Synthesis of non-isothermal water networks including process hot and cold streams

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ABSTRACT

The synthesis problems of non-isothermal water networks have received considerable attention throughout academia and industry over the last two decades because of the importance of simultaneously minimising water and energy consumption [1]. Most papers have addressed this issue only by considering heat integration between hot and cold water streams. In this study, the scope of heat integration is expanded by enabling heat integration of process streams (such as waste gas streams and reactor effluent streams) together with the water network's hot and cold streams. This approach integrates the non-isothermal water network synthesis problem with the classical heat exchanger networks (HENs) synthesis problem by considering them simultaneously as a unified network. A recently proposed superstructure [2] for the synthesis of non-isothermal process water networks is extended to enable additional heat integration options between hot/cold water streams and hot/cold process streams. Within a unified network, heat capacity flow rates and inlet and outlet temperatures are fixed for process streams, and variable for water streams. The complexity of the overall synthesis problem increases significantly when compared to the syntheses of both networks separately. Therefore, solving this types of problem is more challenging. The objective function of the proposed mixed integer nonlinear programming (MINLP) model accounts for operating costs (including fresh water and utilities) and investment costs for heat exchangers and treatment units. The results indicate that by solving a unified network, additional savings in utilities consumption and total annual cost can be obtained, compared to the sequential solution obtained by solving both sub-networks separately. Thus, more efficient water networks can be designed.

KEYWORDS

Water network, heat exchanger network, simultaneous synthesis, superstructure optimisation.

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INTRODUCTION

Process industries use large amounts of water and energy. Water is used as process water, boiler feed water or cooling water, whilst energy is used in mostly in the form of thermal or electric energy. Much effort has been invested by industries in order to increase the efficiency of their processes by reducing the consumption of costly natural resources. However, for most industries there is still room for minimising water and energy consumption. Accordingly, water and energy integration during the design of new processes or analyses and the retrofitting of existing processes have been identified as an important research direction [3]. Systematic approaches are recognized as a useful tool for achieving resource conservation by combining process sub-system networks or the whole processes within an industrial complex.

Systematic approaches have been developed over time, including pinch analysis (PA) and mathematical programming (MP), in order to address the problems of water or/and energy integration. Advantages of both approaches can be combined in order to facilitate the solution of complex problems. PA was first introduced and applied to heat exchanger network (HEN) synthesis [4]. This approach systematically analyses the impact of heat recovery approach temperature (ΔT_{\min}) on utilities usage and uses heuristic rules for designing HENs. Subsequently, it was automatized as a linear programming (LP) transhipment model, determining minimum utilities usage and extended into mixed integer linear programming (MILP), minimising the number of heat exchange matches [5]. This is the first targeting step in a two step methodology in which the HEN was designed using the superstructure approach [6]. The advantage of a mathematical programming approach, in the context of sequential synthesis, whether it is performed by using PA or MP, is that MP is easier to apply to large scale problems. However, both approaches fail to give optimal results because of their sequential nature in which trade-offs between investment and operating costs are not addressed properly. This led to the development of simultaneous approaches [7] and mixed integer nonlinear programming (MINLP) models for simultaneously minimising operating and investment costs. The stage-wise superstructure proposed by Yee and Grossmann [7] was used as a basis for further improvements by considering non-isothermal mixing within HEN stages [8], optimal placement of heaters and coolers [9] or multi-period operations using multiple utilities [10]. Recent research in the field of heat exchanger networks synthesis has focused on retrofitting [11] and synthesis [12] of large scale heat exchanger networks. In these HEN synthesis problems, heat integration between process streams (such as waste gas streams, reactor feed or effluent stream) was performed in order to find optimal HEN design. The reader is referred to recent work by Klemeš and Kravanja [13] covering research progress related to heat integration over the last forty years and review papers presenting heat integration techniques and HEN synthesis [14, 15].

