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A novel MILP approach for simultaneous optimization of water and energy: Application to a Canadian softwood Kraft pulping mill

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Abstract

An optimization methodology based on Mixed Integer Linear Programming (MILP) has been developed for simultaneous optimization of water and energy (SOWE) in industrial processes. The superstructure integrates non-water process thermal streams and optimizes the consumption of water, while maximizing internal heat recovery to reduce thermal utility consumption. To address the complexity of water and energy stream distribution in pulp and paper processes, three features have been incorporated in the proposed SOWE method: **(a)** Non-Isothermal Mixing (NIM) has been considered through different locations to reduce the number of thermal streams and decrease the investment cost by avoiding unnecessary investment on heat exchangers; **(b)** the concept of restricted matches combined with water tanks has been added to the superstructure; and **(c)** the Integer-Cut Constraint technique has been combined with the MILP model to systematically generate a set of optimal solutions to support the decision-making for cost-effective configurations. The performance of the proposed improved MILP approach has been evaluated using several examples from the literature and applied to a Canadian softwood Kraft pulping mill as an industrial case study. The results indicate that this approach provides enhanced key performance indicators as compared to conceptual and non-linear complex mathematical optimization approaches.

Keyword: mathematical programming, combined mass and heat optimization, non-isothermal mixing; process integration; industrial application

1 Introduction

Minimizing the environmental impact of industrial operations means optimizing the use of natural resources, especially water, energy, and raw materials. In the context of climate change, as pointed out by the Conference of Parties in Paris (COP21), the efficient use of energy, water, and other resources is one of the solutions that could substantially reduce industrial Greenhouse Gas (GHG) emissions. The Canadian industrial sector accounts for 30.6% of secondary energy use and 22.1% of secondary energy-related GHG emissions, thus constituting the second largest GHG emitter after transportation (Natural Resources Canada, 2013). Among the possible techniques to improve industrial process efficiency and optimize the use of energy, water, and other resources, process integration is a powerful approach used in various industrial processes, such as petroleum refining as well as in the chemical, food and beverage, petrochemical, and pulp and paper industries. Process integration can be used to find the best design options to minimize the use of thermal energy in a process. Pinch analysis, a simple process integration technique, applies thermodynamic principles to optimize heat recovery systems in industrial facilities. In conducting pinch analysis, process engineers examine the pathways where heat is being used, where it can be recovered, and how it can best be applied across the process. Pinch analysis comprises a diagnosis phase, during which potential for improvement is determined, followed by an optimization phase, during which heat recovery measures that improve energy efficiency are identified. Over the past few decades, process integration has spread into other fields, with the introduction of Mass Integration (MI) or Resource Conservation methodologies. In the first published work on this topic (Takama et al., 1980), water allocation was optimized in a petroleum refinery, using the Complex method developed by Box (1965) and improved by Guin (1968) and by Krus et al. (1992). This method requires only the iterative computation of the design calculations and it is not necessary to find any gradients. This method is capable of optimizing a "black-box" system with few constraints on the optimization function and requiring no knowledge of its derivatives. This method is widely applicable to the optimal design of process systems. The El-Halwagi group contributed significantly to the development of MI methods (El-Halwagi and Manousiouthakis, 1990a, 1990b, 1989). They applied the pinch technique to mass integration. Most works in this field only consider chemical compositions, leaving aside property-based constraints (e.g. viscosity, toxicity, etc.). Shelley and El-Halwagi (2000) were the first to address these problems. Ponce-Ortega et al. (2010) addressed environmental constraints for combined mass and property-based networks. The properties included in their models are chemical composition, density, viscosity, pH, reflectivity, colour, odour, and chemical oxygen demand. They used a relaxation approach to remove bilinear terms.

The ultimate goal of these approaches should not be limited to reducing utility consumption: they should also address raw material consumption. Srinivas and El-Halwagi (1994) had the first publication on combined heat and reactive mass exchange networks. Their proposed method is a two-stage targeting procedure: in the first stage, the minimum operating cost of the network is identified by a Mixed Integer Non-Linear Programming (MINLP) model, while in the second stage, the minimum number of exchangers needed to satisfy this minimum cost is determined. The solution of the first stage is used in two sub-problems (due to decomposition of the original problem) to identify the minimum number of heat and mass exchangers. Papalexandri and Pistikopoulos (1994) addressed the problem of simultaneous synthesis of mass and heat exchange processes with varying flow rates and inlet compositions and concentrations that were modelled using a multi-period MINLP approach.

Mass streams are subjected to heating and/or cooling duties, and in some cases, they are used to produce heat and power (e.g. hydrogen, methane, and sludge). As a result, there is a trade-off between using the mass in the process and consuming it for heat and power generation. Gassner and Maréchal (2010) addressed combined mass and energy integration in syngas upgrading using multicomponent membrane gas separation systems. It was shown that reducing the crude syngas recovery ratio increases the quality of depleted gas that can be used as a hot utility or further recycled in the process. The same approach has been applied in liquid biofuel production (Tock et al., 2010), combined production of sugar and bioethanol (Morandin et al., 2011), hydrogen production from lignocellulosic biomass (Tock and Maréchal, 2012), and most recently, ammonia production (Tock et al., 2015).

The main contribution of combined mass and energy integration comes from the studies on heat-integrated water allocation networks. In addition to the water consumption for heating and/or cooling water systems, water is also used for energy production. This emphasizes the intertwined nature of water and energy. Due to the complexities arising from the nexus between water and energy, there is a need to develop systematic and unified frameworks for modelling and decision-making (Varbanov, 2014).

2 State of the art in simultaneous optimization of water and energy

Several reviews on combined water and energy optimization have been published. Bagajewicz (2000) and Furman and Sahinidis (2002) cover developments in water network design and heat exchanger network design. Foo (2009), Jeżowski (2010), and Ahmetović et al. (2015) reviewed the pinch methods applied in water network design. In the most recent review (Ahmetović et al., 2015), 83 articles are examined and compared, based on the methods' features and functionalities. This paper provides a more recent review, as shown in Tables 1 and 2.

Combined mass and energy integration is one of the major topics in the field of process integration. Water scarcity and tightened environmental policies regarding wastewater disposal, along with the intertwined nature of water and energy have motivated researchers to propose methodologies for simultaneous integration of water and energy. Two main research institutions have initiated early developments in this field: Texas A&M University (El-Halwagi, 1997; Srinivas and El-Halwagi, 1994) and the Centre for Process Integration of the University of Manchester Institute of Science and Technology (Savulescu and Smith, 1998).

Two main methodologies have been considered: conceptual *versus.* mathematical, driven by two main approaches: sequential *versus.* simultaneous. Most of the articles reviewed consider water and energy simultaneously in their methodology. Conceptual approaches use graphical tools and heuristics to obtain the optimized water-energy network. They are preferred by engineering experts, as they can provide insight on the whole procedure and are linked to expert judgment. Conceptual methods have some drawbacks. They cannot guarantee that the global optimum or a good sub-optimal solution will be found, because they do not consider all HEN design options. Furthermore, the application of conceptual methods in large-scale case studies is somewhat difficult, as they are not suitable for large amounts of plant operating data. These drawbacks make mathematical approaches all the more promising.

Mathematical approaches are based on the construction of a superstructure of all possible connections and heat exchanges. The more complete the superstructure, the more complex the network and mathematical formulation. The optimal network will then be selected, while minimizing an objective function (e.g. total cost of water and heat exchanger network, operating costs of the system, number of matches in heat exchanger network) subjected to thermal and water network constraints. A complete MINLP model makes it possible to design detailed heat exchanger and water networks. Binary variables that account for fixed operating/investment costs or existence/non-existence of a network connection can be included.

2.1 Solving techniques

Most simultaneous mass and energy optimization problems are non-linear, with binary variables representing equipment or topological constraints. As a result, the superstructure will be a non-convex MINLP problem, which will be difficult to solve for the global optimum. In parallel to developing these superstructures, researchers looked for ways of solving these problems. The classification proposed by (Jeżowski, 2010) is adapted to address problem-solving techniques.

Linearization: Bilinear terms arise in the mass exchanger network, due to the multiplication of flow rates and contamination loads. For the single-contaminant case, Savelski and Bagajewicz (2000) stated the optimality conditions for which the formulation can be linearized. The necessary conditions for optimality in multi-contaminant cases were proved by Savelski and Bagajewicz (2003) and later adapted by Yang and Grossmann (2012) in their methodology. They proposed a linear model for multi-contaminant cases at the level of utility consumption targeting. Bagajewicz et al. (2002) have also used MILP formulation for simultaneous optimization of water and energy.

Initialization: Another way to find the “global” optimum is to start from a local optimum and then proceed to the global one. All of the methods are based on solving a simplified configuration of the main problem. The first guess can be found through either a stochastic approach (Xiao et al., 2009), solving a linearized MINLP problem, or considering a random initial guess (Zhou and Li, 2015).

Sequential procedure: In this procedure, the MINLP problem will be decomposed into a few sub-problems, and they will be solved sequentially. The variables of one problem will become the parameters of another problem. Many researchers have used this technique for solving their proposed MINLP model. The two-stage strategy consists of a targeting stage and a HEN design stage (Ahmetović and Kravanja, 2012; Bogataj and Bagajewicz, 2008; Chen et al., 2010; Liao et al., 2008, 2011). Leewongtanawit and Kim (2008) proposed NLP-MILP decomposition for solving the simultaneous optimization of water and energy: having fixed the contaminations and temperatures, the model becomes a MILP. The result of this optimization (i.e. binary variables of connections in the water network and heat exchanger network) becomes the input of the NLP model. Consequentially, the result of the NLP model (i.e. temperatures and contamination concentrations) becomes the input of the MILP model. The procedure is solved iteratively until the stopping criteria are reached.

Meta-heuristic: Over the past years, meta-heuristic techniques have emerged as promising techniques for solving problems in process integration approaches. Xiao et al. (2009) used evolutionary strategies and manipulations as the last stage of their method for improving water and heat exchanger network configurations. Liu et al. (2013) used a hybrid algorithm called genetic algorithm combined with simulated annealing developed previously by Yu et al. (2000) for solving the combined water and energy problem. They selected the mass flow rate and mass transfer temperatures of lean streams, the overall outlet concentrations, and the temperature difference contribution of streams as the decision variables.

2.2 Utility integration

Only few publicly available works have addressed systematic utility integration in the combined water and heat network. It should be noted that most plants use steam and cooling water as hot and cold utilities, respectively. The water for steam production should have a high purity for consumption in the boiler; besides, cooling water should be integrated in the water network as it is water and an energy carrier. Kim et al. (2001) addressed the problem of temperature restriction on effluents. They stated that inconvenient mixing of effluents results in inefficient heat recovery and a low driving force for the cooling system. Chew et al. (2007) investigated a particular case of simultaneous water and energy minimization, applied to a chilled water network. Panjeshahi et al. (2009) expanded the method of Kim and Smith (2001) to account for interactions between the cooling network and the heat exchanger network.

2.3 Non-isothermal mixing

There are two types of non-isothermal mixing (NIM): homogeneous and heterogeneous. Homogeneous NIM occurs between two cold streams or two hot streams, while heterogeneous NIM takes place between a hot and a cold stream (Yiqing et al., 2012). Homogeneous NIM cannot decrease utility consumption, but heterogeneous NIM can decrease, increase, or even have no effect at all on utility consumption. Heterogeneous NIM potentially reduces the energy consumption as long as it takes place within the pinch interval and between streams with temperatures in the same pinch temperature range. Non-isothermal mixing has the ability of reducing the number of heat exchangers and hence reducing the investment cost of the system. This is a non-linear problem, due to the multiplication of mass flow streams and their unknown temperature.

There are three main methods for implementing NIM in a water network superstructure, as shown in Figure 1:

Figure 1 here

In Figure 1a (left), direct heat exchange before indirect heat exchange: All the streams are mixed non-isothermally and then heated up or cooled down through a heat exchanger, before entering the operating unit. In Figure 1b (middle), indirect heat exchange before direct heat exchange: The streams from different sources pass through heat exchangers before being mixed non-isothermally. The mixture's temperature and contamination level correspond to the demand of the operating unit. This method is non-linear, due to the unknown mass flows and outlet temperatures of each heat exchanger. George et al. (2011) used DNLP (Non-Linear Programming with Discontinuous Derivatives) for NIM formulation. In Figure 1c (right), the streams are mixed non-isothermally and will then pass through a heat exchanger to reach the required temperature. Only water utility streams are allowed to exchange heat indirectly through heat exchangers. Bogataj and Bagajewicz (2008) have used this method and their superstructure was computed using a NLP (Non-Linear Programming) approach.

Table 1 here

Table 2 here

According to the literature review above, solving optimization problems combining mass and energy integration does not include process operational uncertainties and environmental metrics. In this paper, a novel MILP formulation is proposed for simultaneous optimization of water and energy. Such a formulation includes non-isothermal mixing opportunities, multi-contaminant problems, and integer-cut constraint (ICC) to enable the generation of an ordered list of solutions to the MILP superstructure. Non-isothermal mixing is addressed through pre-defined temperature levels selected thanks to expert insights into the superstructure. ICC will support the decision-maker in selecting the best options with respect to an objective that is not included in the optimization. A second MILP optimization can be performed based on the first-stage results for the HEN conceptual design. This will help identifying promising heat exchange matches in the system that can be investigated and evaluated for practical implementation. The proposed method makes use of non-water thermal streams in the process, which have not been considered in any previous optimization methods. The problems were implemented in AMPL (Fourer et al., 2003). The MILP models are solved using CPLEX solver.

