CHEMICAL ENGINEERING TRANSACTIONS

VOL. 88, 2021

A publication of
AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Yee Van Fan, Jiří J. Klemeš

ISBN 978-88-95608-86-0; **ISSN** 2283-9216

DOI: 10.3303/CET2188191

Synthesis of Heat-Integrated Water Networks: Case Study with Sensitivity Analysis

Nidret Ibrić[a,*], Elvis Ahmetović[a], Zdravko Kravanja[b], Ignacio E. Grossmann

[a] University of Tuzla, Faculty of Technology, Urfeta Vejzagića 8, 75000 Tuzla, Bosnia and Herzegovina
[b] University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova ulica 17, 2000 Maribor, Slovenia
[c] Carnegie Mellon University, Department of Chemical Engineering, 5000 Forbes Avenue, Pittsburgh, 15213 PA, United States
nidret.ibric@untz.ba

This work addresses the synthesis of heat-integrated water networks (HIWNs) by using a superstructure optimisation approach. A recently developed mixed-integer nonlinear programming (MINLP) model and an iterative solution strategy are applied in this work to a case study of HIWN. The objective function of the MINLP model is to minimise the network total annualised cost (TAC) comprising operating and investment costs. As there are trade-offs between operating and investment costs, good solutions can be obtained if the TAC is minimised by simultaneously exploring all water and heat integration opportunities within the network.
A case study with sensitivity analysis is solved by analysing the impact of freshwater and utility costs on the network design and key performance indicators. The results indicate that in cases of low freshwater cost increased freshwater usage is forced and thus lowering wastewater regeneration/recycling and wastewater treatment cost. Increased freshwater flowrate is related to an increase of HEN investment. The high cost of freshwater could produce solutions with lower freshwater consumption compared to base case depending on utility cost and wastewater treatment cost. However, a decrease in freshwater consumption increases wastewater regeneration costs.

1. Introduction

Industrial sector uses large amounts of natural resources (raw materials, fuels, water, and energy) and emits the pollutants to air, water, and soil. The consumption of natural resources and the emission of pollutants into the environment can be significantly reduced by improving water and energy efficiency in industrial processes. Over the last few decades an increasing trend of studies can be noticed that are focused on water and energy efficiency in various industrial processes by using conceptual and mathematical programming approaches. However, it has been demonstrated that mathematical programming approach can better address multiple-contaminant and large-scale problems of heat-integrated water networks (HIWNs) including water-using and wastewater treatment units (Hong et al., 2018). The reader is referred to review paper (Kermani et al., 2018) for more details about mathematical approaches, their key features and solution strategies applied to HIWNs. A recent review paper (Budak Duhbacı et al., 2021) focused on water and energy minimisation in industrial processes by mathematical programming identified several research gaps including sensitivity analysis of case studies of HIWNs. Sensitivity analysis as a tool for studying model outputs in relation to change in the model input parameters has been rarely considered in previous studies. In this way, an analysis can be performed to analyse the changes of the water network design in relation to some critical process parameters (maximum inlet contaminants concentration, operating temperatures etc.) or more often freshwater and utility prices. Ghazouani et al. (2015) introduced a mixed integer linear programming (MILP) model to design heat integrated water allocation network based on the transhipment model for heat integration. The objective function of the model minimises total operating cost of freshwater and utility. Sensitivity analysis is performed by varying freshwater cost and analysing its impact on total cost, freshwater, and utility consumption as well as network configuration. Investment cost for the heat exchangers was not considered. Authors later extended their research to account for simultaneous synthesis of water and heat exchanger network (Ghazouani et al., 2017) by minimising total

Paper Received: 13 May 2021; Revised: 8 July 2021; Accepted: 7 October 2021
Please cite this article as: Ibrić N., Ahmetović E., Kravanja Z., Grossmann I.E., 2021, Synthesis of Heat-Integrated Water Networks: Case Study with Sensitivity Analysis, Chemical Engineering Transactions, 88, 1147-1152 DOI:10.3303/CET2188191

annualised cost now considering and the investment cost for heat exchangers. A sensitivity analysis was performed for analysing number of operating years for return of investment on the total annualised cost. Sujak et al. (2017) presented a two-step holistic approach for designing cost optimal water networks considering different levels of water saving hierarchy (e.g., reuse, recycling, elimination). As part of the proposed methodology, a sensitivity analysis was performed to study an effect of increasing freshwater prices to water minimisation schemes as well as on the economic indicators such as savings, investment, and payback period. However, the approach assumes only isothermal water operations. The main goal of this work is to perform sensitivity analysis of HIWN consisting of water-using and wastewater treatment units with heat losses and gains and to analyse the impact of freshwater and utility costs on the network design, key performance indicators, and total annualised cost (TAC).