Similarly to systematic tools for HEN synthesis, the PA, MP and their combinations were used for the synthesis of non-isothermal water networks. The objective of the synthesis problem was to simultaneously minimise freshwater and utilities (used for water heating and cooling) consumption. Because there are close interactions between water and energy usage within processes [16], reduction of water usage causes reduction in energy usage and vice versa [17]. The research related to the synthesis of non-isothermal water networks began with the development of PA based methodologies for simultaneous water and energy minimisation [18, 19] and later a sequential mathematical programming approach was proposed [20]. However, the water network (WN) and HEN were synthesised separately. Later, simultaneous approaches [21-23] were used for developing optimal network designs and establishing trade-offs between operating and investment costs. Different solution strategies [24] were employed in order to solve complex non-isothermal WN synthesis problems within a

single–step [25] or by using a two–step [26, 27] strategy. Note that in these synthesis problems, heat integration was only performed between water streams in order to find an optimal design for heat–integrated or non–isothermal WN. However, a mixed integer linear programming (MILP) model for simultaneous optimization of water and energy usage (SOWE) developed by Kermani, et al. [28] enables heat integration between water and process thermal streams using a source/demand superstructure representation. The reader is referred to a recently published comprehensive review of contributions over the last fifteen years regarding water and heat integration and the synthesis of non–isothermal WNs [1]. In that paper, the synthesis of process, water, wastewater, and heat exchange networks is highlighted as a possible further direction within this field (see Figure 1). During process synthesis and design, subsystems (such as water networks and heat exchanger networks) are usually implemented separately after an optimal process flow sheet is identified. In a paper by Handani, et al. [29], simultaneous synthesis and design of process and wastewater networks, also known as a multi-network problem, is addressed in order to maximise water reuse when synthesizing process flow sheets.

Our study presents a new conceptual representation that integrates the synthesis problem of non-isothermal water networks with the heat exchanger network synthesis (HENS) problem, including process hot and cold streams. The two networks are considered simultaneously as a unified network. This extends the scope for heat integration between water networks' hot and cold water streams and process hot and cold streams, giving the opportunity for additional savings in utility or investment costs, leading to more efficient WN designs. Firstly, we present a definition of the problem and a description of the superstructure, followed by a description of the solution and modelling approach which will be applied to a case study demonstrating model capabilities and results. Lastly, a modelstatistics is provided and the main conclusions are highlighted.

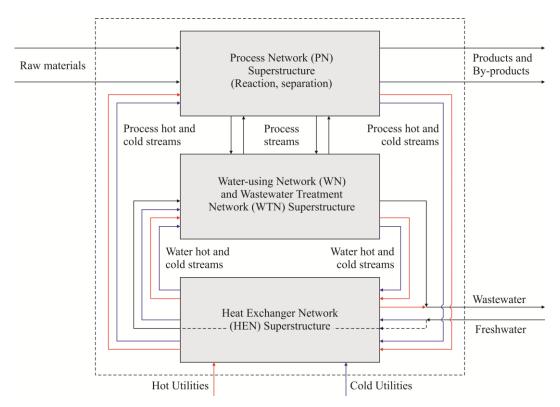


Figure 1. Combined process network, water—using, wastewater treatment network and heat exchanger network [1]

PROBLEM DEFINITION

In order to solve the synthesis problem of a unified non–isothermal water network, including process hot and cold streams, the problem should be defined as follows:

- Set of hot $hp \in HP$ and cold $cp \in CP$ process streams with known heat capacity flow rates and inlet/outlet temperatures,
- Set of freshwater sources $s \in SW$ with the specified temperatures and contaminants $c \in SC$ concentrations,
- Set of process water—using units $p \in PU$ with known operating temperatures and given the maximum inlet/outlet contaminant concentrations,
- Set of wastewater treatment units $t \in TU$ in which wastewater is regenerated and reused if wastewater treatment is included,
- Set of heating stages for cold water streams ($cs \in CS$) and cooling stages for hot water streams ($hs \in HS$),
- Temperatures of hot and cold utilities
- Limiting conditions of temperature and/or contaminant concentrations within the effluent water stream,
- Freshwater and utilities cost as well as investment cost data for heat exchangers and treatment units if wastewater treatment is included.

