for during the evaluation of the "chemical compatibility" so as to avoid assessing cleaning costs of impossible transitions.

In the general case, a *HEX* side can be used for more than two streams during a batch cycle. The costs associated with each "switch" between streams over a batch cycle should therefore be added. Note also that the re-use of *HEX* units between different streams may be associated with possibly significant piping/valving costs, which should be accounted for.

Comments on Figure 8-4 :

1. (see Sub-section 8.3.2);

2. similarly, cleaning costs for the second group **{**H_3, C_4**}** are expressed by a simple 2 x 2 matrix of which only two elements have actually to be evaluated;

3. within the third group **{**H_4, C_3**}**, H_4 potentially includes toxic components, which prevent a cost-effective cleaning without risks, hence the element is shaded in grey.

H.2 Deriving Slice-wise Match Structures

The derivation of the slice-wise match structures requires the following comments :

- **time slice 1 (and 9)** : the base case slice-wise structure is the only possible structure, no other *HEX* can be repiped on C_3-H_1 : e.g. X_4 (C_3-H_4) cannot be repiped from H_4 to H_1, as is the case for X_1 (C_1-H_1) or X_2 (C_2-H_1), which cannot be repiped on their cold side to C_3;
- **time slice 2** : as for time slice 1, the base case slice-wise structure is the only possible structure. The very same arguments hold, and additionally, neither X_3 nor X_9 can be repiped on their cold side to C_3. Note also that resequence is not an issue, since there is only one *HEX* unit on the streams (not a sequence);
- **time slice 3** : the modified slice-wise structure shown on Figure 8-6 includes the repipe of X_7 from H_2 to H_1 (the "switching" from H_2 to H_1 has actually been performed while H_1 did not exist yet, i.e. during time slice 8 of the preceding batch cycle). But one could have also decided not to repipe X_7 at all, or repipe it in another place on the sequence of matches X_1, X_2, X_8 (three additional possible positions). Hence, 5 possible slice-wise structures are associated with the repipe of X_7. What about resequence opportunities ? On C_5, there is no need for resequencing X_7 with X_9, since C_5 is supposed to be an

evaporation stream with low or almost zero temperature increase. Reasons pertaining to not resequencing X_1 with X_3 on C_1, and X_3 and X_9 on H_3, are more "tricky". On the one hand, neither C_1 nor H_3 tolerate resequencing; on the other hand, resequencing could be realized during periods when C_1 is not active (e.g. time slices ≠ 3), or when H_3 is not flowing. But since the *HEXs* X_1, X_3, X_9, if resequenced, would be used only for time slice 3, these resequences would look like "permanent resequences", and are not to be considered as embedded in the present overall match structure. By "permanent resequence", it is meant that the related matches never operate (i.e. are never active) in their original sequence as provided by the overall match structure;

- **time slice 4** : resequencing X_6 with X_{10} on C_2 is feasible, since H_4 and H_5 are heat recovery opportunities (i.e. are not sensitive to transient temperature conditions), and since C_2 is supposed not to be critical to transients conditions (e.g. pre-heating of a feed). Hence, there are 2 possible slice-wise structures. No other *HEX* can be repiped to be used during this time slice. Note that X_9 do not interact with X_6 or X_{10};
- **time slice 5** : considerations for time slice 4 still hold here; the fact that X_9 is not active any more is unimportant, because this match (C_5-H_3) is independent of C_2, H_4, and H_5. Therefore there are also two possible slice-wise structures. It may be worth noting, for the consistency of slice-wise structures 4 and 5, that although it is theoretically possible to work with the sequence $X_6 \Rightarrow X_{10}$ on C_2 during time slice 4, and with the reverse sequence ($X_{10} \Rightarrow X_6$) during time slice 5, this could not be justified in practice, because the temperatures conditions on the sub-system made of C_2, H_4 and H_5 remain identical during both time slices;
- **time slice 6** : on Figure 8-7, both matches X_2 and X_3 are repiped. Repiping X_2 (on its hot side from H_1 to H_2) could have occurred during time slice 4 (*TS 4*) or *TS 5*, when neither H_1 nor H_2 are present, and the reverse could occur during *TS 8*. Repiping X_3 (on both sides, from C_1 to H_2, and from H_3 to C_4) requires that none of streams C_1, C_4, H_2, H_3 be active, which is the case during *TS 5*, and *TS 8*, *TS 9*, *TS 1* for the reverse repipe. Since matches X_2 and X_3 are expected to be active during *TS 3* in their original position (with respect to the overall structure), these repipes are not, *a priori*, "permanent repipes". Note that X_2 and X_3 can be repiped in various sequences on H_2. X_3 may also be repiped in a reverse sequence on C_4 (could also be placed upstream with respect to X_5). Other resequence opportunities (not associated with repipe) could be found on C_2 and H_5. On C_2, X_6 and X_{10} could be found in a reverse sequence, but resequencing could not take place during *TS 6*, since "resequence sensitive" streams are present in the matches (*HEN*) downstream on C_2 (e.g. H_2, C_4). If