2. Problem description

Given the number of superstructure elements it is required to synthesise the optimal HIWN design with the given process and environmental constraints by minimising the TAC of the network. Process constraints include operating temperatures, maximum inlet and outlet concentrations, and mass load of contaminants of process water-using units. Operating temperature and contaminants removal ratio in wastewater treatment units is also given. Environmental constraints include temperature and contaminant concentrations in the wastewater stream discharged into the environment.

3. Methodology

A mathematical programming approach and an optimisation model based on a HIWN superstructure are used in this work. The recently proposed HIWN superstructure shown in Figure 1 (Ibrić et al., 2021) consists of: freshwater sources *s*; process water-using units *p* (fixed mass load units); wastewater treatment units *t* (fixed removal ratio units); heating/cooling stages *ws* and wastewater discharge. The superstructure elements are interconnected enabling water reuse, regeneration and recycling as well as heat integration between hot and cold water streams. Heat integration occurs within heating/cooling stages consisting of a predefined maximum number of hot/cold streams identified by a convex hull formulation. In this way a controlling element is introduced into the model to reduce the complexity of the network when dealing with large-scale HIWNs.

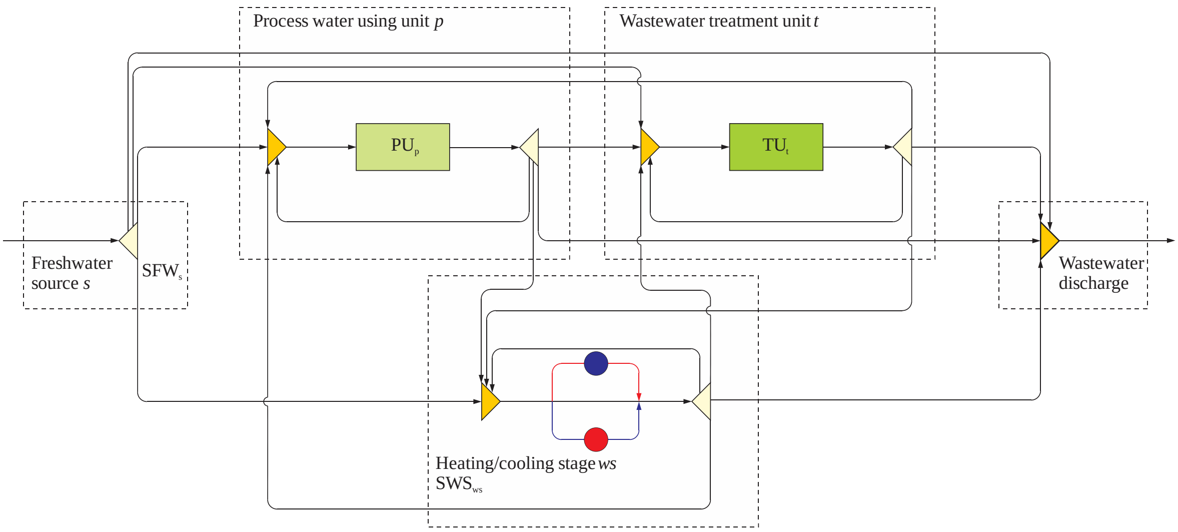

Figure 1: Superstructure design

Based on the proposed superstructure shown in Figure 1, a mixed integer nonlinear programming model (MINLP) was developed (Ibrić et al., 2021) and a three-step solution strategy proposed enabling solution of the problem (Figure 2). The overall model consists of three models: water network model (M1), heat integration model (Duran and Grossmann, 1986) (M2) and heat exchanger network model (Yee and Grossmann, 1990) (M3). In step 1 of the strategy, combined models M1 and M2 (M1-2) are solved by minimizing the linear operating cost of the network for heat recovery approach temperatures (HRATs) lower and greater than the exchanger minimum approach temperature (EMAT). The main goal of this step is to set lower and upper bounds on the utility consumption for the next step of the solution strategy. Step 2 combines M1 and M3 models minimizing

linearized total annualised cost (TAC). The promising heat exchange matches (match (i, j)) are identified between hot streams i and cold streams j. This limits the number of heat exchange matches $z(i, j)$ within step 3 of the strategy that combines M1 and M3 models minimising the nonlinear objective function and finding the optimal network design.
The proposed solution procedure is solved in iterations to generate a set of locally optimal solutions from which the best one is selected. Different HRAT values are randomly generated within each iteration for setting the upper bound on utility consumption providing different initialization points for the following optimisation steps. Based on various problems solved by the proposed solution procedure, it should be highlighted that the targeting Steps 1 and 2 are very important for determining freshwater and utility consumption and selecting promising matches thus reducing the complexity of the overall synthesis model solved in the Step 3.

