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Synthesis of Heat-Integrated Water Networks with Exergoeconomic Criteria

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This paper considers the exergy analysis of Heat-Integrated Water Networks (HIWNs) rarely addressed in the literature. Two objective functions were analyzed, with the first minimizing the total annualized cost (TAC) and the second minimizing the exergy losses of the network. The exergetic objective function minimizes exergy losses due to non-isothermal mixing, heat exchange, and exergy losses due to friction. The HIWN was optimized under a constant pressure assumption. However, exergy losses due to pressure drops are considered to balance network complexity. The proposed nonlinear programming (NLP) model and iterative solution strategy showed that by using exergetic criteria as an objective function, good solutions could be obtained compared to the solution of the mixed integer nonlinear programming (MINLP) model minimizing the TAC. The advantage is that exergy-based model is an NLP, and cost data for the utilities and equipment are not required.

1. Introduction

Global water and energy consumption continuously increase due to increasing industrial, domestic and agricultural demands. This increasing demand adds to emissions of greenhouse gases and pollution of existing freshwater resources. Accordingly, there is a need to conserve water and energy, which is a main priority for many industries. Water is a natural resource essential to process industries such as chemical, pharmaceutical, food, and others. In energy production industries, it is critical for hydropower production and as cooling water in thermal or nuclear power plants. Process water is used for various purposes, such as cleaning, washing, scrubbing, and absorption, as well as water in the final products from food and pharmaceutical industries. Water and energy are closely related, and reducing freshwater consumption reduces energy for heating and cooling. This can be achieved systematically using Pinch Analysis (PA) (Savulescu et al., 2005) and Mathematical Programming (MP) (Bagajewicz et al., 2002). In PA methods, water and energy targeting is performed separately from water and Heat Exchanger Network (HEN) design using tools such as two-dimensional grid diagrams (Savulescu et al., 2005), temperature versus concentration diagrams (Martínez-Patiño et al., 2011), or water energy balance diagrams (Leewongtanawit and Kim, 2009). Thus, obtaining a design with minimum cost is difficult because a good trade-off between freshwater, utility consumption, and HEN investment is not achieved with these approaches. Targeting models for simultaneous water and energy minimization (Yang and Grossmann, 2013) can also help find theoretical limits to resource consumption but do not estimate the total cost of the network. This issue was addressed in (Nemet et al., 2022) with a targeting model to find minimum freshwater and utility consumption that can find promising matches for heat exchange and provide a corresponding cost estimate for the heat exchangers. This is the state of the art for targeting based on PA methods, but its usefulness is moreso in generating theoretical water and energy targets and bounds on performance rather than practical and real solutions. MP methods aim at more practical, real solutions. For example, Ahmetović and Kravanja (2012) used a sequential approach to first synthesize a Water Network (WN) under the assumption of constant temperatures using the global optimization solver BARON. In the second step, the HEN is synthesized using a stage-wise superstructure (Yee and Grossmann, 1990). Kermani et al. (2019) solved three sub-problems sequentially and iteratively to generate a set of potential solutions implementing integer cut constraints. The first problem minimizes operating costs by selecting potential thermal matches, and the second problem minimizes the number of thermal matches given the Heat Recovery Approach Temperature

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(HRAT). In the final step, the optimum HEN design with minimum investment cost is determined by solving a nonlinear programming (NLP) model. In an alternative, simultaneous approach, freshwater and utility consumption are minimized simultaneously with the investment cost for heat exchangers optimizing the exchanger's minimum approach temperature. This can be achieved using multistep approaches consisting of targeting and design steps (Ibrić et al., 2014) or a single-step simultaneous approach (Ibrić et al., 2022) simultaneously combining WN with the HEN. The downside is that the complexity of MP problems grows rapidly with the scale of the HIWN. It can quickly become intractable to find global solutions or even local ones. Our goal is to develop methods with the scalability of PA and yet attain the rigorous, practical solutions of MP approaches.