required, the resequence could occur at the end of *TS 5*. On H_5, the resequence of X_5 with X_6 would be a "permanent resequence": C_4 (matched to H_5 by X_5) does not tolerate resequence, meaning that resequencing when C_4 is present (*TS 6* and *TS 7*) is not feasible (resequence could occur during any other time slice). But since a resequence of X_5 and X_6 would only concern *TS 6* and *TS 7*, and the fact that a resequence during these two time slices is not feasible, a resequence of X_5 and X_6 (compared to the original sequence from the overall structure) would be a "permanent resequence", which is not acceptable (the reverse sequence of X_5 and X_6 will only be modelled by a related overall structure). With the feasible repipe and resequence opportunities mentioned above (including the case when X_2 and X_3 are not repiped, i.e. are "inactive"), there are a total of 32 feasible slice-wise structures for time slice 6;

- **time slice 7** : as for *TS 6*, X_2 and X_3 can be repiped, while X_6 and X_{10} may appear in the original sequence or resequenced. Taking into account each feasible structural change leads to 16 feasible slice-wise structures for this time slice;
- **time slice 8** : H_4 is the only stream present, so no process-to-process match can be used;
- **time slice 9** : as time slice 1.

H.3 Optimal Re-use of *HEX* Area

H.3.1 Optimal Re-use of *HEX* Area to Minimize Utility Costs

The installed *HEX* areas $A_{ppO\ m}$ of the overall match structure have to be optimally used (operated) during each time slice to minimize the utility requirements [1]. Except for very simple (slice-wise) *HEX* structures, finding the active areas $A_{pp\ l,m}$ (with $A_{pp\ l,m} \leq A_{ppO\ m}$) which minimize the utility requirements is not a straightforward task. The following simple example is merely intended to illustrate the problem.

Consider **Table H-1** listing the streams present during one time slice of a batch process. Assume that for the heat integration of this time slice, a *HEN* including 3 matches is available, of which the structure and the areas are inheritated from another time slice. **Figure H-1** represents four possible ways of re-using the available *HEN* to minimize the utility requirements :

1. In a multiple utility context, the total costs of utilities have to be minimized.

Stream Name	T supply [°C]	T target [°C]	CP [kW/°C]	Heat Rate [kW]	h [W/m²°C]
C1	25	170	10	-1450	2000
C2	90	210	15	-1800	2000
H1	160	40	20	2400	2000
H2	250	120	12	1560	2000

Table H-1 A time slice including 4 process streams.

a) situation before area adjustment (base case *HEN*), i.e. when total available area for each match is used, leading to the fact that the target temperature of C_2 is exceeded, requiring cooling;

b) case in which the target temperature of C_2 is satisfied by adjusting the area of X_3;

c) case in which the target temperature of C_2 is satisfied by adjusting the area of X_2;

d) optimal case of area adjustment using the *Solver* tool (*GRG2* implementation) of *Microsoft Excel*, showing that the objective function (the costs of utilities subject to the constraints of no reverse utility) can be improved by further reducing X_2 area, up to a point where hot utility on C_2 is needed, while the cooling requirement of H_2 cancels out.