3 SOWE methodology

Simultaneous Optimization of Water and Energy (SOWE) introduces a novel superstructure that integrates process thermal streams and optimizes the consumption of water, while maximizing internal heat recovery to reduce thermal utility consumption. Three important concepts related to specific issues in pulp and paper processes have been developed and incorporated in the SOWE methodology, namely: **(a) non-isothermal mixing** that has been considered at different locations to reduce the number of thermal streams and decrease investment costs by avoiding unnecessary investment on heat exchangers; **(b) restricted matches and water tanks** that have been added to the superstructure to adapt it to the pulp and paper case studies; and **(c) integer-cut constraint technique**, which has been combined with the MILP model to systematically generate a set of optimal solutions to support decision-making for cost-effective configurations. The SOWE methodology is based on seven successive steps: (1) plant characterization; (2) quantification of qualitative constraints; (3) modelling; (4) preliminary targeting; (5) optimization problem-solving; (6) identification and evaluation of energy and water reduction opportunities; and (7) projects selection and roadmap implementation. These steps are detailed in section 3.3.

3.1 Problem statement

Two sets of water unit operation parameters ($\mathrm{P_{out}^{WN}}$, $\mathrm{P_{in}^{WN}}$) are given. Each unit j in $\mathrm{P_{in}^{WN}}$ needs water at temperature $\mathrm{T_j}$, with a maximum allowed contamination level of $\mathrm{C_j^{k,max}}$ and a flow rate of $\mathrm{m_j}$. Each unit i in $\mathrm{P_{out}^{WN}}$ provides water at temperature $\mathrm{T_i}$, with a contamination level of $\mathrm{C_i^{k,max}}$ and a flow rate of $\mathrm{m_i}$. Furthermore, sets of hot and cold non-water process streams ($\mathrm{P^H}, \mathrm{P^C}$) are also considered. They are characterized by inlet temperatures ($\mathrm{T_{p,in}^H}, \mathrm{T_{p,in}^C}$), outlet temperatures ($\mathrm{T_{p,out}^H}, \mathrm{T_{p,out}^C}$), and heat loads ($\mathrm{Q_p^H}, \mathrm{Q_p^C}$), respectively. Thermal hot and cold utilities ($\mathrm{U^H}, \mathrm{U^C}$) are also available in case the energy within the system is not sufficient to satisfy energy demands. In addition, multiple fresh-water sources and waste-water sinks ($\mathrm{U_{out}^{WN}}$, $\mathrm{U_{in}^{WN}}$) are given. Multiple water utilities are needed in order to respond to the demand of water having different qualities. Further, different waste-water sinks accept waste at different contamination levels, according to different wastewater treatment facilities. The objective is to reduce water and energy consumption in the system, while satisfying heat and mass demands.

3.2 MILP formulation

The superstructure proposed in this paper is based on a MILP model. It includes the water network, the heat network (using a heat cascade model), and connections between the two (i.e. incorporating the water thermal streams within the heat cascade model).

An innovative linearized formulation of the NIM has been integrated in the superstructure, combining the above-mentioned methods. The idea involves fixing the temperature at which non-isothermal mixing takes place based on pre-defined values. The primary source of these temperatures is the set of inlet/outlet temperatures based on the current operating conditions of the process. A variation of these temperatures is possible, but must consider the operating limitations of the mill. Figure 2 shows a simple superstructure for two water network utilities (i.e. wastewater disposal and freshwater), and two water network processes (one demand and one source). The contamination levels are not shown, for the purpose of simplicity. This simple model contains four (4) temperatures, namely $\mathrm{T_i}, \mathrm{T_j}, \mathrm{T_{fw}}, \mathrm{T_{ww}}$. All possible interconnections are formulated.

Figure 2 here

The objective function (Eq. 1) is to minimize the total cost of the network. It includes operating costs and annualized investment costs. Operating costs consist of freshwater consumption, wastewater production, as well as hot and cold utility consumption. Annualized investment costs include the investment cost of the utilities. Additionally, a ranking factor (i.e. penalizing) is attributed to each thermal stream in the water network. This factor is an estimated investment cost corresponding to a fictitious counter-current heat exchanger in which the thermal stream is passing. The minimum approach temperature is assumed constant for each stream. The detailed mathematical formulation is provided in Appendix A.

Objective function

$$= \min \left\{ \begin{array}{c} \left(\sum_{\mathrm{fw} \in \mathrm{U}_{\mathrm{out}}^{\mathrm{WN}}} \boldsymbol{m}_{\mathrm{fw}} . \mathrm{C}_{\mathrm{fw}} + \sum_{\mathrm{ww} \in \mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}} \boldsymbol{m}_{\mathrm{ww}} . \mathrm{C}_{\mathrm{ww}}\right) \times \mathrm{t}_{\mathrm{operating}} \\ + \\ \left(\sum_{\mathrm{u} \in \mathrm{U}^{\mathrm{H}}} \boldsymbol{f}_{\mathrm{u}}^{\mathrm{H}} . \mathrm{q}_{\mathrm{u}}^{\mathrm{H}} + \sum_{\mathrm{u} \in \mathrm{U}^{\mathrm{C}}} \boldsymbol{f}_{\mathrm{u}}^{\mathrm{C}} . \mathrm{q}_{\mathrm{u}}^{\mathrm{C}}\right) \times \mathrm{t}_{\mathrm{operating}} \\ + \\ \dfrac{\mathrm{i}.(1+\mathrm{i})^{\mathrm{n}_{\mathrm{year}}}}{(1+\mathrm{i})^{\mathrm{n}_{\mathrm{year}}}-1} . \times \left(\begin{array}{c} \sum_{\mathrm{u} \in \mathrm{U}^{\mathrm{H}}} \left(\boldsymbol{y}_{\mathrm{u}}^{\mathrm{H}} . \mathrm{I}_{\mathrm{f,u}}^{\mathrm{H}} + \boldsymbol{f}_{\mathrm{u}}^{\mathrm{H}} . \mathrm{I}_{\mathrm{p,u}}^{\mathrm{H}}\right) \\ + \\ \sum_{\mathrm{u} \in \mathrm{U}^{\mathrm{C}}} \left(\boldsymbol{y}_{\mathrm{u}}^{\mathrm{C}} . \mathrm{I}_{\mathrm{f,u}}^{\mathrm{C}} + \boldsymbol{f}_{\mathrm{u}}^{\mathrm{C}} . \mathrm{I}_{\mathrm{p,u}}^{\mathrm{C}}\right) \end{array} \right) \\ + \\ \dfrac{\mathrm{i}.(1+\mathrm{i})^{\mathrm{n}_{\mathrm{year}}}}{(1+\mathrm{i})^{\mathrm{n}_{\mathrm{year}}}-1} \times \left(\sum_{\mathrm{i} \in \mathrm{P}^{\mathrm{WN}} \cup \mathrm{U}^{\mathrm{WN}}} \left(\sum_{\mathrm{t} \in \mathrm{T}} \boldsymbol{m}_{\mathrm{i,t}} . \mathrm{I}_{\mathrm{p,i,t}}^{\mathrm{WN}}\right)\right) \end{array} \right\}$$

(Eq. 1)

Where:

$$\mathrm{I}_{\mathrm{p,i,t}}^{\mathrm{WN}} = \mathrm{k}_1 + \mathrm{k}_2 \log\left(\frac{\mathrm{q}_{\mathrm{i,t}}^{\mathrm{WN}}}{\mathrm{U}.\Delta\mathrm{T}_{\mathrm{lm,i,t}}}\right) + \mathrm{k}_3 \left(\log\left(\frac{\mathrm{q}_{\mathrm{i,t}}^{\mathrm{WN}}}{U.\Delta\mathrm{T}_{\mathrm{lm,i,t}}}\right)\right)^2 \quad \text{(Eq. 2)}$$

$\mathrm{k}_1, \mathrm{k}_2$, and k_3 are parameters that must be taken into account to determine the cost of a counter-current heat exchanger. In a more detailed model, the cost of piping can also be added to account for distances in the plant (Chew et al., 2008).

$$C_{\mathrm{i,j}}^{\mathrm{piping}} = \mathrm{D}_{\mathrm{i,j}} \left(\sum_{\mathrm{t} \in \mathrm{T}} \sum_{\mathrm{t'} \in \mathrm{T}} \left(\mathrm{I}_{\mathrm{f}}^{\mathrm{piping}} \times \boldsymbol{y}_{\mathrm{i,j,t,t'}} + \mathrm{I}_{\mathrm{p}}^{\mathrm{piping}} \times \boldsymbol{m}_{\mathrm{i,j,t,t'}}\right)\right) \quad \text{(Eq. 3)}$$

$$\forall\, \mathrm{i} \in \mathrm{P}_{\mathrm{out}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{out}}^{\mathrm{WN}} \text{ and } \forall\, \mathrm{j} \in \mathrm{P}_{\mathrm{in}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}$$

Where: $\boldsymbol{y}_{\mathrm{i,j,t,t'}} . \mathrm{m}_{\mathrm{i,j,t,t'}}^{\mathrm{min}} \leq \boldsymbol{m}_{\mathrm{i,j,t,t'}} \leq \boldsymbol{y}_{\mathrm{i,j,t,t'}} . \mathrm{m}_{\mathrm{j}}$

3.3 Step-by-step approach to address complex industrial problems

A step-wise approach that embeds the mathematical formulation above is proposed to tackle large and complex industrial problems:

1. *Plant characterization*

   The first step consists of characterizing the industrial site and understanding the processes involved, as well as their specificities. This step is crucial, as the subsequent steps rely on a deep understanding of the nature of the processes and their mode of operation. Three elements are important to integrate at this stage:

   a) Establishment of project priorities, mill champion, and study objectives: active partnership, constant communication, and participation of mill personnel are key factors of success to produce a quality process integration study at an industrial site, and one that will facilitate the implementation of the energy and water savings opportunities identified using the SOWE methodology.

   b) Data collection: This step focuses on collecting necessary and sufficient data from the process. It should be carried out in collaboration with the mill personnel. It involves defining the problem and gathering data in order to build a representative mill model. For water networks, the only data that must be obtained relates to outlet and inlet water streams and their qualities. Recycling, reusing, and regenerating water streams can be excluded, as the superstructure is able to generate these connections and add them to the optimization problem automatically.

   c) Mill simulation model: A simulation model based on mass and energy balances can be an additional tool to facilitate model definition. Access to a reconciled simulated model of the mill will help in the extraction of a coherent set of data to use in the definition of the mathematical model. Such a model will also help in simulating the energy and water savings opportunities and correctly assessing related impacts on the process.

2. *Quantification of qualitative constraints*

If no data is available on the quality of mass streams (e.g. water contamination), this step aims at introducing recycling and reusing opportunities by applying the concept of restricted matches. Therefore, regular communication with engineering experts on possible and feasible matches is necessary to better incorporate conceptual criteria into mathematical programming of the SOWE methodology.

The concept of restricted matches has been introduced to account for contamination levels and mill topology constraints. The latter include economic and process topology limitations (e.g. recycling between two unit operations or a heat exchange between two streams can be beneficial or disadvantageous, depending on economic or physical location limitations). Moreover, the concept of restricted matches does not require the use of contamination levels, which are rarely measured in pulp and paper processes.

In order to apply this concept, a level of restriction, $\mathrm{RM^k}_\mathrm{i}$, is defined for each unit, using binary values (0 meaning no connection is allowed between a source water unit operation and demand water unit operation, while 1 allows the connection). Equation (Eq. 4) constrains any match having the parameters:

$$\sum_{t,t' \in T} \sum_{i \in \mathrm{P^{WN}_{out}}\ \mathrm{U^{WN}_{out}}} \mathrm{RM^k}_\mathrm{i} \times \boldsymbol{m}_{\mathrm{i,j,t,t'}} \geq \mathrm{RM^k}_\mathrm{j} \times \mathrm{m_j} \qquad \forall j \in \mathrm{P^{WN}_{in}} \cup \mathrm{U^{WN}_{in}} \qquad \text{(Eq. 4)}$$

3. *Modelling*

The mathematical model is built using the data collected or extracted from the simulation model of the mill. The mathematical modelling used the MILP formulation described in the present publication (Section 3.2). As in the pulp and paper industry, the contaminant levels are rarely made fully available, the model has been sufficiently made flexible to include contaminant levels if available and uses the concept of restricted matches in the case that contaminant levels are not provided.

4. *Preliminary targeting*

   Before any optimization, one can evaluate the preliminary water and energy targets of the whole process. This provides a lower bound for the subsequent step. Due to the inclusion of process constraints, these targets can never be reached in real scenarios.