The goal of the synthesis problem is to minimise the total annual costs of the unified process heat exchanger and water network, subject to the given process and environmental constraints. As a result, the optimum network design should be obtained with water network topology and HEN design allowing heat exchange between hot/cold water streams and hot/cold process streams.

The following assumptions were used in order to simplify the synthesis problem:

- water heat capacity is constant and independent of the stream temperatures
- individual heat transfer coefficients are constant for water and process streams and utilities
- single hot utility (steam) and cold utility (cooling water) is available
- fixed mass loads of contaminants transferred to water streams are given
- fixed removal ratios of each contaminant within treatment units, if wastewater treatment units are considered
- counter-current shell and tube heat exchangers are used
- process is continuous.

SUPERSTRUCTURE

Figure 2 shows the proposed superstructure of a unified non–isothermal water network including process hot and cold streams. A recently proposed compact superstructure [2] for the synthesis of non–isothermal water network has now been extended in order to explore heat integration opportunities of water streams within the water network with the process hot and cold streams (see Figure 2). This approach integrates synthesis problems of non–isothermal water networks with classical heat exchanger networks (HEN) by considering them simultaneously as a unified network.

Process streams are referred to as water non related streams (such as reactor feed, reactor effluent, and gaseous waste streams). Several sub-networks can be identified within the proposed superstructure, including a water network (WN), a wastewater treatment network (WTN), and a heat exchanger network (HEN). The WN enables water reuse options between process water—using units. The WTN enables regeneration of wastewater streams,

regeneration reuse and regeneration recycling. As can be seen from Figure 2, HEN consists of two sub–networks. The first is the WN–HEN sub–network where direct heat exchange by non–isothermal mixing as well as indirect heat exchange for water streams is enabled. The second sub–network is a process and heat exchanger network (PN–HEN), where only indirect heat exchange (heat exchange through heat exchangers) is enabled for process hot and cold streams. Note that indirect heat exchange between two sub–networks, WN–HEN and PN–HEN, is possible, enabling heat integration of water streams with process streams. This extends the scope of heat integration and opens possibilities for additional energy savings.

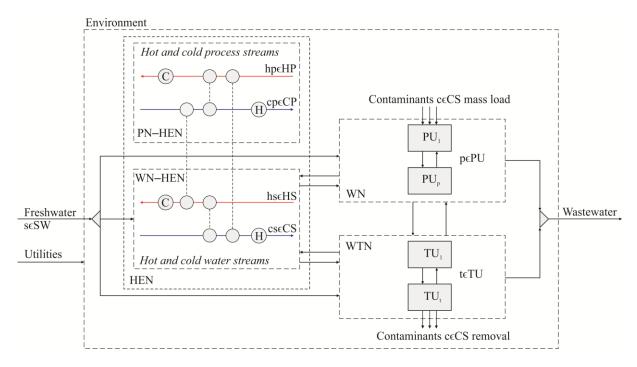


Figure 2. Superstructure of the unified non-isothermal water network including process hot and cold streams

SOLUTION APPROACH AND MODELLING

A recently proposed two–step iterative solution strategy [2] was used for solving the synthesis problem shown in the previous section. In the first step, the water network model (M1) was combined with a simultaneous optimisation and heat integration model (M2) proposed by Duran and Grossmann [30]. The combined nonlinear programming (NLP) model (M1+M2) problem was solved by minimising the operating costs of the network including freshwater, hot and cold utilities and wastewater treatment, if included, at a fixed heat recovery approach temperature (HRAT). Within the first step, simultaneous optimisation of the water network was performed including heat integration of hot/cold water streams with hot/cold process streams. By solving the first NLP model problem, an initialisation for variables (including flow rates and contaminant concentrations) and lower and upper bounds on freshwater and utility usage were provided for the second design step. In the second step, the water network model (M1) was combined with the heat exchanger networks synthesis model (M3) proposed by Yee, et al. [31]. The combined mixed integer nonlinear programming (MINLP) model (M1+M3) problem was solved with the objective of minimising the total annual cost of the network. Within the second step, WN as well as HEN designs were considered simultaneously, enabling heat integration of water streams with the process hot and cold streams. A detailed explanation of the iterative procedure used to obtain multiple locally optimal solutions is given in our recent publication [2]. A General Algebraic Modelling System (GAMS) [32] was used as a tool for creating a generalised model of the superstructure given in Figure 2. AlphaECP solver was used for solving the NLP model and SBB for MINLP model problems. Note that this model enables solving three types of problems: the heat exchanger network synthesis problem including process hot and cold streams, the non–isothermal water network problem and a unified network problem comprising the two previously mentioned problems, as shown later in this paper. The synthesis problems were solved on a computer with 2.67 GHz Intel i5 processor with 8 GB of RAM.