Significant differences in the active areas of matches X_2 and X_3 (as well as the *HEX* duties) between cases b), c) and d) can be observed.

It is worth reminding (refer to Section 7.6) that the free availability of excess area (inheritated from other, more area-demanding time slices) may lead to *HENs* which significantly deviate from the *HENs* that would be obtained using the standard Pinch Design Method [2]. Heat transfer from the below-pinch region to the above-pinch region may exist, corresponding to heat being transferred with very small temperature differences.

2. *HENs* designed with the Pinch Design Method feature temperature driving force distributions between the matches which are not too different from the vertical heat transfer model as given by composites curves, avoid heat transfer across the pinch and meet the ΔT_{min} constraint for any match.

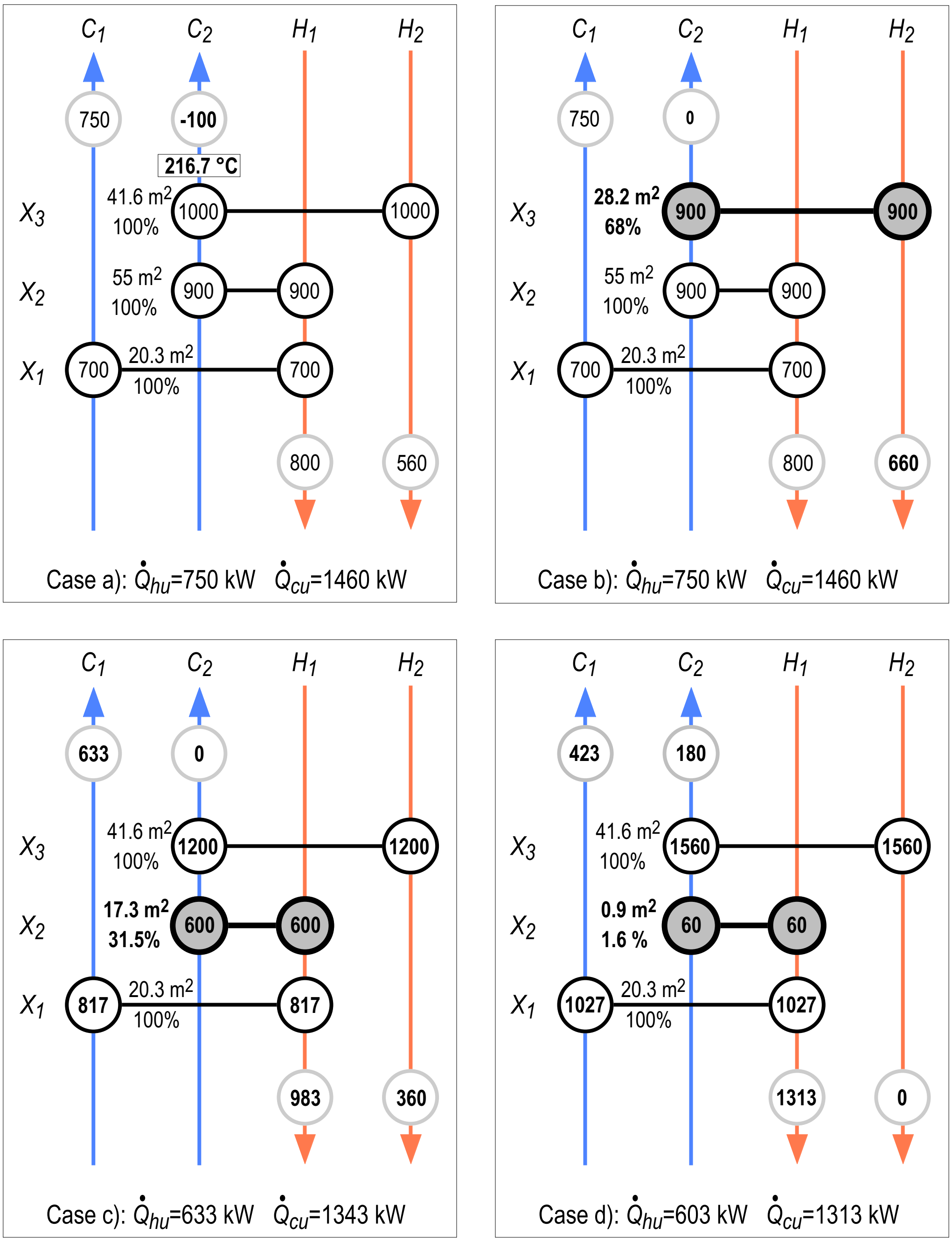


Figure H-1 Base case *HEN* (a) and three possible area adjustments (b, c, d) (see comments in the text).