5. *Optimization problem-solving*

   Solving the optimization problem consists of two sequential MILP formulations:

   SOWE formulation with integer-cut constraint (ICC)

   The proposed SOWE superstructure is a MILP model consisting of integer variables and continuous variables. It is possible to find alternative optimal solutions to a MILP problem if more than one set of stated variables can satisfy the same value of the objective function. These alternatives can be useful, as they allow the decision-maker to find all of the solutions to the problem. These solutions need to be classified in terms of operating and capital costs. Therefore, an integer cut constraint functionality, incorporated in the solving algorithm, was used.

   Heat Load Distribution

   SOWE-ICC will provide several water networks in the increasing order of the MILP objective function. For each of these solutions, the set of all hot and cold thermal streams in the network can be listed (i.e. water thermal streams, utility thermal streams, and process thermal streams).

At this stage, Heat Load Distribution (HLD) will be applied as a preliminary step, prior to the detailed design of the heat exchanger network.

HLD is formulated as a MILP model, based on minimizing the total number of connections among all hot and cold streams (Marechal et al., 1989; Mian et al., 2016). HLD answers two main questions:

a. Which streams are connected to each other?

b. What are the related heat loads of these connections?

$\dot{\boldsymbol{Q}}_{ikj}$ is defined as the heat from hot streams ‘i’ in heat cascade interval ‘k’ to cold stream ‘j’ in the intervals ‘k’ and below. The objective function is to minimize the total number of connections between hot and cold streams. In the most general representation, a penalty cost (p_{ij}) can be linked to each connection for ranking purposes.

$$\min_{y_{ij},\dot{\boldsymbol{Q}}_{ikj}} \sum_{i \in HS} \sum_{j \in CS} p_{ij} . \mathbf{y}_{ij} \qquad \text{(Eq. 5)}$$

Thermal balance of hot streams in each temperature interval:

$$\sum_{j \in CS} \dot{Q}_{ikj} = \dot{Q}_{ik} \qquad \forall i \in HS, \forall k \in TI \qquad \text{(Eq. 6)}$$

Thermal balance of cold streams:

$$\sum_{i \in HS} \sum_{k \in TI} \dot{Q}_{ikj} = \dot{Q}_j \qquad \forall j \in CS \qquad \text{(Eq. 7)}$$

The upper and lower bounds on the heat transfer:

$$\sum_{k \in TI} \dot{Q}_{ikj} - y_{ij} . \dot{Q}_{ij}^{max} \leq 0 \, , \qquad \forall i \in HS, \forall j \in CS \qquad \text{(Eq. 8)}$$

$$\sum_{k \in TI} \dot{Q}_{ikj} - y_{ij}.\dot{Q}_{ij}^{min} \geq 0 \qquad \forall i \in HS, \forall j \in CS \tag{Eq. 9}$$

Feasibility of the connection:

$$\sum_{i \in HS} \sum_{r=1}^{k} \dot{Q}_{irj} - \sum_{r=1}^{k} \dot{Q}_{jr} \geq 0 \qquad \forall j \in CS, \forall k \in TI \tag{Eq. 10}$$

$$\dot{Q}_{ikj} \geq 0 \qquad \forall j \in CS, \qquad \forall i \in HS, \qquad \forall k \in TI \tag{Eq. 11}$$

Moreover, the total heat transfer from all the hot streams in intervals k and below should be lower than the total heat required by the cold streams in those intervals:

$$\sum_{i \in HS} \dot{Q}_{ikj} - \sum_{r=k}^{k_{end}} \dot{Q}_{jr} \leq 0 \qquad \forall j \in CS, \forall k \in TI \tag{Eq. 12}$$

6. *Identification and evaluation of energy and water reduction opportunities*

Several HLD results are available for different optimal water networks. Energy and water reduction opportunities can be extracted at this stage. Recycling and reduction opportunities in the water network and large heat exchanges are targeted to identify opportunities that should be evaluated for economical, physical, and thermodynamic feasibilities. This step should be conducted in collaboration with mill personnel. Any unfeasible project can be discarded or added as a constraint if a subsequent iteration is performed.

7. *Project selection and implementation roadmap*

The most promising projects are selected. The impacts and interactions with other projects are also detailed at this step. A sequence of implementation with short-medium and long-term vision is also proposed. Once again, this step must be completed in close collaboration with mill personnel.

4 Validation of SOWE methodology using standard test cases

Although the proposed SOWE methodology was designed to tackle complex problems, a first validation was conducted using three standard test cases commonly used by the scientific community involved in this area. The first test case is a single-contaminant problem compared to a conceptual approach, as introduced in (Savulescu et al., 2005a, 2005b). The second example is a single-contaminant problem compared to a MILP sequential approach, introduced in (Bagajewicz et al., 2002). The third case is a multi-contaminant problem compared with a MINLP approach from (Dong et al., 2008). A series of key performance indicators, including energy and water targets, as well as a HEN structure and economics have been evaluated for the three test cases. It was observed that most state-of-the-art methodologies are able to reach the minimum energy and water target (i.e. fresh water consumption and hot and cold utility consumption). Therefore, the emphasis is placed on network indicators, such as the number of thermal flows, the number of water streams, and the number of non-isothermal mixing points. Table 3 summarizes the network indicators for the 3 test cases, based on benchmarking SOWE methodology with others. Overall, the number of thermal flows and the number of mixing points (i.e. the number of water streams) are reduced. This results in a simplified network that can enable SOWE applications for industrial case studies.

Table 3 here

5 Industrial application

Available test cases in the literature aim at evaluating the performance of the proposed methodologies on simplified examples for demonstration/proof-of-concept purposes. To our knowledge, none of the reviewed papers refers to an industrial case study. Due to highly constrained optimization problems and the complex operational structures of industrial processes, conventional optimization methods are not often directly applicable. This is mainly due to:

- A high number of process streams within the system, which will result in complexities of the network and higher computational time.
- Process topology constraints (i.e. physical locations and restricted exchanges).
- Lack of available and/or reliable data (i.e. having insufficient measurements for mathematical modelling purposes). For example, the contamination levels of the water network involved in the actual industrial production systems need to be taken into account, to identify potential practical and plausible recovery solutions.

The pulp and paper industry was chosen as the first potential industrial application of the SOWE methodology. This industry is energy-intensive, and a large amount of energy is transferred to complex fresh water and contaminated water networks, making it the ideal candidate to validate the performance, robustness, and reliability of the SOWE methodology. To address the specific configurations of water and heat exchanger networks of the pulp and paper processes, two novel concepts have been included in the SOWE methodology: water tanks and restricted matches, to address the lack of industrial data related to water contamination levels. These concepts were first tested on a simplified pulp and paper process configuration, including the most important pulping unit operations of a Canadian Kraft pulping mill. A real industrial case study is then presented to illustrate the potential of the SOWE methodology.

5.1 Simplified industrial case study

A simplified Kraft pulping mill case study was chosen to illustrate the potential application of SOWE, using the concepts of restricted matches and water tanks. Data on streams are provided in Table 4, which includes the available hot process thermal streams and process water streams of the five (5) main Kraft departments (i.e. stock preparation, washing, bleaching, pulp machine, and recausticizing).

Given that quantitative contamination levels of water streams are unavailable, qualitative restrictions are defined and modelled using the concept of restricted matches. The following operational constraints are considered:

1. Outlet of recausticizing, washing, and bleaching cannot be recycled.
2. Outlet of the pulp machine can only be recycled in the washing section or sent to the sewer.
3. Outlet of the stock preparation can only be recycled in the bleaching section or sent to the sewer.
4. No fresh water can be used to dilute the wastewater streams.
5. No recycling can take place within each tank.
6. A connection is possible from the cold water tank to the hot water tank, either directly or through a heat exchanger.

Table 4 here

The number of water tanks added to the superstructure corresponds to the number of tanks available in the existing process. However, it is possible to define additional tanks that could be considered as new equipment with a capital cost associated. In the present example, only existing tanks were defined, namely warm and hot water tanks.

In the current operating conditions, 137 kg/s of fresh water is used to meet the water demands while cooling down the process hot streams. Moreover, 3,392 kW of hot utility is used to heat up the water in order to satisfy water demands. The wastewater is rejected at 58.6^{o}C to the effluent stream, which – for environmental reasons – should be later cooled down to 30^{o}C by 136 kg/s of fresh water. In total, 273 kg/s of water should be consumed.

The results are presented in Table 5. It shows that by using the SOWE methodology, the total water consumption will be reduced by 17%, while no thermal hot utility is used. Total cost decreases by 34%, which is mainly due to the high potential of integrating thermal streams and water streams at the same time and decreasing operating costs.

Table 5 here

The current water network and the optimal water network, developed using the SOWE methodology, are shown in Figure 3 and Figure 4, respectively. Note that the SOWE methodology-based solution is one among many that can be generated using integer-cut constraint. In the current condition (Figure), most of the non-water thermal streams are being used to heat up and feed the fresh water into water tanks. However, as it can be seen, about 22 kg/s of water from the warm water tank and 5 kg/s of water from the hot water tank are directed to wastewater disposal. This, combined with the fact that there are no recycling options, increases fresh water use and, consequently, hot utility consumption. An improved water network configuration and better water recycling methods produced through the application of the SOWE methodology demonstrate how all process heating demands can be satisfied by available non-water thermal streams (Figure). The number of mixings (including non-isothermal mixings) has increased from 9 (all NIM) to 11 (of which 10 are NIM), due to a better use of the available heat in water streams.

Figure 3 here

Figure 4 here

The heat load distribution formulation has been applied to the water network in Figure , and the result is presented in Figure 5. From this result, one can observe the connections between hot and cold streams and extract any promising heat exchange, such as the one between non-water process stream “2” and outlet of cold water tank, which has the second highest heat load (~ 8,058 kW). This connection should be further evaluated for geographical or thermodynamic feasibilities. Using the simplified Kraft mill model, the adapted SOWE methodology combined with ICC and HLD has been tested successfully. In the next section, an actual large-scale pulp and paper mill is considered.

Figure 5 here

5.2 Industrial case study

The industrial case study addressed in this paper is a large-scale pulp and paper mill located in Canada, producing up to 1,000 air-dry-tonnes of Kraft pulp per day. Figure shows a general representation of the main sections of the Kraft pulping process. Each section can have water, heating, or cooling demands. The clean cold water is used in all of the mill's departments for cooling or dilution purposes. The cooling water is then stocked in warm and hot water tanks and distributed to the processes. Steam (represented as "S" in Figure 6) is used to compensate for the temperature drop resulting from the injection of clean cold water. Moreover, water can be recovered from some sections, such as washing or bleaching, to be reused within other sections of the mill. The existing water-heat network of this mill consists of the following sets:

- Twenty-three (23) cold process streams that are currently heated using steam.
- Twenty (20) hot process streams that are currently cooled within the water network.
- Six (6) waste hot streams that can be recovered for heating purposes.
- Hot utility is steam produced in the mill at two (2) different pressure levels: medium (10-12 bar) and low pressure (5 bar).
- Four (4) water tanks, namely the fresh water (20°C), treated warm water (28°C), raw warm water (52°C), and treated hot water (60°C) tanks. The latter act as hubs in which water streams can be mixed and used in other processes.

- Nine (9) water unit operations on the demand side, and five (5) on the source side.
- A fresh water source.
- Waste water disposal.

Figure 6 here

The data encompasses the main hot and cold process thermal streams (Table 6 and Table 7), as well as the water process streams of the main departments (Table 8). Thermal losses (waste heat) in the effluents are also included, as they contribute to the heat recovery potential (Table 9).

Tables 6 to 9 here

Due to the high number of units and streams involved, three assumptions were made to simplify data extraction and build the related mathematical model:

- The water unit operations with their corresponding temperatures and maximum allowed inlet or outlet contaminations should be extracted. The MILP superstructure will automatically generate all of the thermal streams within the water network and add them to the optimization problem.
- Streams passing in heat exchangers (in series) are combined into a single grassroots stream (i.e. hot streams that pass through three heat exchangers for the desuperheating, condensation, and subcooling stages are modelled as one stream). Phase changes are still modelled with the corresponding heat load.
- Hot thermal streams with unknown (i.e. unmeasured) temperatures are replaced by the corresponding cooling water streams from heat exchangers. This adds two units of water demand and water supply to the problem.

In the current state of the mill, the cold non-water process streams are heated up with steam, while the hot non-water process streams are cooled down in the water network. As a result, there is no heat integration between hot and cold process streams, which results in high consumption of water and steam. The water process operations are satisfied in the water network, but any heating required in the water network is satisfied by steam.

5.2.1 Model constraints definition

Similar to the previous standard test case, there is no measurement of the quality of water unit operations (e.g. quality of water in the outlet of the washing section or minimum quality of water necessary for the bleaching section). Kraft pulping mills are rarely equipped with water quality monitoring techniques. To mitigate this challenge, several recycling and reuse streams can be incorporated in the model, using the concept of restricted matches. The options to restrict or free any connection are commonly decided by an expert panel, in order to make informed decisions that take into account the mill's operational conditions. Figure 7 illustrates the proposed matches in the water network. This concept can be further applied to heat exchanges among thermal streams, resulting from economic, geographical, or process-specific constraints.

Figure 7 here

5.2.2 Targeting and water network

Table 10 shows the utility consumption for both the current condition of the mill and the result of applying the SOWE methodology. It can be observed that both water and hot utility consumption were simultaneously reduced by 34% and 21%, respectively.