CASE STUDY

This section presents a case study in order to demonstrate solutions of the formulated synthesis problem. Firstly, sequential solutions of separate networks are presented following the simultaneous solution of the integrated networks. The synthesis problem includes three process water—using units, and two hot and two cold process streams. The process water—using unit's data were taken from the literature [21] and are given in Table 1. Data for the hot and cold process streams are also taken from the literature [7] and given in Table 2. Additional required parameters and cost data are given in Table 3.

Table 1. Process units' operating data for Example [21]

Process	Contaminant	Maximum inlet	Maximum outlet	Temperature
unit	mass load	concentration	concentration	(°C)
	(g/s)	(ppm)	(ppm)	
PU_1	5	50	100	100
PU_2	30	50	800	75
PU_3	50	800	1,100	100

Table 2. Process streams' data [7]

Stream	Inlet temperature	Outlet temperature	Heat capacity flow
	(°C)	(°C)	rate (kW/K)
Hot 1	170	60	30
Hot 2	150	30	15
Cold 1	20	135	20
Cold 2	80	140	40

Table 3. Operating parameters and cost data [21]

Parameter	
Temperature of freshwater, °C	20
Temperature of wastewater, °C	30
Inlet and outlet temperatures of cooling water, °C	10 and 20
Temperature of hot utility (steam), °C	150
Freshwater cost, \$/t	0.375
Cold utility cost (cooling water), \$/(kW·y)	388
Hot utility cost, \$/(kW·y)	189
Fixed cost for heat exchangers, \$	8,000
Area cost coefficient for heat exchangers, \$/m ²	1,200
Cost exponent for heat exchangers	0.6
Individual heat transfer coefficients for water streams, process streams and utilities, kW/(m ² ·K)	1
Specific heat capacity of water, kJ/(kg·K)	4.2
Plant operating hours, h	8,000

Sequential approach (Case 1)

<u>PN-HEN</u>. Firstly, a heat exchange network problem including only process hot and cold streams was solved separately by using the data given in Table 2. The optimal HEN design obtained by integrating hot and cold process streams is given in Figure 3. The network consists of four heat exchangers and one cooler with a HEN investment cost of 155,170 \$/y. A hot utility is not required in the network design and 400 kW of cold utility is consumed. The total annual cost of the network is 230,770 \$/y. The same network design was obtained by Yee and Grossmann [7] with a small difference in heat loads and heat exchanger areas caused by using different utility and heat exchanger costs, as well as individual heat transfer coefficients. Note that the same optimal solution can be obtained by using the BARON global optimisation solver [33] (Branch and Reduce Optimisation Navigator), so that that the solution obtained is a global optimum.

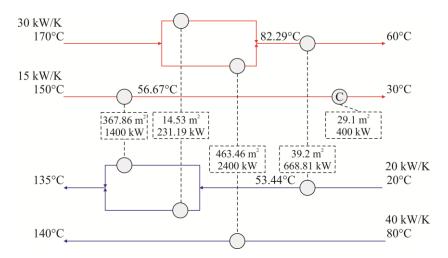


Figure 3. Optimal network design for process heat exchange network

<u>WN+WN-HEN</u>. Figure 4 shows the optimal design of a non–isothermal water network obtained by solving the proposed model problem and excluding process streams from the network design. The optimal network design exhibited a minimum freshwater (77.273 kg/s) and a minimum hot utility consumption of 3,245.5 kW. Two heat exchangers and two heaters are included in the optimal network design with a HEN investment cost of 331,049 \$/y. The total annual cost of the networks is 2,424,830\$/y.