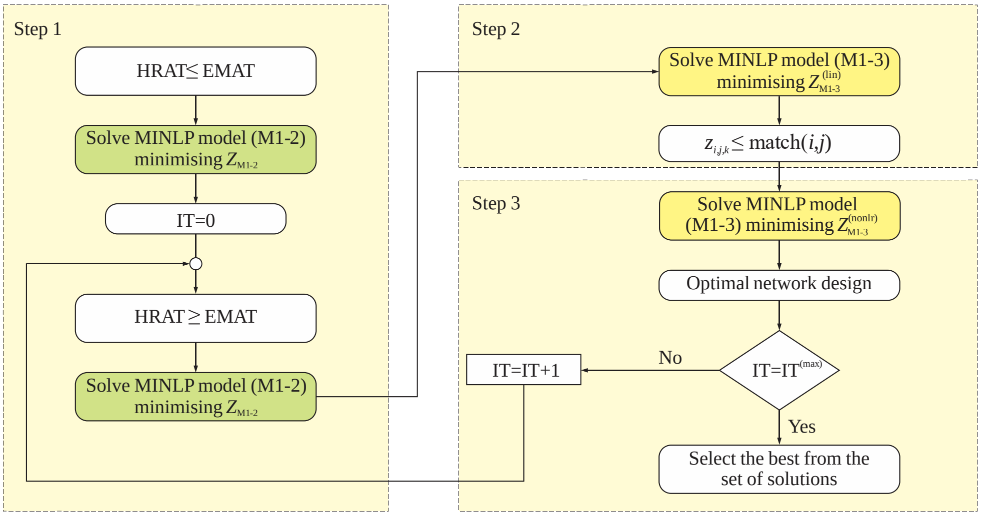

Figure 2: Flowchart of the solution strategy

By using the presented solution strategy, the basic sensitivity analysis is performed for different prices of freshwater and utility to obtain a set of solutions for each case. The base cost for freshwater and utility is varied ± 50 % to analyse an impact to water networks design and key performance indicators such as freshwater and utility consumption, as well as operating and investment cost.

4. Case study

When designing HIWNs two types of problems exist, threshold and pinched (Ibrić et al., 2013). In the later, both hot and cold utilities are required, and hence stronger connection exists between freshwater and utilities consumption. This case study is an example of multi-contaminant pinched HIWNs consisting of two water-using units and a single wastewater treatment unit taken from the literature (Bogataj and Bagajewicz, 2008). The data for the water-using units is given in Table 1. As can be seen the inlet and outlet temperatures of water-using units are different accounting for heat losses and gains and the problem is pinched.

Table 1: Process water-using units' data

Process unit	Contaminants mass load (kg/h)			Contaminants maximum inlet concentration (ppm)			Contaminants maximum outlet concentration (ppm)			Temperature (°C)	
	A	B	C	A	B	C	A	B	C	In	Out
PU_1	6	3	4	5	150	100	50	200	200	25	35
PU_2	5	8	1	150	120	60	300	150	300	100	85

Freshwater temperature is 20 °C and the temperature of wastewater discharged into the environment is 30 °C. Hot utility is fresh steam at temperature 126 °C and cold utility is cooling water with inlet and outlet temperatures 15 °C and 20 °C. The base cost of freshwater is 2.5 $/t. The base cost of hot and cold utility is 260 $/(kW·y) and 150 $/(kW·y). The shell and tube heat exchanger cost ($/y) as function of heat exchanger area (m^2) is given by equation $10{,}000+860\cdot(\text{Area})^{0.75}$. Individual heat transfer coefficients for water streams and hot utility are 1 kW(m^2·K) and 5 kW(m^2·K). Treatment unit operating and investment data are given in Table 2. Annualisation factor for the treatment unit investment cost is 1. Specific heat of water streams is 4.186 kJ/(kg·K). The total plant annual operating time is 8,322 h.