To do this, we note that most objective functions in MP approaches are the minimum total annualized cost (TAC). These require cost estimates for resources and equipment that are sometimes unreliable and are almost always nonlinear and sometimes even discrete. It is a major contributor to the computational difficulty of finding the optimal solution. For this reason, a few papers studied the use of exergy as a useful thermodynamic metric that aids in design. For example, Dong et al. (2014) presented a simultaneous optimization approach of an integrated heat, mass, and pressure exchange networks and applied it to a modified HIWN problem considering pressure exchange networks. Exergo-economic optimization was performed to minimize economic cost per unit exergy of the final water flows. Meramo and González-Delgado (2023) analyzed heat-integrated water regeneration networks with different objectives: minimizing TAC, minimizing exergy losses, and a twodimensional approach in searching for a solution with a good trade-off between the first two scenarios. Both recognized the value of exergy but still required the use of TAC and retained the same scalability challenges associated with the use of nonlinear TAC. We propose using exergetic objective functions without the use of TAC in an MP approach for synthesizing a HIWN. The objective function minimizes exergy losses by introducing exergy losses due to friction to balance network complexity with thermo-mechanical exergy losses of the overall system. The proposed objective function does not rely on cost data for resources and equipment and provides an alternative approach to solving HIWN problems which solves much more quickly and leads to very similar rigorous solutions to the more computationally intensive TAC-based MP approaches.

2. Problem statement

Figure 1 shows a representation of the synthesis problem of the HIWN. Water is supplied to process waterusing units ($p \in P$) with the freshwater sources $s \in S$, and wastewater is available for reuse. Process units operate at a specified temperature and given maximum inlet contaminants $k \in K$ concentration. Water can be directly used within water-using units or heated/cooled within a heat exchanger network (HEN). The water network (WN) and heat exchanger network (HEN) are interconnected, enabling heat integration of water streams by direct heat exchange. Within the HEN, indirect heat exchange opportunities are enabled within heat exchangers ($e \in E$), heaters ($h \in H$), and coolers ($c \in C$). The hot utility is low-pressure steam, and the cold utility is cooling water. Wastewater is discharged into the environment at a specified temperature. The objective is to find the optimum HIWN design by minimizing economic (TAC) or exergetic (exergy losses) criteria.



Figure 1: Problem representation of the HIWNs

3. Superstructure and modeling

In this work, a recently published paper (Ibrić et al., 2022) is extended regarding superstructure design and mathematical modeling to include an exergy analysis of HIWN. The superstructure proposed by Ibrić et al.

(2022) consisted of a single set of heat exchange systems ($e \in E$) consisting of heat exchanger, a heater and a cooler. The coolers and heaters are present in the superstructure, even if not required for specific problems. The superstructure has been modified to define separate sets for heat exchangers ($e \in E$), heaters ($h \in H$), and coolers ($c \in C$). This enables more control over the superstructure design and facilitating the solution to the problem.

3.1 Objective function

In this paper, two objective functions were analyzed. The objective economic function given by Eq(1) minimizes TAC, including operating costs for the freshwater, utilities, pumping for overcoming pressure drop per unit length of pipes, and annualized investment costs for the heat exchangers.

$$\min \sum_{s} FS_{s}C_{s}H + \sum_{h} q_{h}C_{HU} + \sum_{c} q_{c}C_{CU} + C_{el}H \sum N_{pump} + \underbrace{af\sum_{exc} (z_{exc}a + bA_{exc}^{n})}_{exc}$$
(1)

The exergetic objective function minimizes thermo-mechanical exergy losses related to non-isothermal mixing and heat exchange and exergy losses due to friction, as given by Eq(2).

$$\min\sum_{s} FS_{s}e_{s} + \sum_{h} m_{h}^{(HU)} \Delta e_{HU} + \sum_{c} m_{c}^{(CU)} \Delta e_{CU} - FWWe_{WW} + \sum_{c} E_{loss,p}$$
(2)

The classic TAC economic objective function considers both the continual costs of operation (the terms without the underbar) balanced with the one-time costs of capital (the terms with the underbar), with their relative influence weighted by the annualization factor *af*. The capital costs term factors in both nonlinear costs associated with heat exchanger size, but also costs of "existence" such that there is a cost penalty associated with the discrete number of exchangers (and the number of network connections) at any size.