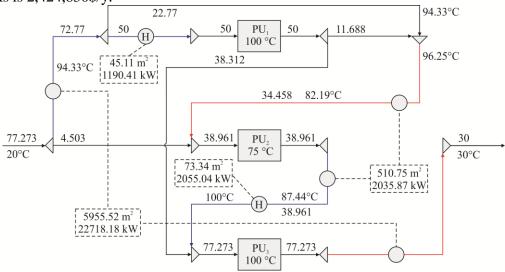


Figure 4. Optimal network design for non-isothermal water network

Simultaneous approach (Case 2)

Combining and simultaneously solving separate network problems as an integrated network could obtain a potentially better solution because of more heat integration opportunities within the integrated network. However, the complexity of the problem increases as a larger number of hot and cold streams is involved in heat integration. The optimum network design obtained by using the proposed model is shown in Figure 5.

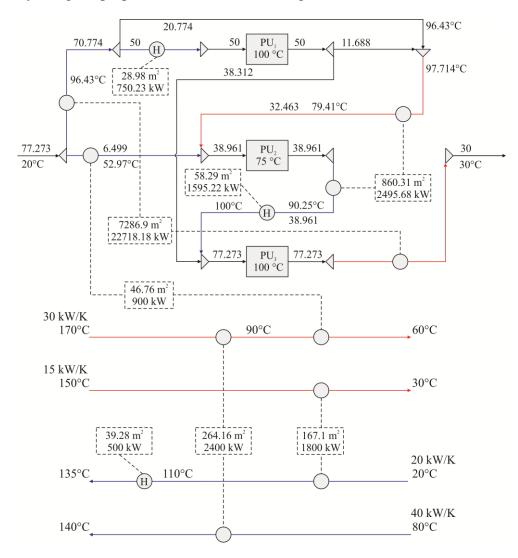


Figure 5. Optimal network design of a unified non-isothermal water network including process hot and cold streams

The minimum freshwater consumption was obtained (77.273 kg/s) which is the same as for the network design given in Figure 4. Note that the topology of the water network design (Figure 5) obtained by simultaneously solving two network problems is the same as that given in Figure 4, in which the water network was synthesised separately, whilst some small differences exist in some flow rates and temperatures at the end of heat exchangers. However, the HEN design related to the process streams has been significantly changed. The hot process stream with a heat capacity flow rate of 30 kW/K and inlet temperature of 170 °C has been integrated with a cold freshwater stream (see Figure 5), recovering 900 kW of heat. Note also that in Figure 5, cold utility was not consumed, compared to the optimum network design given in Figure 3. The consumption of cold utility was reduced by 400 kW, and consequently equal reduction of hot utility was achieved within the unified network design. The hot utility

consumption was 2,845.5 kW. Surprisingly, the reduction of hot and cold utilities did not lead to a significant increase in HEN investment (see Table 4) when compared to the investment in heat exchangers for individual networks. The TAC of the network was 2,426,712 \$/y. Table 4 shows a comparison of the results for the sequential (Case 1) and simultaneous (Case 2) approaches. The TAC of the unified network was reduced by approximately 8.6%. Note that all values given in Table 4 were obtained by using lower bounds on exchanger minimum approach temperatures of 1 °C in order to find their optimum values.

Table 4. Comparison of the results for separate networks and a unified network

Parameter	Case 1	Case 2	Difference between Case 1 and Case 2	Percentage of improvement
Freshwater consumption, kg/s	77.273	77.273	0	0
Hot utility consumption, kW	3,245.5	2,845.5	400	12.3
Cold utility consumption, kW	400	0	400	100
Number of heat exchangers	9	8	1	11.1
Operating costs, \$/y	2,169,382	1,938,582	230,800	10.6
HEN investment cost, \$/y	486,219	488,131	-1,192	-0.4
Total annual cost, \$/y	2,655,601	2,426,713	228,888	8.6

MODEL STATISTICS

This section provides a brief description of model statistics. Only data for the second MINLP model are given.