Table 10 here

These reductions are mainly made possible through the optimization of the water network. The new network is less complex, having a reduced number of shipments of water among water unit operations. This facilitates industrial implementation. Table 11 shows indicators of the water network, comparing the current case with an optimized solution based on the SOWE methodology.

Table 11 here

5.2.3 Heat load distribution and identification of opportunities

The HLD method was applied to the water network, and the results are shown in Figure 8. To account for the physical locations of the constraints, the mill was divided into four (4) locations, namely:

- Location 1: digester, washing, and bleaching
- Location 2: pulp machine
- Location 3: concentration, stripping, and recausticizing
- Location 4: power boilers

Figure 8 here

Heat integration between these locations is favoured through the water network only. The hot utility (i.e. steam) can provide heat to all four locations.

For each location, the heat load distribution shows the connections between streams and the related heat loads of these connections. All of these connections serve to reach the energy and water targets defined earlier in Table 10. Several types of heat exchanges can be observed by looking at the heat load distribution:

- Classical usage of a hot utility to heat cold streams: Injecting steam in the steaming vessel (~5.7 MW) (Location 1) or non-avoidable steam usage in the dryer (~19.4 MW) (Location 2).
- New heat recovery opportunity: Preheating warm water from 52°C to 60°C by condensing the flash steam of an evaporator (~9.2 MW) (Location 3).
- Unusual heat exchanges: Using the flash steam from the evaporator in the concentration section instead of the hot utility (~15.4MW) (Location 3). Unusual heat exchanges should be presented and discussed with mill personnel in order to assess their feasibility.

- Unfeasible exchanges such as preheating wood chips with a hot stream other than steam (~1.1 MW) (Location 3). When unfeasible exchanges are identified, they could be added as a constraint to the model for the next round of optimization.

6 Concluding remarks and future outlook

A novel MILP superstructure for simultaneous optimization of water and energy is proposed. It accounts for non-isothermal mixing alternatives and can address multi-contaminant problems. Furthermore, non-water thermal streams can also be added to the problem and exchange heat with water thermal streams, using the heat cascade formulation.

Three test cases from the literature were presented, and the results were compared with different methodologies. In all cases, the minimum targets were reached. The number of hot and cold thermal streams was reduced, through the correct implementation of non-isothermal mixing in the superstructure.

In order to apply the methodology to large-scale cases, several concepts were integrated into the methodology: water tanks and restricted matches. In addition, two mathematical techniques were incorporated to generate a set of solutions to guide decision-makers: integer-cut constraints to generate an ordered set of solutions, and heat load distribution to provide a list of preliminary and promising connections in the heat network, prior to the detailed design of the heat exchanger network. This adapted methodology was applied on a simplified Kraft process and on a real Kraft process, and the result indicates promising opportunities for industrial application of the methodology.

Future work will focus on expanding the methodology by adding the design of the heat exchanger network. It will also focus on detailing the last steps of our methodology, which concern the identification and evaluation of energy and water reduction opportunities and the project selection and implementation roadmap.

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Nomenclature

Abbreviations

Adt	Air-dried ton
AMPL	A Mathematical Programming Language
C	Cold
DNLP	Nonlinear Programming with Discontinuous Derivatives
FW	Fresh Water
FWT	Fresh Water Tank
GA-SA	Genetic Algorithm combined with Simulated Annealing
GHG	Green House Gas
H	Hot
HE(N)	Heat Exchanger (Network)
HLD	Heat Load Distribution
HW	Hot Waste
ICC	Integer Cut Constraint
(N)LP	(Non-)Linear programming
MI	Mass Integration

MI(N)LP	Mixed Integer (Non-)Linear Programming
NIM	Non-Isothermal Mixing
RM	Restricted Matches
RWWT	Raw Warm Water Tank
SOWE	Simultaneous Optimization of Water and Energy
TAC	Total Annualized Cost
THWT	Treated Hot Water Tank
TWWT	Treated Warm Water Tank
W	Water
WN	Water Network
WWTN	Wastewater Treatment Network

Sets

CS	Set of all cold thermal streams (HLD)
HS	Set of all hot thermal streams (HLD)
$\mathrm{P}_{\mathrm{out}}^{\mathrm{WN}}$	Set of source process water unit operations
$\mathrm{P}_{\mathrm{in}}^{\mathrm{WN}}$	Set of demand process water unit operations
P^{WN}	Set of process water unit operations $\left(\mathrm{P}_{\mathrm{out}}^{\mathrm{WN}} \cup \mathrm{P}_{\mathrm{in}}^{\mathrm{WN}}\right)$
P^{H}	Set of hot non-water processes
P^{C}	Set of cold non-water processes
T	Set of temperatures in water network
TI	Set of temperature intervals (HLD)
$\mathrm{U}_{\mathrm{out}}^{\mathrm{WN}}$	Set of freshwater sources
$\mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}$	Set of wastewater sinks
U^{WN}	Set of utility water unit operations $\left(\mathrm{U}_{\mathrm{out}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}\right)$
U^{H}	Set of hot non-water utilities
U^{C}	Set of cold non-water utilities

Parameters

$c_{p,i}$	Heat capacity of water unit operation i	[kJ/(kg.K)]
C_{fw}	Cost of source freshwater unit fw	[USD/kg]
C_{ww}	Cost of sink wastewater unit ww	[USD/kg]
$C_j^{k,max}$	Maximum allowed contamination level k to inlet water unit j	[-]
$C_i^{k,max}$	Maximum allowed contamination level k outlet of water unit i	[-]
$D_{i,j}$	Distance between process water unit operation (water utilities) i and j	[m]
I_f^{piping}	Fixed cost of water piping	[USD/m]
I_p^{piping}	Proportional cost of water piping	[USD/(m.kg)]
$I_{f,u}^{H}$	Fixed investment cost of hot non-water utility u	[USD]
$I_{p,u}^{H}$	Proportional investment cost of hot non-water utility u	[USD/unit]
$I_{f,u}^{C}$	Fixed investment cost of cold non-water utility u	[USD]
$I_{p,u}^{C}$	Proportional investment cost of cold non-water utility u	[USD/unit]
i	Interest rate	[-]
m_i	Mass flowrate of source process water unit operation i	[kg/s]
m_j	Mass flowrate of demand process water unit operation j	[kg/s]
$m_{i,j,t,t'}^{min}$	Minimum mass flowrate allowed between unit i and j from temperature T_t to $T_{t'}$	[kg/s]
n_{year}	System life-time	[yr]
n_r	Number of temperature intervals	
q_u^H	Heat load of hot non-water utility stream	[kW/unit]
q_u^C	Heat load of cold non-water utility stream	[kW/unit]
Q_p^H	Heat load of hot non-water process stream p	[kW]
Q_p^C	Heat load of cold non-water process stream p	[kW]
$\dot{Q}_j$	Heat load of cold stream j (HLD)	

$\dot{\mathrm{Q}}_{\mathrm{ik}}$	Heat load of hot stream i in temperature interval k (HLD)	
$\mathrm{RM^{k}}_{\mathrm{i}}$	Restricted match at level k for unit i	
$\mathrm{t_{operating}}$	Operating time	[hr]
$\mathrm{T^{H}_{p,in}}$	Inlet temperature of hot non-water process stream p	[K]
$\mathrm{T^{C}_{p,in}}$	Inlet temperature of cold non-water process stream p	[K]
$\mathrm{T^{H}_{p,out}}$	Outlet temperature of hot non-water process stream p	[K]
$\mathrm{T^{C}_{p,out}}$	Outlet temperature of cold non-water process stream p	[K]
$\mathrm{T_{i}}$	Temperature of source process water unit operation i	[K]
$\mathrm{T_{j}}$	Temperature of demand process water unit operation j	[K]
$\mathrm{T_{fw}}$	Temperature of source freshwater unit fw	[K]
$\mathrm{T_{ww}}$	Temperature of sink wastewater unit ww	[K]
U	Overall heat-transfer coefficient	kW/(m$^{2\mathrm{o}}$C)

Indices

fw	Source freshwater utility
i	Source water unit operation, or hot stream (HLD)
j	Demand water unit operation, or cold stream (HLD)
k	Contamination level, temperature interval (HLD)
p	Process unit
t, t'	Temperature
u	Hot/cold utility
ww	Sink wastewater utility

Calculated parameters

$\mathrm{c^{k,max}_{i,t}}$	Contamination k of unit i at temperature T_t	
$\mathrm{c^{k,max}_{i,j,t,t'}}$	Contamination k of unit i at temperature T_t going to unit j at temperature $T_{t'}$	
$\mathrm{f^{H,min}_{u}}$	Minimum size of hot utility u	[-]

$\mathrm{f_u^{H,max}}$	Maximum size of hot utility u	[-]
$\mathrm{f_u^{C,min}}$	Minimum size of cold utility u	[-]
$\mathrm{f_u^{C,max}}$	Maximum size of cold utility u	[-]
$\mathrm{I_{p,i,t}^{WN}}$	Proportional investment cost of water unit operation $\mathrm{P_i^{WN}}$ from T_i to T_t	[USD]
$\mathrm{q_{i,t}^{WN}}$	Heat load of water stream from temperature T_i to temperature T_t	[kJ/kg]
$\mathrm{q_{i,t,r}^{WN}}$	Heat load of water stream from temperature T_i to temperature T_t in interval r	[kJ/kg]
$\mathrm{q_{u,r}^{H}}$	Heat load of hot non-water utility stream at temperature interval r	[kW]
$\mathrm{q_{u,r}^{C}}$	Heat load of cold non-water utility stream at temperature interval r	[kW]
$\mathrm{Q_{p,r}^{H}}$	Heat load of hot non-water process stream p in temperature interval r	[kW]
$\mathrm{Q_{p,r}^{C}}$	Heat load of cold non-water process stream p in temperature interval r	[kW]
$\dot{Q}_{ij}^{max}$	Maximum allowed heat exchange between cold stream j and hot stream i	[kW]
$\dot{Q}_{ij}^{min}$	Minimum allowed heat exchange between cold stream j and hot stream i	[kW]
$\dot{Q}_{ik}$	Heat load of hot stream i in temperature interval k	[kW]
$\mathrm{\Delta T_{lm,i,t}}$	Minimum approach temperature for stream from T_i to T_t	[K]

Continuous variables

$\boldsymbol{C}_{\mathrm{j}}^{\mathrm{k}}$	Contamination level k inlet to water unit *j*	[-]
$\boldsymbol{C}_{i,j}^{piping}$	Cost of piping from unit i to unit *j*	[USD]
$\boldsymbol{f}_u^C$	Size of cold non-water utility stream u	[-]
$\boldsymbol{f}_u^H$	Size of hot non-water utility stream u	[-]
$\boldsymbol{m}_{i,j,t,t'}$	Mass flowrate between unit i and *j* from temperature T_t to $T_{t'}$	[kg/s]
$\boldsymbol{m}_{i,t}$	Mass flowrate from water unit operation i at T_i going to T_t	[kg/s]
$\boldsymbol{m}_{j,t}$	Mass flowrate at T_t going to water unit operation *j* at T_j	[kg/s]
$\boldsymbol{m}_{fw}$	Mass flowrate of freshwater utility fw	[kg/s]
$\boldsymbol{m}_{fw,t}$	Mass flowrate of unit fw at T_{fw} going to T_t	[kg/s]

$\boldsymbol{m}_{ww}$	Mass flowrate of wastewater utility ww	[kg/s]
$\boldsymbol{m}_{ww,t}$	Mass flowrate at T_t going to mixer ww at T_{ww}	[kg/s]
$\boldsymbol{R}_r$	Cascaded heat at interval r	[kW]
$\dot{\boldsymbol{Q}}_{ikj}$	Heat exchange from hot stream i at interval k to cold stream j at interval k and below (HLD)	[kW]

Binary variables

$\boldsymbol{y}_u^H$	Binary variable for the existence of hot utility u	[-]
$\boldsymbol{y}_u^C$	Binary variable for the existence of cold utility u	[-]
$\boldsymbol{y}_{i,t}$	Binary variable for the existence of water unit operation i at T_t	[-]
$\boldsymbol{y}_{j,t}$	Binary variable for the existence of water unit operation j at T_t	[-]
$\boldsymbol{y}_{fw}$	Binary variable for the existence of waste sink fw	[-]
$\boldsymbol{y}_{ww}$	Binary variable for the existence of waste sink ww	[-]
$\boldsymbol{y}_u$	Binary variable for the existence of utility u	[-]
$\boldsymbol{y}_{i,j,t,t'}$	Binary variable for existence of a connection from unit i at T_i to unit j at T_j	[-]
$\boldsymbol{y}_{ij}$	Binary variable for the existence of a connection between hot stream i and cold stream j (HLD)	[-]

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Appendix A Extended mathematical formulation

A.1 Water network

The mathematical representation of the water network is presented here. Figure A-1 outlines the different parameters and variables in the water network. The set of temperatures, T, is given as:

$$\mathrm{T} = \left\{\mathrm{T_i} | \mathrm{i} \in \mathrm{P_{out}^{WN}} \cup \mathrm{U_{out}^{WN}}\right\} \cup \left\{\mathrm{T_j} | \mathrm{j} \in \mathrm{P_{in}^{WN}} \cup \mathrm{U_{in}^{WN}}\right\} \qquad \text{(Eq. A-1)}$$