The exergetic objective function is structured analogously; the continual thermo-mechanical exergy losses from operation (the terms without the underbar) are compared against an term representing the exergetic losses associated with network complexity (the terms with the underbar). The thermo-mechanical exergy losses are calculated as exergy inlet to the system with fresh water and utilities minus the exergy outlet with the wastewater stream, assuming constant system pressure. These thermo-mechanical exergy losses inherently include losses for non-isothermal mixing and exergy losses in heat exchangers, heaters, and coolers. Deng et al. (2023) already showed that the exergy of utilities could be used as a proxy for the utility value and the exergy losses can be used as a direct analogous substitute for utility cost in the exergy objective function. However, if only the thermo-mechanical exergy losses due to non-isothermal mixing and heat exchange are minimized, solutions with high capital investment and many network connections would be obtained, which is undesirable. Therefore, in this work, the exergy loss due to friction is introduced (underbar), to balance the network complexity. Friction losses make a good predictor of the number of network connections (more connections require more pipes). The term assumes a constant pressure loss per unit pipe length for simplicity. This paper estimates the thermo-mechanical exergy of water streams by fitting data from the literature (Deng et al., 2023).

3.2 Solution strategy

The mathematical programming model with the objective function minimizing the TAC given by Eq (1) (OBJ-1) is an MINLP model solved by the SBB solver using Conopt4 as an NLP sub-solver. The second mathematical programming model, with the objective function given by Eq (2) (OBJ-2), is an NLP model solved with the Conopt4 as an NLP solver. Models are solved by using the General Algebraic Modeling System (GAMS, 2021), with a single-step iterative solution strategy proposed by Ibrić et al. (2022). This strategy provides random initialization to the optimization variables between lower and upper bounds generated based on initial data.

4. Example

The proposed model is demonstrated with a typical literature example (Bogataj and Bagajewicz, 2008) with data for the process water-using units given in Table 1. Freshwater is available at 20 °C and 0 ppm contaminants, and wastewater is discharged into the environment at 30 °C. Other network design data and cost parameters are taken from the literature (Ibrić et al., 2022).

Optimization problem with economic objective function (OBJ-1) was solved for the investment annualization factor (*af*) equal to 1. Exergy losses for the optimal network design were calculated after the optimization. In addition, the same problem was solved with the exergetic objective function (OBJ-2). The TAC of the optimal design chosen was calculated after the exergetic optimization. Ultimately, the solutions obtained by the exergy objective function are almost, but not exactly, identical to the solutions obtained by the economic one. The optimum network design for the objective function minimizing TAC is given in Figure 2. The network exhibits

minimum freshwater consumption of 25 kg/s and a hot utility consumption of 1,050 kW, with a network design including one heat exchanger and one heater. The heat exchanger recovers 5,530 kW of heat from the wastewater stream to preheat freshwater from 20 °C to 82 °C. The external hot utility is required to deliver freshwater at a maximum operating temperature of 100 °C. Exergy losses of non-isothermal mixing and heat exchange are 87.97 and 160.65 kW. The exergy losses due to friction are 58.56 kW per unit length of pipes. Total exergy losses for the optimal design are 307.19 kW, and the TAC of the network is 846,927 \$/y.