Table 5 shows model statistics, including a number of equations, continuous and discrete variables, hot and cold streams and the CPU times required for obtaining the best local solutions. Also, a number of stages within the stage—wise superstructure [7] used for the HEN design are given for all cases, as well as the optimality tolerance for finding the solutions.

Note that considering the unified network (Figure 1) significantly increases the number of continuous as well as discrete variables (see

Table 5). Accordingly, the synthesis problem to be solved becomes more complex, requiring increased computational time. The solver terminated solution was obtained for the case of a unified network when optimality tolerance (1%) was reached. However, computational effort was significantly increased when compared to solutions obtained for individual networks.

In addition, the number of hot and cold streams and the number of stages within the stage—wise superstructure [7] affects models' complexity. A heat exchange network problem that includes 2H and 2C streams was solved within 2 HEN stages. Accordingly, the synthesis problem was relatively simple and was solved within 1 s (see Table 5). Although the maximum number of hot and cold streams within the superstructure for the non–isothermal water network was 5H and 5C, the problem can be easily solved within the 1 HEN stage (9 s), because not all streams were selected in the final design. Figure 4 shows that only 2H and 3C streams were selected in the final design, out of a maximum of 5H and 5C streams. The same

solution was obtained by solving for a non-isothermal water network within 2 HEN stages but this required more computational time (224 s). However, within a unified network, the complexity of the problem increases significantly. This is mainly because of the uncertain parameters (heat capacity flow rates and temperature) of hot and cold water streams combined with the increased number of HEN stages when considering a WN design.

Table 5. MINLPs model statistics for separate networks and a unified network

Parameter	Heat exchange	Non-isothermal	Unified network
	network	water network	
No. of equations	85	275 (370)	570
No. of continuous variables	73	395 (480)	712
No. of discrete variables	12	35 (60)	112
CPU time, s	1	9 (224)	6,094*
No. of stages within the HEN superstructure [7]	2	1 (2)	2
No. of hot (H) – cold (C) streams	2H-2C	5H-5C	7H-7C
Optimality tolerance, %	0	0	1

^{*}time limit for model solving was set to be 7,200 s. Values in brackets obtained with 2 HEN stages.

CONCLUSIONS

In this paper we present a novel superstructure and corresponding MINLP model for the synthesis of unified non-isothermal water networks including process hot and cold streams. The proposed approach combines two networks, a heat exchanger network including process hot and cold streams and a non–isothermal water network, which have usually been treated as separate networks within the literature. The proposed unified network introduces new heat integration opportunities between hot and cold process streams and hot and cold water. However, the complexity of the problem increased significantly with a combined MINLP model and was much more difficult to solve when compared to individual networks, as shown in the model statistics. By solving for two networks simultaneously, a different design was produced and a significant saving (8.6%) obtained in total annualised cost. Research is underway to propose solution strategies for solving more complex problems, including a larger number of process water-using units, process hot and cold streams, and the inclusion of wastewater treatment.

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NOMENCLATURE

Indices

c contaminant

cp cold process stream

cs heating stage for cold water streams

hp hot process stream

hs cooling stage for hot streams

cold process stream

i hot process stream

p process unit

s freshwater source

t treatment unit

Sets

j

CP cold process stream

CS heating stages for cold water streams

HP hot process stream

HS cooling stages for hot water streams

PU process unitSC contaminant

SFW freshwater source

TU treatment unit

Abbreviations

GAMS General Algebraic Modelling System

HEN heat exchanger network LP linear programming

MILP mixed integer linear programming

MINLP mixed integer nonlinear programming

NLP nonlinear programming

TAC total annual cost
WN water network

WTN wastewater treatment network

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