Figure A-1 here

<u>Initials splitters</u>: Mass balance and contamination equality hold for each initial splitter on the source side.

$$\mathrm{m_i} = \sum_{\mathrm{t \in T}} \boldsymbol{m}_{\mathrm{i,t}} \qquad \forall\, \mathrm{i} \in \mathrm{P_{out}^{WN}} \cup \mathrm{U_{out}^{WN}}$$

$$\mathrm{c_{i,t}^{k,max}} = \mathrm{c_i^{k,max}} \qquad \forall\, \mathrm{i} \in \mathrm{P_{out}^{WN}} \cup \mathrm{U_{out}^{WN}}, \qquad \mathrm{t} \in \mathrm{T}$$

<u>Middle splitters</u>: Mass balance and contamination equality hold for each middle splitter on the source side.

$$\boldsymbol{m}_{\mathrm{i,t}} = \sum_{\mathrm{t' \in T}} \sum_{\mathrm{j \in P_{in}^{WN} \cup U_{in}^{WN}}} \boldsymbol{m}_{\mathrm{i,j,t,t'}} \qquad \forall\, \mathrm{i} \in \mathrm{P_{out}^{WN}} \cup \mathrm{U_{out}^{WN}}, \qquad \mathrm{t} \in \mathrm{T}$$

$$\mathrm{c_{i,j,t,t'}^{k,max}} = \mathrm{c_i^{k,max}} \qquad \forall\, \mathrm{i} \in \mathrm{P_{out}^{WN}} \cup \mathrm{U_{out}^{WN}}, \qquad \mathrm{j} \in \mathrm{P_{in}^{WN}} \cup \mathrm{U_{in}^{WN}}, \qquad \mathrm{t, t'} \in \mathrm{T}, \quad \mathrm{k} \in \mathrm{C}$$

<u>Middle mixers</u>:

Mass balance:

$$\sum_{\mathrm{i \in P_{out}^{WN} \cup U_{out}^{WN}}} \sum_{\mathrm{t' \in T}} \boldsymbol{m}_{\mathrm{i,j,t',t}} = \boldsymbol{m}_{\mathrm{j,t}} \quad \forall\, \mathrm{j} \in \mathrm{P_{in}^{WN}} \cup \mathrm{U_{in}^{WN}}, \mathrm{t} \in \mathrm{T}$$

Middle mixers are non-isothermal mixers. The formulation is given below. The inlet and outlet temperatures of the mixers are fixed and are given by set T.

$$\sum_{\mathrm{i} \in \mathrm{P}_{\mathrm{out}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{out}}^{\mathrm{WN}}} \sum_{\mathrm{t}' \in \mathrm{T}} \boldsymbol{m}_{\mathrm{i,j,t',t}} . \mathrm{T}_{\mathrm{t}'} = \boldsymbol{m}_{\mathrm{j,t}} . \mathrm{T}_{\mathrm{t}} \quad \forall \, \mathrm{j} \in \mathrm{P}_{\mathrm{in}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}, \mathrm{t} \in \mathrm{T}$$

Final mixers:

Mass balance:

$$\mathrm{m}_{\mathrm{j}} = \sum_{\mathrm{t} \in \mathrm{T}} \mathbf{m}_{\mathrm{j,t}} \qquad \forall \, \mathrm{j} \in \mathrm{P}_{\mathrm{in}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}$$

The general multi-contaminant problem is a non-linear formulation, due to the multiplication of mass flow and contamination levels. As proven by (Yang and Grossmann, 2012), by fixing the contamination levels at their maximum allowable levels, the minimum fresh water target achieved is the same as the optimum predicted by the non-linear equation, under a specific condition (i.e. at least one contamination level reaches its maximum, as well as for all the process units with nonzero water reuse streams).

$$\sum_{\mathrm{i} \in \mathrm{P}_{\mathrm{out}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{out}}^{\mathrm{WN}}} \sum_{\mathrm{t}' \in \mathrm{T}} \sum_{\mathrm{t} \in \mathrm{T}} \boldsymbol{m}_{\mathrm{i,j,t',t}} \times \mathbf{c}_{\mathrm{i,j,t',t}}^{\mathrm{k}} \leq \boldsymbol{m}_{\mathrm{j}} \times \mathbf{c}_{\mathrm{j}}^{\mathrm{k}} \qquad \forall \, \mathrm{j} \in \mathrm{P}_{\mathrm{in}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}$$

$$\sum_{\mathrm{i} \in \mathrm{P}_{\mathrm{out}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{out}}^{\mathrm{WN}}} \sum_{\mathrm{t}' \in \mathrm{T}} \sum_{\mathrm{t} \in \mathrm{T}} \boldsymbol{m}_{\mathrm{i,j,t',t}} \times \mathrm{c}_{\mathrm{i,j,t',t}}^{\mathrm{k,max}} \leq \boldsymbol{m}_{\mathrm{j}} \times \mathrm{c}_{\mathrm{j}}^{\mathrm{k,max}} \quad \forall \, \mathrm{j} \in \mathrm{P}_{\mathrm{in}}^{\mathrm{WN}} \cup \mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}$$

***Overall mass balance*:**

$$\sum_{\mathrm{j} \in \mathrm{P}_{\mathrm{in}}^{\mathrm{WN}}} \mathrm{m}_{\mathrm{j}} + \sum_{\mathrm{ww} \in \mathrm{U}_{\mathrm{in}}^{\mathrm{WN}}} \boldsymbol{m}_{\mathrm{ww}} = \sum_{\mathrm{i} \in \mathrm{P}_{\mathrm{out}}^{\mathrm{WN}}} \mathrm{m}_{\mathrm{i}} + \sum_{\mathrm{fw} \in \mathrm{U}_{\mathrm{out}}^{\mathrm{WN}}} \boldsymbol{m}_{\mathrm{fw}}$$

A.1.1 Connections between the water network and the heat cascade network

$$q_{\mathrm{i,t}}^{\mathrm{WN}} = \mathrm{c_{p,i}}.(\mathrm{T_t} - \mathrm{T_i}) \qquad \forall\, \mathrm{i} \in \mathrm{P_{out}^{WN}} \cup \mathrm{U_{out}^{WN}}, \qquad \mathrm{t} \in \mathrm{T}$$

$$q_{\mathrm{j,t}}^{\mathrm{WN}} = \mathrm{c_{p,i}}.\left(\mathrm{T_j} - \mathrm{T_t}\right) \qquad \forall\, \mathrm{j} \in \mathrm{P_{in}^{WN}} \cup \mathrm{U_{in}^{WN}}, \qquad \mathrm{t} \in \mathrm{T}$$

A.1.2 Logical constraints

1. Size of each stream after initial splitter in water network:

$$\boldsymbol{y}_{\mathrm{i,t}} \times \mathrm{m_{i,t}^{min}} \leq \boldsymbol{m}_{\mathrm{i,t}} \leq \boldsymbol{y}_{\mathrm{i,t}}.\mathrm{m_i} \qquad \forall\, \mathrm{i} \in \mathrm{P_{out}^{WN}}, \qquad \forall\, \mathrm{t} \in \mathrm{T}$$

2. Size of each stream after middle mixer in water network:

$$\boldsymbol{y}_{\mathrm{j,t}} \times \mathrm{m_{j,t}^{min}} \leq \boldsymbol{m}_{\mathrm{j,t}} \leq \boldsymbol{y}_{\mathrm{j,t}} \times \mathrm{m_j} \qquad \forall\, \mathrm{j} \in \mathrm{P_{in}^{WN}}, \qquad \forall\, \mathrm{t} \in \mathrm{T}$$

3. Size of source utilities in water network:

$$\boldsymbol{y}_{\mathrm{fw}} \times \mathrm{m_{fw}^{min}} \leq \boldsymbol{m}_{\mathrm{fw}} \leq \boldsymbol{y}_{\mathrm{fw}} \times \mathrm{m_{fw}^{max}} \qquad \forall\, \mathrm{fw} \in \mathrm{U_{out}^{WN}}$$

$$\boldsymbol{y}_{\mathrm{fw}} \times \mathrm{m_{fw}^{min}} \leq \boldsymbol{m}_{\mathrm{fw,t}} \leq \boldsymbol{y}_{\mathrm{fw}} \times \mathrm{m_{fw}^{max}} \qquad \forall\, \mathrm{fw} \in \mathrm{U_{out}^{WN}}, \qquad \forall\, \mathrm{t} \in \mathrm{T}$$

4. Size of sink utilities in water network:

$$\boldsymbol{y}_{\mathrm{ww}} \times \mathrm{m_{ww}^{min}} \leq \boldsymbol{m}_{\mathrm{ww}} \leq \boldsymbol{y}_{\mathrm{ww}} \times \mathrm{m_{ww}^{max}} \qquad \forall\, \mathrm{ww} \in \mathrm{U_{in}^{WN}}$$

$$\boldsymbol{y}_{\mathrm{ww}} \times \mathrm{m_{ww}^{min}} \leq \boldsymbol{m}_{\mathrm{ww,t}} \leq \boldsymbol{y}_{\mathrm{ww}} \times \mathrm{m_{ww}^{max}} \qquad \forall\, \mathrm{ww} \in \mathrm{U_{in}^{WN}}, \qquad \forall\, \mathrm{t} \in \mathrm{T}$$

5. Size of hot utilities in heat cascade network:

$$\boldsymbol{y}_{\mathrm{u}} \times \mathrm{f_u^{H,min}} \leq \boldsymbol{f}_{\mathrm{u}}^{\mathrm{H}} \leq \boldsymbol{y}_{\mathrm{u}} \times \mathrm{f_u^{H,max}} \qquad \forall\, \mathrm{u} \in \mathrm{U^H}$$

6. Size of cold utilities in heat network:

$$\boldsymbol{y}_{\mathrm{u}} \times \mathrm{f}_{\mathrm{u}}^{\mathrm{C,min}} \leq \boldsymbol{f}_{\mathrm{u}}^{\mathrm{C}} \leq \boldsymbol{y}_{\mathrm{u}} \times \mathrm{f}_{\mathrm{u}}^{\mathrm{C,max}} \qquad \forall\, \mathrm{u} \in \mathrm{U}^{\mathrm{C}}$$

A.1.3 Heat cascade model

The thermal streams of the heat network and the water network will contribute to heat integration. The heat cascade formulation is given below. Figure A-2 shows the heat balance for temperature interval r.

$$\begin{aligned}\boldsymbol{R}_{\mathrm{r}} = \boldsymbol{R}_{\mathrm{r}-1} &+ \left(\sum\nolimits_{\mathrm{u} \in \mathrm{U}^{\mathrm{H}}} \boldsymbol{f}_{\mathrm{u}}^{\mathrm{H}} \times \mathrm{q}_{\mathrm{u,r}}^{\mathrm{H}} - \sum\nolimits_{\mathrm{u} \in \mathrm{U}^{\mathrm{C}}} \boldsymbol{f}_{\mathrm{u}}^{\mathrm{C}} \times \mathrm{q}_{\mathrm{u,r}}^{\mathrm{C}}\right) \\ &+ \left(\sum\nolimits_{\mathrm{p} \in \mathrm{P}^{\mathrm{H}}} Q_{\mathrm{p,r}}^{\mathrm{H}} - \sum\nolimits_{\mathrm{p} \in \mathrm{P}^{\mathrm{C}}} Q_{\mathrm{p,r}}^{\mathrm{C}}\right) \\ &+ \left(\sum\nolimits_{\mathrm{i} \in \mathrm{P}^{\mathrm{WN}} \cup\, \mathrm{U}^{\mathrm{WN}} \mid \mathrm{q}_{\mathrm{i,t,r}}^{\mathrm{WN}} \geq 0} \sum\nolimits_{\mathrm{t} \in \mathrm{T}} \boldsymbol{m}_{\mathrm{i,t}} \times \left|\mathrm{q}_{\mathrm{i,t,r}}^{\mathrm{WN}}\right| \right. \\ &\left. - \sum\nolimits_{\mathrm{i} \in \mathrm{P}^{\mathrm{WN}} \cup\, \mathrm{U}^{\mathrm{WN}} \mid \mathrm{q}_{\mathrm{i,t,r}}^{\mathrm{WN}} \leq 0} \sum\nolimits_{\mathrm{t} \in \mathrm{T}} \boldsymbol{m}_{\mathrm{i,t}} \times \left|\mathrm{q}_{\mathrm{i,t,r}}^{\mathrm{WN}}\right|\right) \quad \forall\, \mathrm{r} = 1, \dots, \mathrm{n}_{\mathrm{r}}\end{aligned}$$

To close the balance, the first and the last heat cascades are set to zero.

$$\boldsymbol{R}_0 = 0, \boldsymbol{R}_{n_r} = 0$$

Figure A-2 here

List of captions

Figure 1. Alternatives for non-isothermal mixing implementation

Figure 2. Superstructure of combined water and energy network

Figure 3. Current water network of the simplified Kraft process

Figure 4. Optimal water network of the case study, based on the SOWE methodology

Figure 5. HLD results of the case study representing the matches and their corresponding heat loads