Process unit	Contaminant mass load (g/h)	Maximum inlet contaminant concentration (ppm)	Maximum outlet contaminant concentration (ppm)	Temperature (°C)
P1	2,000	0	100	40
P2	5,000	50	100	100
P3	30,000	50	800	75
P4	4,000	400	800	50



Figure 2: Optimal network design with economic criteria

Reference	Freshwater consumption (kg/s)	Hot utility consumption (kW)	HEN investment (\$/y)	TAC (\$/y)	TAC including pumping (\$/y)
Bogataj and Bagajewicz (2008)	25	1,050	146,748	812,598	-
lbrić et al. (2014)	25	1,050	134,227	800,077	-
Yan et al. (2016)	25	1,050	131,525	797,375	-
lbrić et al. (2022)	25	1,050	131,527	797,377	-
This paper OBJ-1	25	1,050	134,227	800,077	846,927
This paper OBJ-2	25	1,050	134,795	800,645	847,008

Table 2: Comparison of the results with the literature

Figure 3 shows the optimum network design with the exergetic objective function. The solution is selected from the set shown in Figure 4 obtained using an iterative solution strategy. Figure 4 shows the TAC for each solution calculated after the exergetic optimization that corresponds to the minimum exergy losses. The solution with minimum exergy losses can be easily identified. However, alternative local solutions with different network designs can also be analyzed. The optimum network exhibits the same freshwater and utility consumption as the network with minimum TAC. The network design includes the same number of heat exchangers and heaters and a similar network design. The network exhibits the same number of non-isothermal mixing points (five) and one less splitting point (four) compared to the network shown in Figure 2. Exergy losses of non-isothermal mixing

and heat exchange are 88.12 and 160.50 kW. In addition, the exergy losses due to friction are slightly reduced from 58.56 to 57.95 kW. The TAC of the optimal design with minimum exergy losses is 847,008 \$/y, which is comparable with the objective of minimizing the TAC of the network. Table 2 shows a comparison of the results with those from the literature. TAC, including pumping cost were not compared as those are not optimized in other studies. However, the design with minimum TAC is the same as in previous studies (lbrić et al., 2014), and given electricity cost 0.1 \$/(kWh), the network would give the same TAC by including pumping.



Figure 3: Optimal network design with exergetic criteria



Figure 4: Set of solutions obtained for the objective function minimizing exergy losses

5. Conclusions

This paper presented an alternative approach for synthesizing Heat Integrated Water Networks (HIWNs) with an exergetic objective function. The objective function of the nonlinear programming (NLP) model minimizes thermo-mechanical exergy losses of the system and exergy related to frictional pressure drop to balance network complexity. The NLP model requires less computational effort to be solved compared to the mixed integer nonlinear programming (MINLP) model with economic objective function and finds designs essentially equal in quality to those of the cost-based approaches. The solution obtained with exergetic objective function is within 0.04 % of the best solution in the literature when minimizing total annualized cost. In addition, the exergetic objective function is not reliant on the cost of utilities and equipment. The model can be modified to include wastewater regeneration units for distributed wastewater treatment. In addition, the non-constant pressure of water streams can be considered by including pressure change networks.

Nomenclature

a – fixed cost coefficient, \$ A_{exc} – heat exchanger area, m² af – annualization factor for the investment, b – area cost coefficient, \$/m² C_{CU} – cost of cold utility, \$/(kW y)

 C_{el} – cost of electricity, \$/(kW h) C_{HU} – cost of hot utility, \$/(kW y) C_s – cost of freshwater, \$/kg Δe_{CU} – exergy change of cold utility, kJ/kg Δe_{HU} – exergy change of hot utility, kJ/kg e_s – exergy of freshwater, kJ/kg e_{ww} – exergy of wastewater, kg/kg $E_{loss,mix}$ – exergy loss of mixing, kW $E_{loss,exc}$ – exergy loss of heat exchangers, kW $E_{loss,p}$ – exergy loss due to friction, kW FS_s – freshwater consumption, kg/s FWW – wastewater flowrate, kg/s H – plant operating hours, h/y $m_c^{(CU)}$ – mass flowrate of cold utility, kg/s $m_h^{(HU)}$ – mass flowrate of hot utility, kg/s N_{pump} – energy, kW n – heat exchanger cost exponent, q_c – cold utility consumption, kW q_h – hot utility consumption, kW z_{exc} – binary variable representing heat exchangers

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