H.3.2 Reducing the Active Heat Transfer Area

As the adjustment of the *HEX* area is an important aspect for an automated batch *HEN* design, the following simple example, maybe quite obvious, is meant to illustrate the principle. It involves the case of the match X_{pp1} of example process

EP-1 (refer to Figure 7-3). The size of X_{pp1} is set to 6.3 m^2 during the time slice 4 (**Figure H-2**, case a), while X_{pp1} is re-used between the same pair of process streams for the time slices 2 and 3 (**Figure H-2**, case b), requiring only 3.9 m^2. With

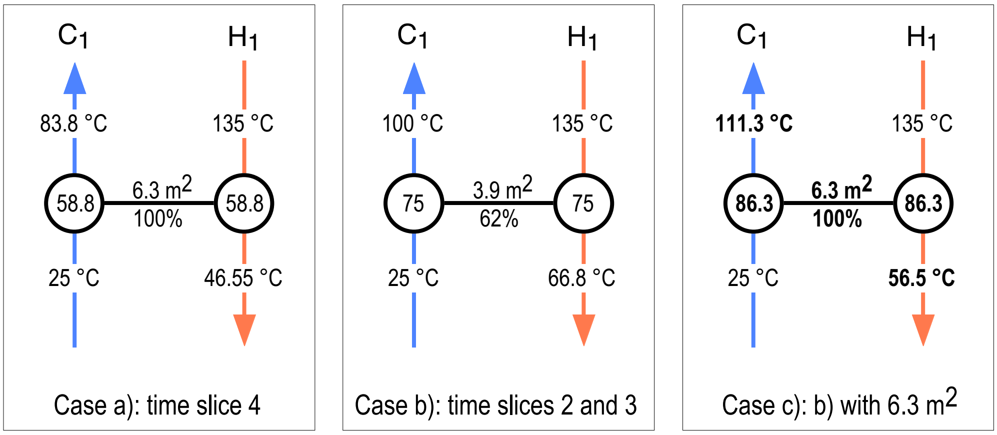


Figure H-2 Re-use of match X_{pp1} across time slices (see comments in the text).

excess area on X_{pp1} (6.3 instead of 3.9 m^2) during these latter time slices, the target temperature of stream C_1 (100 °*C*) would be exceeded by 11.3 °*C* and C_1 would then require cooling (**Figure H-2**, case c).

Figure H-3 illustrates how the apparent area of X_{pp1} is reduced when by-passing

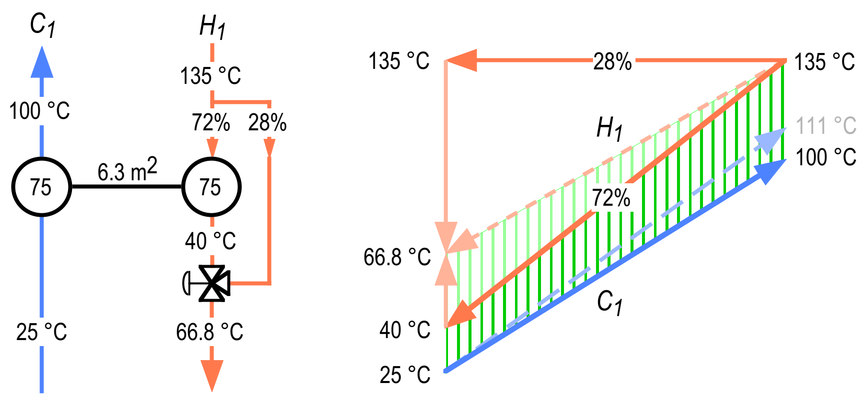


Figure H-3 Using a by-pass to decrease the active area of a *HEX*.

part of the flowrate, and hence decreasing the effective logarithmic mean temperature difference ΔT_{lm}. In this case, a by-pass factor of about 28 % reduces the active area from 6.3 to 3.9 m^2. Note that the above case implicitly assumes that the heat transfer film coefficient is not influenced by the reduction of the flowrate through the *HEX*.