Figure 6. General view of the Kraft pulping process

Figure 7. Proposed water superstructure for recycling and reuse of water for the industrial case

Figure 9. HLD results of the water network

Figure A-1. Graphical representation of the superstructure

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Table 1. Comparison of articles on combined water and energy integration (network)

Table 2. Comparison of articles on combined water and energy integration (mathematical approaches)

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Table 10. Preliminary targeting of the industrial case

Table 11. Characterization of the water network of the industrial case

Table 1. Comparison of articles on combined water and energy integration (network)

	Methodology			**Approach**[1]			**Energy features**			**Network features**		
Articles	Conceptual	Mathematical	Combined	Separate	Sequential	Simultaneous	Non-water thermal streams	Utility streams	Contaminants[2]	Non-isothermal mixing	Storage (water tanks)	HEN
Current article			X		X	X	X	X	M	X	X	
(Ghazouani et al., 2015)			X			X		X	S	X		X
(Liu et al., 2015)		X			X	X			S	X		
(Zhou and Li, 2015)		X				X		X	M	X		X
(Zhou et al., 2015)		X				X		X	S	X		
(Liao et al., 2015)	X					X			S	X		X
(Zhao et al., 2015)	X				X				S	X		X
(Pintarič et al., 2014)		X				X		X	M	X	X	X
(Tan et al., 2014)			X			X		X	M	X		X
(Jiménez-Gutiérrez et al., 2014)		X				X		X	M	X		X
(Ibrić et al., 2014a)		X				X		X	M	X		X
(Ibrić et al., 2014b)		X			X	X		X	M	X		X
(Hou et al., 2014)	X					X			M			X
(Ahmetović et al., 2014)		X				X		X	M	X		X
(Ahmetović and Kravanja, 2014)		X				X	X	X	M	X		X
(Ibrić et al., 2013)		X			X	X		X	M	X		X
(Liu et al., 2013)			X		X	X		X	S	X		X
(Chew et al., 2013)		X				X		X	S	X		
(Ahmetović and Kravanja, 2013)		X				X		X	M	X		X
(Rojas-Torres et al., 2013)		X				X		X	M			X
(Yang and Grossmann, 2012)		X				X			M			X
(Martínez-Patiño et al., 2012)	X					X			S	X		X
(Sahu and Bandyopadhyay, 2012)			X		X			X	M	X		X
(Ahmetović and Kravanja, 2012)		X			X	X		X	M			X
(Boix et al., 2012)		X			X			X	S	X		X
(George et al., 2011)		X			X			X	M	X		X
(Wan Alwi et al., 2011)	X					X			S			X
(Martínez-Patiño et al., 2011)	X				X				S	X		X
(Liao et al., 2011)		X				X		X	S	X		X
(Chen et al., 2010)		X				X			M	X	X	
(Polley et al., 2010)	X			X					S			X
(Ataei and Yoo, 2010)			X		X			X	M	X		X
(Kim et al., 2009)		X				X		X	M			X
(Manan et al., 2009)	X				X			X	S	X		X
(Xiao et al., 2009)		X				X		X	M			X
(Leewongtanawit and Kim, 2009)	X				X				S	X		X
(Isafiade and Fraser, 2009)		X				X		X	M			X
(Feng et al., 2009)		X			X				M	X		
(Liao et al., 2008)		X			X			X	S	X		
(Bogataj and Bagajewicz, 2008)		X				X		X	M	X		X
(Dong et al., 2008)		X				X		X	M	X		X
(Leewongtanawit and Kim, 2008)		X				X		X	M	X		X
(Savulescu et al., 2005a, 2005b)	X					X		X	S	X		X
(Bagajewicz et al., 2002)		X			X				S	X		X

[1] in terms of water and energy integration

[2] contaminants: S – single; M – multiple

Table 2. Comparison of articles on combined water and energy integration (mathematical approaches)

	Objective functions				**Formulations**					**Additional features**		**Solution strategy**				
Articles	Targeting	Operating cost	Total annualized cost	Number of connections	LP	MILP	NLP	MINLP	DNLP	WWTN	Flow/heat loss/gain	Linearization	Initialization	Sequential	Meta-heuristic	Global optimization
Current article			X	X		X					X	X		X		
(Ghazouani et al., 2015)		X				X								X		
(Liu et al., 2015)		X						X						X		
(Zhou and Li, 2015)			X					X		X			X	X	X	
(Zhou et al., 2015)			X					X			X					X
(Pintarič et al., 2014)	X	X	X	X				X		X		-	-	NA	-	-
(Tan et al., 2014)		X						X								X
(Jiménez-Gutiérrez et al., 2014)			X		X		X	X				X		X		
(Ibrić et al., 2014a)		X	X				X	X					X	X		
(Ibrić et al., 2014b)		X	X				X	X					X	X		
(Ahmetović et al., 2014)			X					X		X			X	X		
(Ahmetović and Kravanja, 2014)			X					X					X	X		
(Ibrić et al., 2013)		X	X				X	X					X	X		
(Liu et al., 2013)			X					X						X	X	
(Chew et al., 2013)		X	X					X								X
(Ahmetović and Kravanja, 2013)			X				X	X						X		X
(Rojas-Torres et al., 2013)			X					X								X
(Yang and Grossmann, 2012)	X				X		X			X		X		X		
(Sahu and Bandyopadhyay, 2012)	X				X						X	X				
(Ahmetović and Kravanja, 2012)	X		X				X	X					X	X		
(Boix et al., 2012)	X		X			X		X		X		X	X	X		
(George et al., 2011)	X	X			X				X			X				X
(Liao et al., 2011)		X	X	X		X		X				X	X	X		
(Chen et al., 2010)	X	X	X			X		X		X				X		
(Ataei and Yoo, 2010)			X				X				X			X		
(Kim et al., 2009)			X					X								X
(Xiao et al., 2009)			X					X						X	X	
(Isafiade and Fraser, 2009)			X					X		X		-	-	NA	-	-
(Feng et al., 2009)	X							X						X		
(Liao et al., 2008)	X			X				X				X		X		
(Bogataj and Bagajewicz, 2008)	X		X				X	X		X			X	X		
(Dong et al., 2008)			X					X		X			X	X	X	
(Leewongtanawit and Kim, 2008)			X			X	X	X			X	X	X	X		
(Bagajewicz et al., 2002)	X			X	X	X						X		X		

Table 3. Validation of SOWE methodology using standard test cases

	Network indicators			
Test cases *versus* SOWE	**# of thermal flows**	**# of heat exchangers**	**area (m^2)**	**# of mixers (NIM)**
Single-contaminant test case by Savulescu et al., (2005a, 2005b)				
Savulescu et al., (2005a, 2005b)	9	5	4,531	9 (4)
SOWE	7	7	3,410	9 (3)
Single-contaminant test case with LP sequential approach by Bagajewicz et al., (2002)				
Bagajewicz et al., (2002)	14	12	4,092	21 (10)
SOWE	7	10	3,564	17 (8)
Multi-contaminant test case by Dong et al., (2008)				
Dong et al., (2008)	7	6	960.1	4 (2)
SOWE	6	6	568.8	6 (3)

Table 4. Operating data for the simplified Kraft pulp case study

Process Water Streams	T_{in} (°C)	T_{out} (°C)	m (kg/s)	**Process Thermal Streams**	T_{in} (°C)	T_{out} (°C)	Q (kW)
1. Pulp Machine	50	50	10	1	65	64	-7,560
2. Bleaching	70	70	20	2	95	50	-10,920
3. Washing	65	65	35	3	75	40	-2,205
4. Stock Preparation	62	62	25	4	59	30	-1,050
5. Recausticizing	35	35	20	5	80	65	-630
Water Utilities				**Thermal Utility**			
Fresh water	-	10	-	Hot utility	120	120	-
Waste water	-	30	-	Cold utility	10	35	-
Tanks							
Warm water tank	62	62	-				
Cold water tank	35	35	-				

Table 5. Key performance indicators for the simplified Kraft pulp mill case study

Key Performance Indicators	Units	Reference Case	SOWE
Fresh water	kg/s	137	104 (-24%)
Hot utility	kW	3,392	0 (-100%)
Cold utility[1]	kW (kg/s)	14,270 (136)	12,795 (122)
Total water consumption (fresh water + cooling water)		273	226 (-17%)
Waste outlet temperature	°C	54.8	59.4
Network Indicators[2]			
Number of thermal streams: total	-	15	10
Number of heat exchangers	-	8	8
Total area of HEs	m^2	2,978	3,620
Number of mixers (NIM)		9 (9)	11 (10)
Financial Indicators			
Operating cost	USD/yr	1,369,407	712,535 (-48%)
Investment cost	USD/yr	0	187,073
Total cost	USD/yr	1,369,407	899,607 (-34%)

[1] Cold utility required to cool down waste streams to 30°C. (The cold utility is assumed as fresh water from 10°C to 35°C.) A counter-current heat exchanger is assumed.

[2] One heat exchanger is considered for cooling down the waste stream.

Table 6. Kraft pulp data: Hot and cold process streams

Section/Stream ID	Type*	T_{in} (°C)	T_{out} (°C)	Heat Load (kW)
Digester				
Chip bin heater	C	20	55	3,290
Steaming vessel	C	55	123	13,585
Upper liquor heater	C	122	150	4,810
Lower liquor heater	C	146	160	5,750
Washer liquor heater	C	126	165	4,060
Black liquor flash tank 1	H	128	128	5,350
Black liquor flash tank 2	H	93	93	9,960
Turpentine condenser	H	123	60	1,915
Bleaching				
Steam mixer 1	C	70	75	1,860
Pulp heater	C	75	77	2,520
Steam mixer 2	C	72	80	2,630
Steam mixer 3	C	73	87	3,100
ClO_2 heater	C	5	43	4,185
Pulp machine				
Wash water heater	C	66	88	1,640
White water exchanger	C	66	88	1,670
Dryer	C	42	95	26,510
Room air preheater	C	21	25	210
Dryer air preheater	C	25	42	310
Economizer	C	38	66	4,365
Air preheater	C	20	21	70
Dryer exhaust - chimney	H	92	68	4,745
Evaporators, concentrators, and recovery boiler				
Evaporator heater (1st eff.)	C	119	139	33,390
Concentrator heater	C	106	111	16,220
Boiler air preheater	C	106	111	16,220
Black liquor heater	C	111	129	1,300
Stripping and ClO_2				
Stripping column heater	C	97	155	4,460
ClO_2 heater before reactor	C	65	75	3,170
* C: cold stream, H: hot stream				

Table 7. Kraft pulp data: Cooling water streams and corresponding process hot streams

Section	**From***	**To***	**Type***	**T_{in} (°C)**	**T_{out} (°C)**	**Heat Load (kW)**
Evaporators						
Primary condenser	FWT	FHD	W	20	50	22,650
			H	119	55	
Secondary condenser	FWT	FHD	W	20	30	2,360
			H	119	30	
Inter/After condenser	FWT	FWT	W	20	30	600
			H			
Flash Heat Double (FHD)						
Flash heat double cooler	-	RWWT	W	46	54	9,045
			H	65	65	
Non-condensable gas cooler	FWT	FWT	W	21	25	460
			H	81	81	
Inter/After condenser	FWT	FWT	W	20	30	1,340
			H			
ClO2 plant						
ClO2 cooler	FWT	FWT	W	20	24	560
			H	71	25	
Recausticizing						
Green liquor cooler	FWT	FWT	W	20	33	180
			H	93	25	
Bearing cooler	FWT	FWT	W	20	31	385
			H	80	40	
Pulp Machine						
Water cooler	FWT	Press shower	W	20	25	70
			H	120	105	
Cooler	FWT	Economizer	W	20	36	1,605
			H	46	30	
Stripping						
Reflux condenser	FWT	RWWT	W	20	60	4,365
			H	101	80	
Recovery Boiler						
Main surface condenser	TWWT	THWT	W	28	78	13,670
			H	89	88	
Auxiliary surface condenser	TWWT	THWT	W	28	70	3,080
			H	89	88	
Fan cooler	TWWT	THWT	W	28	38	1,340
			H	48	38	
Washing						
Cold blow cooler	FWT	FWT	W	20	34	2,930
			H	77	70	

*FWT: fresh water tank; RWWT: raw warm water tank; TWWT: treated warm water tank; THWT: treated hot water tank; H: hot process stream; W: water

Table 8. Kraft pulp data: Water unit operations

Section	Stream ID	T(℃)	Flowrate (kg/s)
Demand side			
Bleaching	Washers	60	69
ClO_2 plant	Absorption tower	13	29.8
	Showers	20	6.7
Recausticizing	Vacuum pump	20	16.7
	Pressure disc filter	60	6.7
Pulp machine	Vacuum pump	20	48.0
	Shower	45	6.5
	Recycled white water	71	578
Washing	Washers	60	69
Source side			
Recovery boiler	Smelt spout cooler	45	16
Contaminated condensate	Inlet of recausticizing	85	22
Recausticizing	Vacuum pump	36	16.7
Pulp machine	Vacuum pump	36	48
	White water outlet	66	666