Table 2: Wastewater treatment unit data

Treatment unit	Removal percent of contaminants (%)			Investment cost coefficient (IC)	Operating cost coefficient (OC)	Cost exponent	Temperature (°C)	
	A	B	C				In	Out
TU_1	75	90	90	20,000	0.95	0.78	40	37

The base costs are varied ± 50 % to analyse the influence of freshwater and utility costs on the total annualised cost (TAC) and design of the HIWN. Table 3 shows detailed optimisation results for the case study. The base case study produces the identical solution to those reported in the literature (Hong et al., 2018) with the minimum TAC of 5,038,794 $/y. The freshwater consumption is 27.778 kg/s. Figure 3 shows the optimal network design for the base case. Two heat exchangers, heater and a cooler exist within the network with the HEN investment cost 176,096 $/y. Heat integration occurs between the hot wastewater stream and cold freshwater stream (116.28 kW) and between the process water-using unit PU_2 outlet and inlet streams (2,701.24 kW). Additional heater is required to preheat the water at the inlet to PU_2 to 100 °C requiring 1,905.32 kW of hot utility and one cooler to cool down the wastewater stream to a temperature of 30 °C requiring 697.67 kW of cold utility. The optimal network design comprises wastewater regeneration-recycling of wastewater streams with the total amount of wastewater treated 41.667 kg/s. Optimisation results for the case with low freshwater cost (1.25 $/t) show the increased freshwater consumption. This is especially the case for the low freshwater cost (- 50 %) and high utility cost (+ 50%) where the network design exhibits a freshwater consumption of 37.589 kg/s. The consumption of hot (1,820.26 kW) and cold (117.19 kW) utility is reduced compared to base case. The cost of wastewater treatment is also reduced with the decreased flowrate of water through the treatment unit (33.656 kg/s vs. 41.667 kg/s). The amount of recycled water is significantly reduced to 0.707 kg/s (see Figure 4). Note that due to low freshwater cost a part of freshwater is used for diluting the wastewater to reduce the wastewater treatment operating and investment cost. The optimal network design exhibited the same number of heat exchangers, heaters, and coolers as in the base case with the increased investment cost for HEN (206,856 $/y). With the increase of freshwater flowrate, the amount of water entering and leaving heat exchangers increases and thus the heat load of heat exchangers and heat exchange area also increases.

For the case with high freshwater cost (+50 %) and low utility cost (- 50 %) the optimal network design is the same as for the base case with freshwater consumption 27.778 kg/s. The HEN and TU investment costs are also identical. The TAC of the network is 5,779,027 $/y. The increase in freshwater price does not reduce freshwater consumption compared to the base case. Further decrease in freshwater consumption would significantly increase flowrate of water through the wastewater treatment unit and thus wastewater treatment operating and investment cost. However, freshwater consumption also relates to the utility price as well as wastewater treatment operating, and investment cost related to wastewater flowrate. The annualisation investment factor influence on the network design should also be investigated as it relates to the trade-off between investment and operating cost.