By-passing may in principle be used on either side of a *HEX*. To select on which side it is best applied in practice, the following criteria should be considered :

- **temperature sensitivity** : at the output of the by-passed *HEX* side, the by-passed stream fraction is mixed with the direct stream fraction (passing through the *HEX*). By definition, these two stream fractions are not at the same temperature: the direct stream "exceeds" the final mixing temperature, while the by-passed stream remains "below" the mixing temperature (refer e.g. to Figure H-3). The extent to which the mixing temperature is exceeded may be a problem [3] with temperature-sensitive products such as food products (brewing, dairy, etc.), bio-engineering products, flavour & fragrance, etc. The by-pass should preferably be used on the side which is least temperature sensitive;
- **ease of cleaning** : by-pass requires pipes and valves, which need to be cleaned. Some processes (in particular in food processing) are subject to severe design guidelines which prohibit the use of control valves on sterile product streams, since perfect cleaning of these valves is difficult to guarantee;
- **sensitivity of film coefficient to a decrease of the flowrate** : the by-pass should preferably be placed on the side showing the least sensitivity of the heat transfer film coefficient, in other words the side with the highest margin to laminar flow;
- **existing piping & valving** : savings can be made on equipment costs if piping and valving for resequence or repipe already exist;
- **required quality of temperature control** : this criteria could also determine the side where by-pass should be applied.

Note that depending on the type of *HEX* to be used and the required flexibility, a *HEX* unit could be split into several partial, serially connected sub-units whose areas match the different area requirements. On plate & frame *HEXs* for example, this subdivision can easily be realized using intermediate ports (inlet-outlet connections), while all plates are hold on one single frame [4]. In this way, and with on/off by-pass of unnecessary sub-units, the drawbacks associated with area adjustment using partial by-pass are avoided, but this is obtained at the expense of increased capital costs.

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3. Unless a safe margin with respect to the target temperature of the sensitive product can be ensured in any case.
4. On plate & frame *HEXs* for example, this subdivision can easily be realized using intermediate ports (inlet-outlet connections), while all plates are hold on one single frame.

Appendix I

FURTHER WORK

100 % indirect heat integration and 100 % direct heat integration are two limiting cases of a more general, mixed direct-indirect heat integration. The actual comparison of of these modes cannot be based on profitability (e.g. total batch costs) solely but requires that their behaviour with respect to the schedule fluctuations, and more generally to flexibility issues, are also taken into account. Moreover, in an optimization perspective, the schedule variations [1] should not be considered as an afterthought, but ultimately be simultaneously included in the optimization models.

Several milestones remain to be passed before achieving the above objective. These milestones involve practical issues as well as methodological developments.

I.1 Practical Issues

Essential methodological issues of indirect as well as direct heat integration have been addressed in this work, considering the schedule as is. For the indirect mode, the following practical issues should be considered :

1. recoding of existing *IHRS* model in *C++* [2] while accounting for the changes introduced by the proposed extended *IHRS* model (refer to Appendix E);
2. implementation of the graphical tools and methods described in Chapter 4;

1. Other fluctuations may also be found (e.g. mass flowrate variations, changing supply or target temperatures) but are expected to have a significantly smaller influence on the optimal trade-off between direct and indirect heat integration.
2. To circumvent the computing time limitations arising from the interpreted *Matlab* code, and make the optimization framework applicable in engineering practice.