Table 9. Kraft pulp data: Thermal waste streams

Section/Stream ID	Type*	T_{in} (°C)	T_{out} (°C)	Heat Load (kW)
Bleaching				
Alkaline bleach effluent	HW	82	35	14,852
Acid bleach effluent	HW	71	35	11,492
Pulp machine				
Dryer exhaust	HW	68	35	9,643
Evaporators				
Combined condensate	HW	89	35	4,608
Combine condensate to recausticizing	HW	85	71	1,475
*HW: hot waste				

Table 10. Preliminary targeting of the industrial case

			Current condition of the mill	**SOWE**
Steam consumption	5 bar	MW	136	131 (-3.6%)
	10-12 bar	MW	41	9 (-79%)
Total hot utility		MW	177	140 (-21%)
Water consumption		kg/s	592	390 (-34%)

Table 11. Characterization of the water network of the industrial case

	Current condition of the mill	**SOWE**
Tank		
Steam used in the tanks	Yes	No
NIM above 10°C	Yes	Yes
Overflow	Yes	No
NIM above 10°C	Yes	Yes, but less
Dilutions		
NIM above 10°C	Yes	Yes, but less
Water network indicators		
Number of heat exchangers	43	34

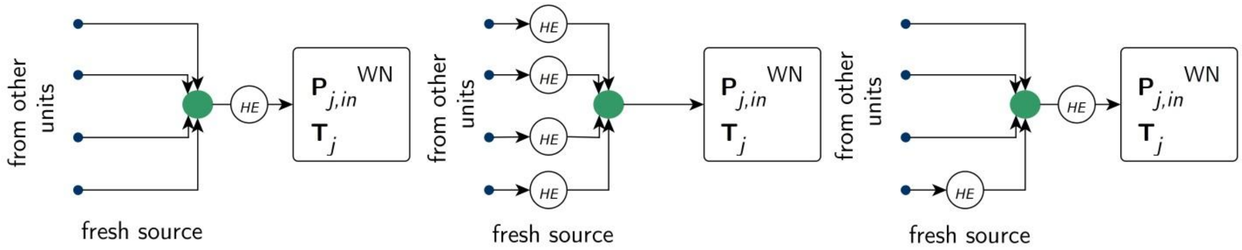

Figure 1. Alternatives for non-isothermal mixing implementation

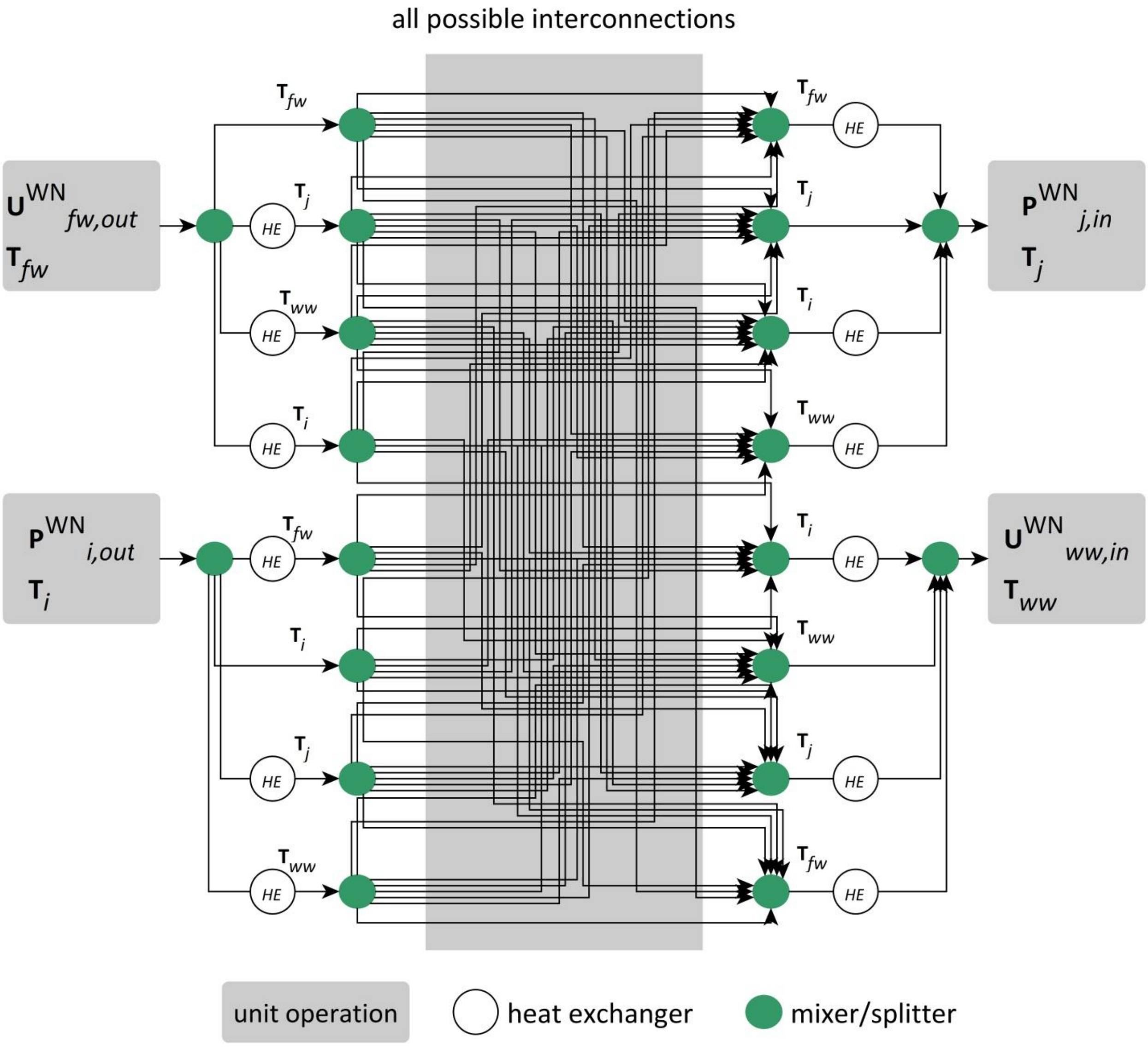

Figure 2. Superstructure of combined water and energy network

Figure 3

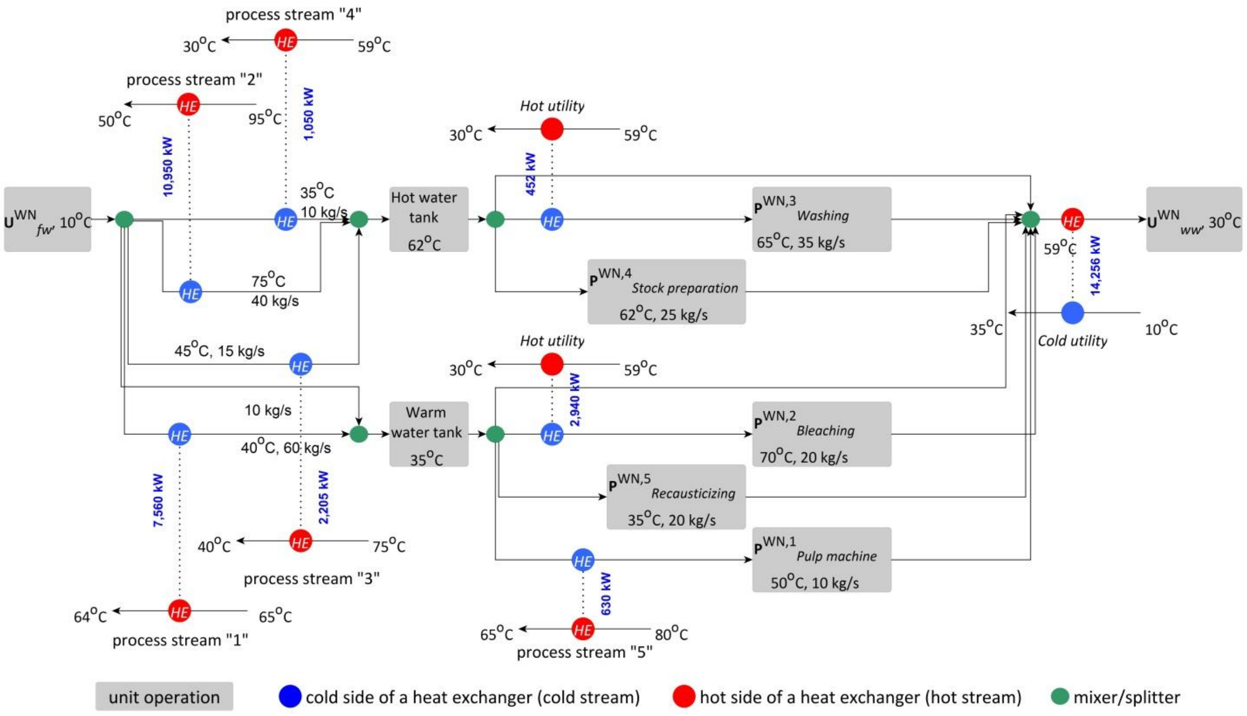

Figure 3. Current water network of the simplified Kraft process

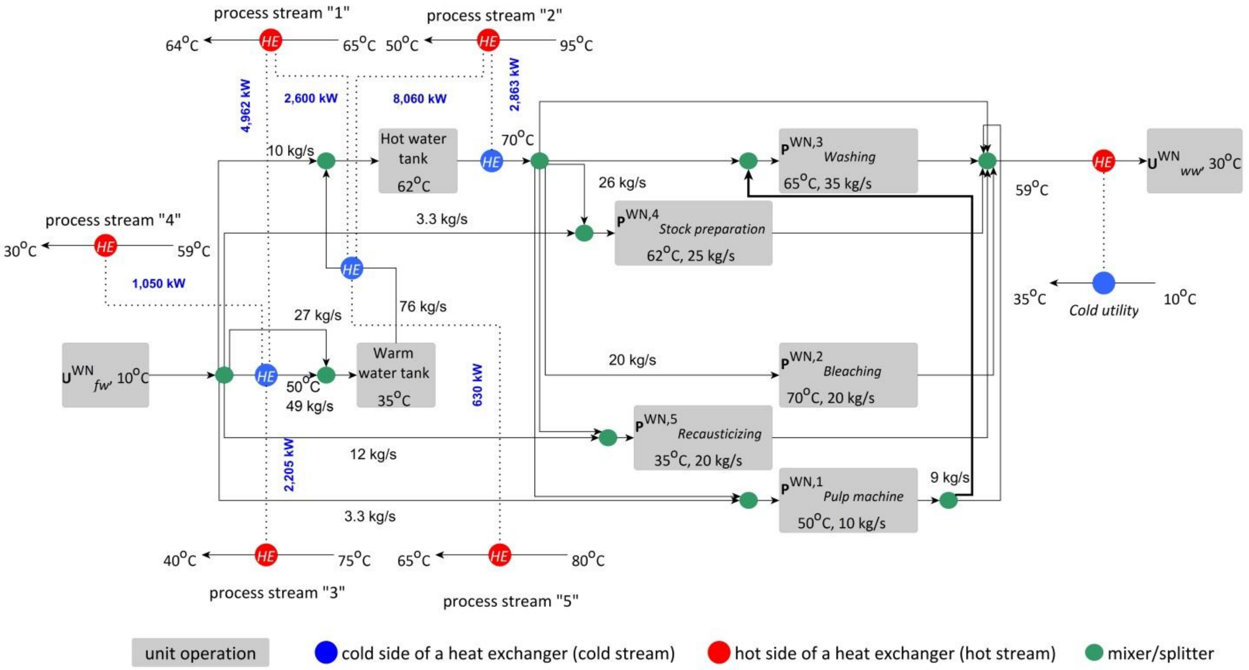

Figure 4. Optimal water network of the case study, based on the SOWE methodology

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Figure 5

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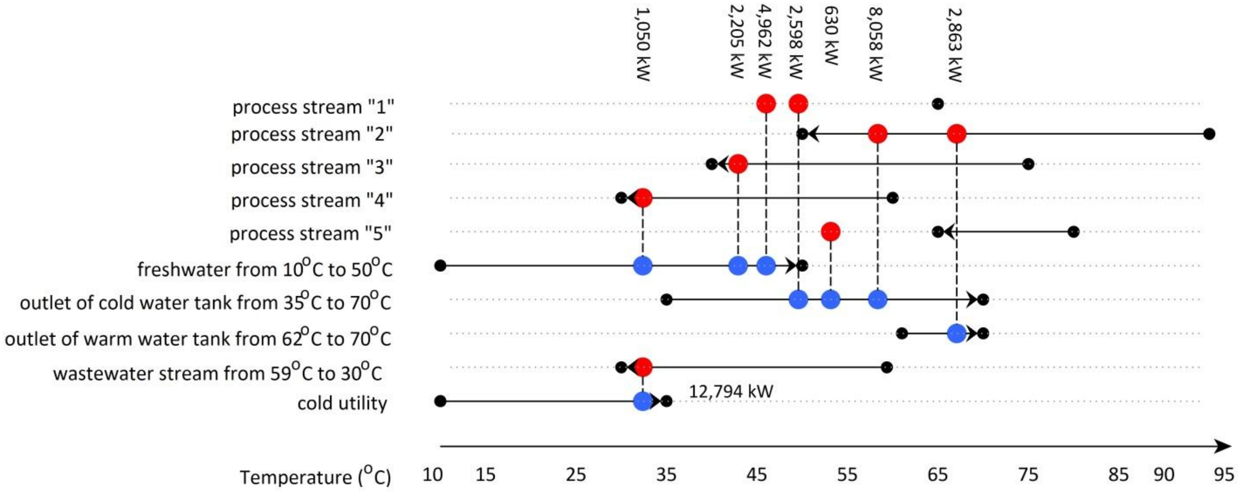

Figure 5. HLD results of the case study representing the matches and their corresponding heat loads

Figure 6

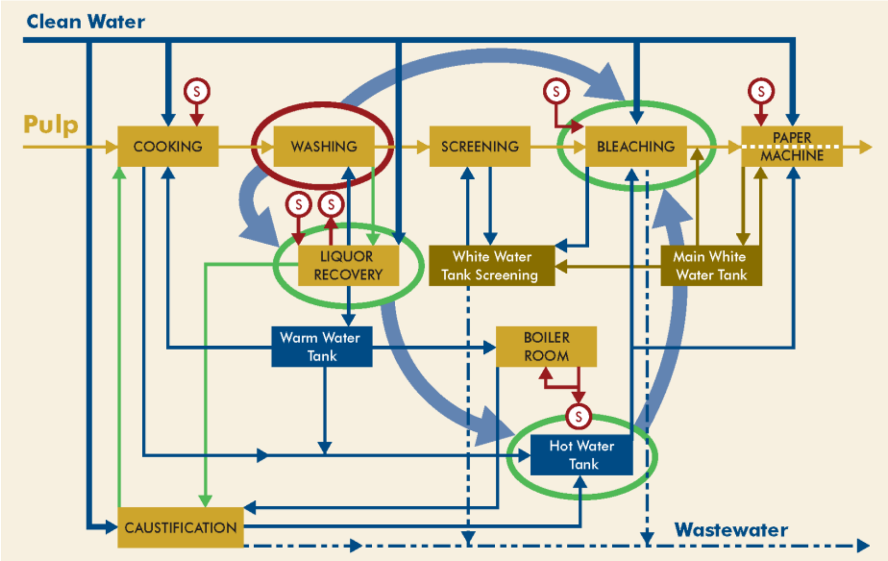

Figure 6. General view of the Kraft pulping process

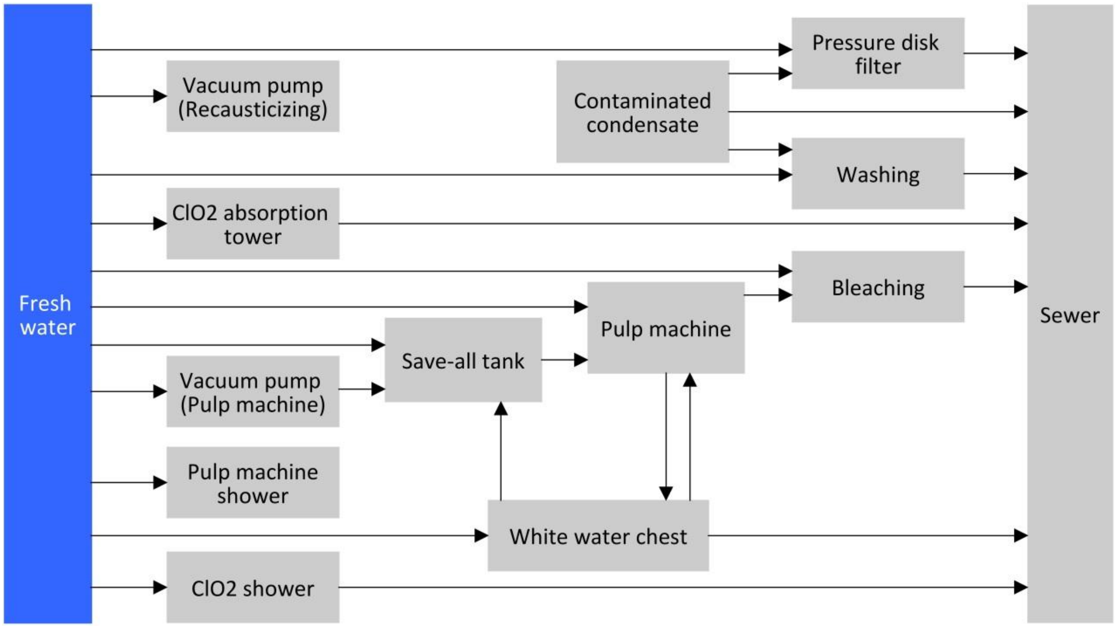

Figure 7. Proposed water superstructure for recycling and reuse of water for the industrial case

Figure 8

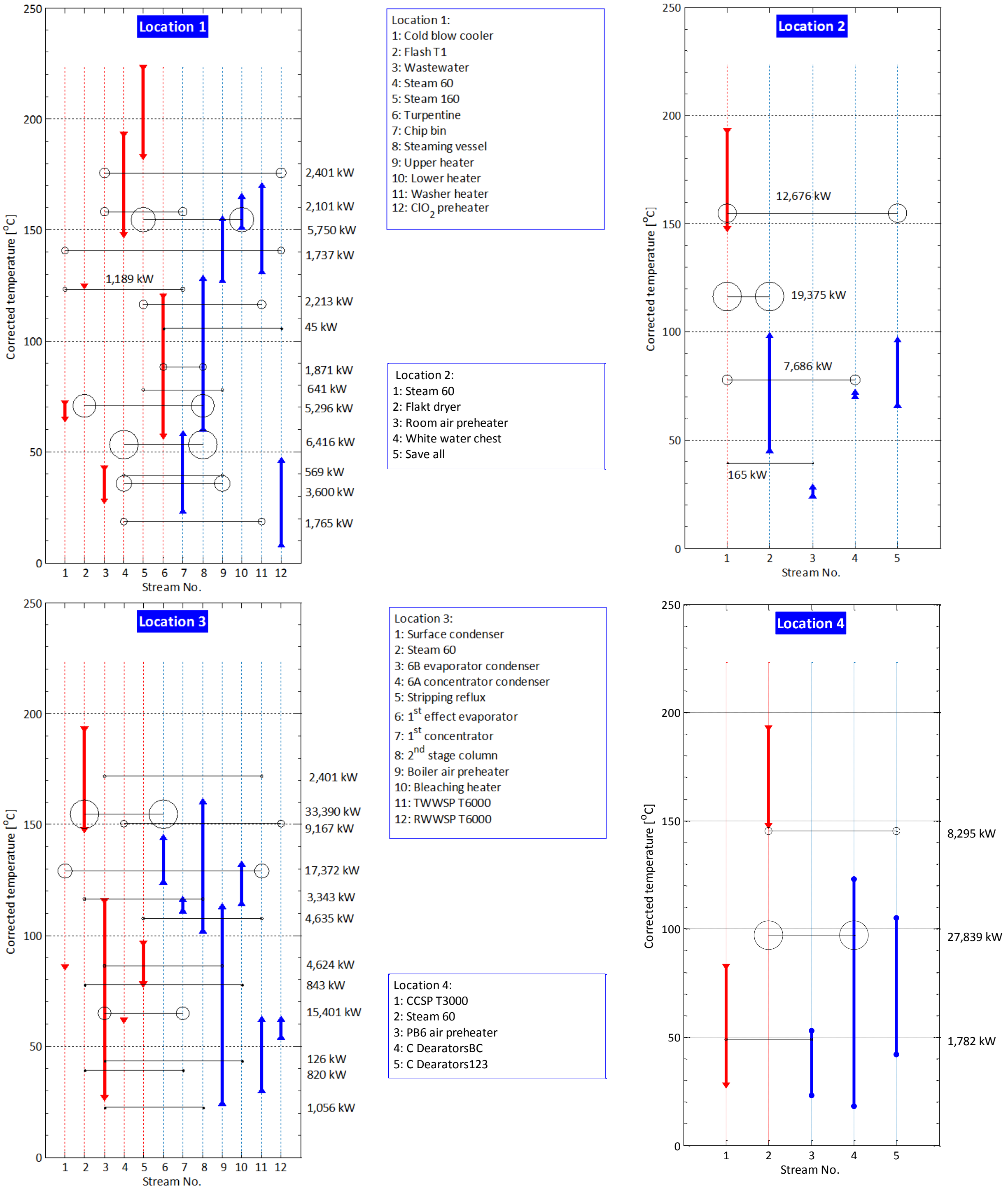

Figure 8. HLD results of the water network

Figure A-1

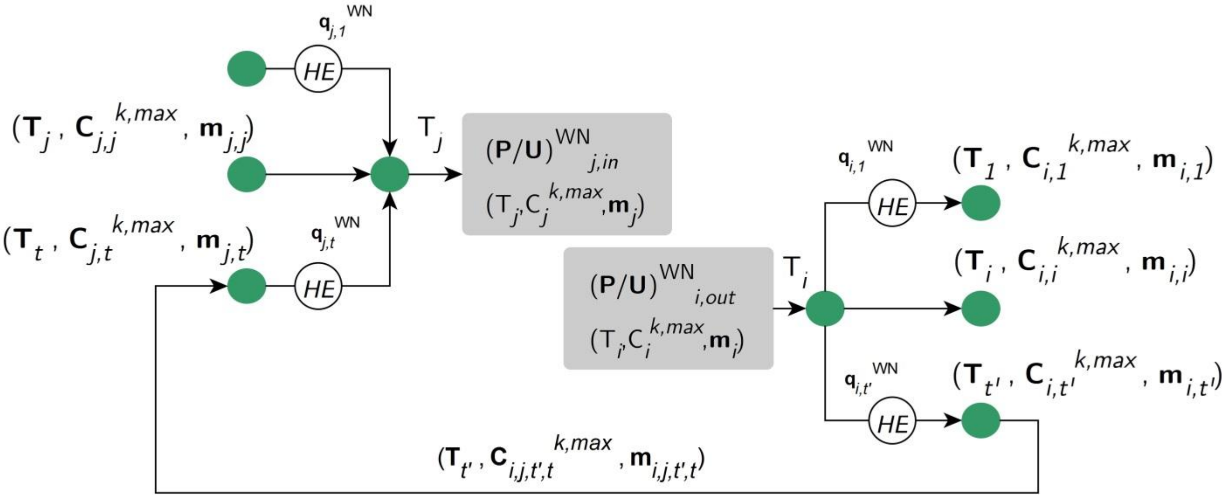

Figure A-1. Graphical representation of the superstructure

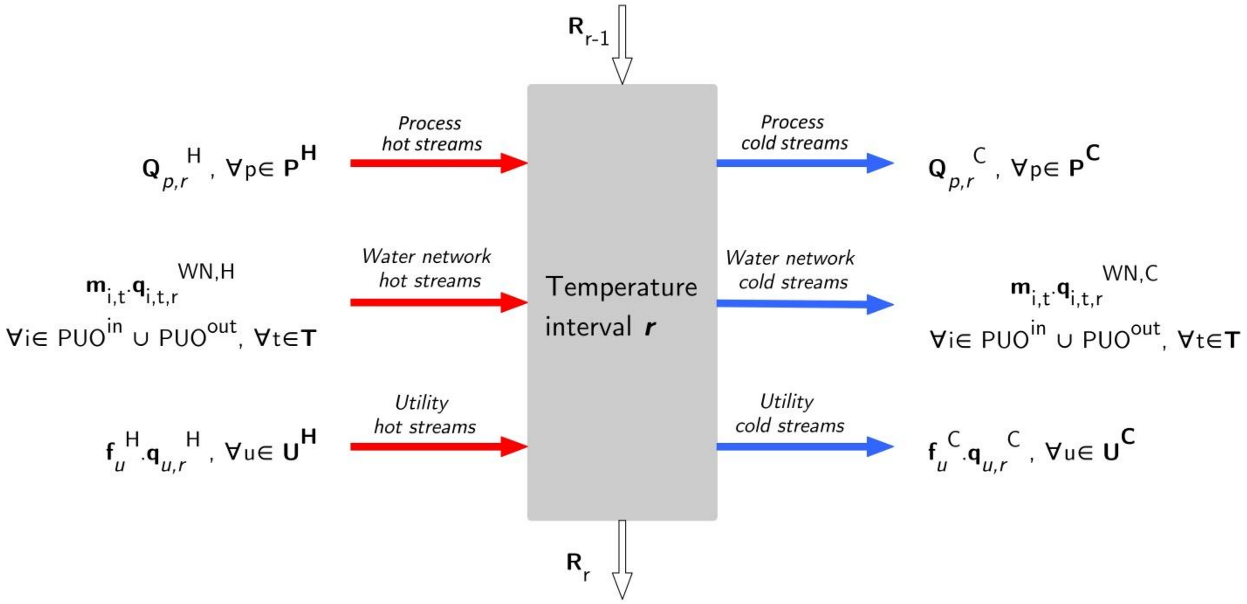

Figure A-2. Heat cascade model at interval *r*