3. extension of the process-storage match structure to include cascaded configurations of process streams, as suggested in Sub-section 4.4.1 (checking for such configurations should be restricted to promising opportunities obtained by targeting);
4. accounting for multiple utilities and for separate and/or hybrid heat storage systems, e.g. for cases in which the use of a single heat storage fluid within a single heat storage system is a questionable compromise (these issues actually include practical and methodological aspects).

The proposed *GA* based synthesis framework for direct batch *HENs* must be implemented and validated [3]. In both frameworks, piping costs must be taken into account.

These two *GA* based synthesis frameworks shall be applied to several industrially relevant batch processes [4]. The possible causes of schedule variations, their propagation and the applied/possible strategies to avoid or limit the detrimental effects (occurring with or without heat integration) of these variations must be given due consideration. Systematic optimization runs should be made for the main schedule variations.

I.2 Methodological Developments

The following methodological issues are foreseen as being particularly relevant :

1. the introduction of stream splitting in the direct overall match structure, as well as in the indirect heat recovery schemes to account for beneficial direct matches;
2. the development of a targeting method for mixed direct-indirect heat integration for screening the major opportunities, and a complementary analysis with the insight obtained by the targeting and the synthesis approaches of direct as well as of indirect heat integration;
3. suitable ways to specify the schedule fluctuations and the applicable techniques to control/alleviate their propagation [5];

3. The methodological issues summarized in Section 8.7 must to be previously solved.
4. Each process must be provided with a complete description in order to be used as a benchmark problem. Detailed cost functions and economic data, as well as the practical constraints should be included to allow the analysis of the feasibility and the practical relevance of the obtained heat integration solutions to be achieved.
5. Although contributions in this field already exist (e.g. *Kotjabasakis*, 1988; *Klemes* et al., 1994), methods to model this variability and to account for its effects are definitely needed (an up-to-date literature review must be achieved).

4. based on the previous analysis, a quantitative measurement of the robustness (insensitivity to schedule variations) of a direct match should be proposed [6];
5. strategies to analyse the indirect heat integration schemes and identify the beneficial direct heat exchange matches to be introduced (the aim is to screen the major structural issues) [7].

6. One default method would be to simulate the behaviour of a given heat integration solution over a large number of cycles including a representative set the various situations (base cases) in order to define the reasonable cost-effective contingency to be introduced in the heat integration solution. The feasibility and relevance of this approach must be analysed and tested. The identification of base cases is another open issue. The methods used for design under uncertainty must be reviewed in the perspective of their applicability to this type of problem. This approach still considers the schedule variability as an afterthought.
7. The cases studies mentioned in the previous section should provide inspiration to devise and test such techniques. One possible technique consists in the analysis and comparison of heat flows in direct and indirect heat integration solutions; the proportion of heat which actually contributes (on the average, accounting for schedule variations) to the storage capacity could be a starting point for cost/benefits analysis of various direct matches.

CURRICULUM VITAE

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Education

1992 Postgraduate Studies in Energy Engineering at the S*wiss Federal Institute of Technology - Lausanne* (*EPFL*)

1982 Diploma Degree of Electrical Engineering at *EPFL*

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Professional Experiences

1992-00 Research assistant at the *Laboratory for Industrial Energy Systems* (*LENI*) of *EPFL*, developing methods and codes for the heat integration of batch processes and achieving numerous industrial energy analysis & integration studies, coordinator of the *"Swiss National Team"* for the *IEA Implementing Agreement on Process Integration*

1990-92 Director of *InfoEnergie*, an information & consulting office on pilot & demonstration projects for energy efficient technologies in industry

1985-89 Scientific collaborator at *Centre Suisse d'Electronique et de Microtechnique* (*CSEM SA*) in *Neuchâtel*, *Switzerland*, in charge of the development of integrated temperature sensors in *CMOS* technology (patented), and of the test of non-volatile memories (*EEPROMs*)

1982-85 Research assistant at *Laboratory of Applied Thermal Engineering* & *Turbomachinery* (*LTA*) at *EPFL*, investigating automatic control of floor heating systems, collaborating to high temperature solar collector testing, and developing electronic measuring and positioning systems

Teaching Experiences

1992-00 Supervision of student projects and diploma theses, introductory short courses in energy integration, computer aided training sessions