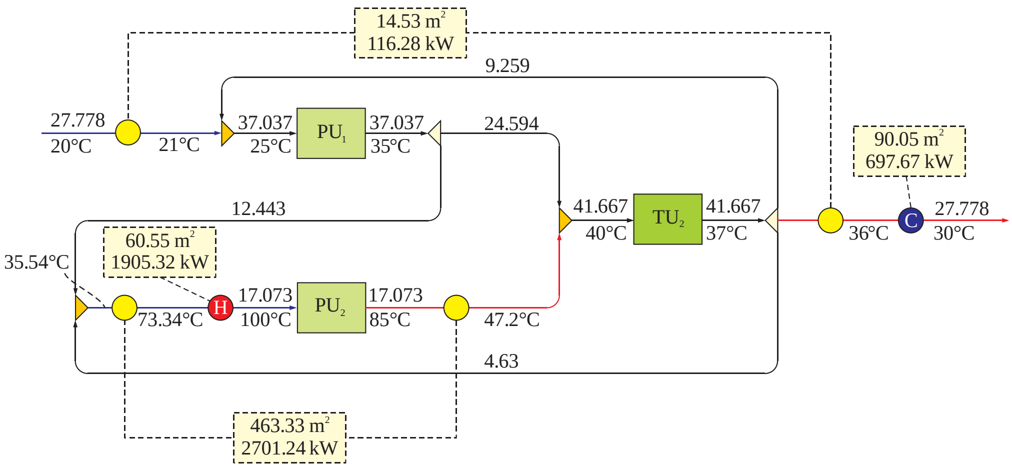

Figure 3: Optimal network design for the base case

Table 3: Optimisation results for the case study

Freshwater cost ($/t)	Parameter	Unit	Hot/cold utility cost ($/(kW·y))		
			- 50 % 130/75	Base case 260/150	+ 50 % 390/225
1.25 (- 50 %)	TAC	$/y	3,607,988	3,894,642	4,152,127
	FW consumption	kg/s	31.25	31.25	37.589
	HU consumption	kW	1,886.38	1,886.38	1,820.26
	CU consumption	kW	552.32	552.32	117.19
	HEN investment	$/y	188,104	188,104	206,856
	TU investment	$/y	908,829	908,829	843,445
	TU operating	$/y	1,054,120	1,054,120	957,897
2.5 (Base case)	TAC	$/y	4,738,776	5,038,794	5,426,952
	FW consumption	kg/s	27.778	27.778	27.778
	HU consumption	kW	1,905.32	1,905.3	2,191.47
	CU consumption	kW	697.66	697.67	813.94
	HEN investment	$/y	176,096	176,096	192,726
	TU investment	$/y	996,279	996,279	996,279
	TU operating	$/y	1,185,885	1,185,885	1,185,885
3.75 (+ 50 %)	TAC	$/y	5,779,027	6,079,552	6,505,758
	FW consumption	kg/s	27.778	27.778	27.329
	HU consumption	kW	1,905.3	1,905.3	1,979.34
	CU consumption	kW	697.67	697.67	790.75
	HEN investment	$/y	176,096	176,096	151,072
	TU investment	$/y	9,962,79	996,279	1,056,266
	TU operating	$/y	1,185,885	1,185,885	1,278,194

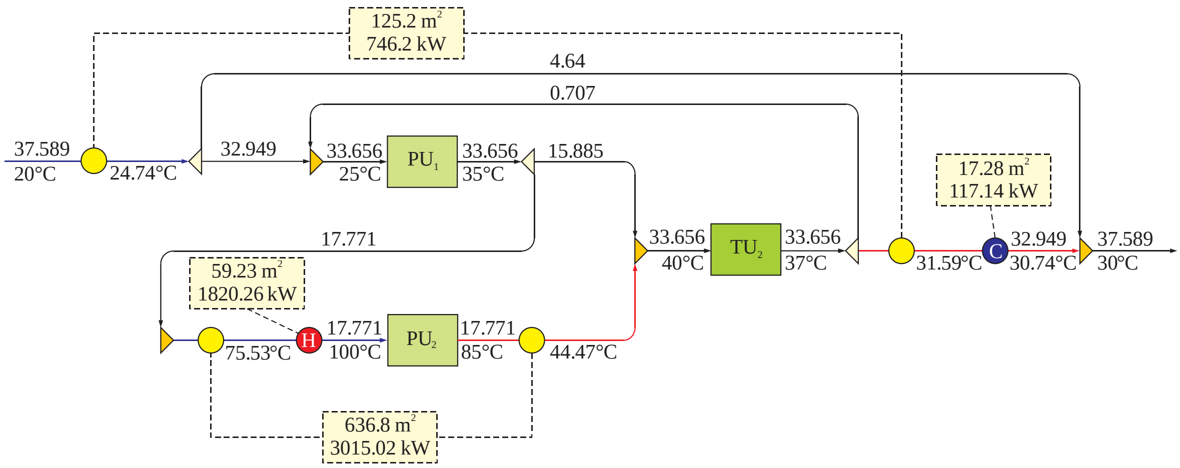

Figure 4: Optimal network design for the case of low water cost (- 50 %) and high utility cost (+ 50 %).

5. Conclusions

This paper presents a mathematical programming approach for the synthesis of heat-integrated water networks (HIWNs). The recently proposed MINLP model and the three-step solution strategy were used to generate a set of solutions by performing a sensitivity analysis for different costs of freshwater and utility. The pinched problem of HIWN was considered comprising heat losses/gains and thus requiring hot and cold utility consumption. The base case solution presented in this work is in agreement with the solutions reported in the literature with the freshwater consumption (27.778 kg/s) and hot/cold utility consumption (1,905.3 kW and 697.67 kW). The optimisation results for the case with low water cost (- 50%) and high utility cost (+ 50 %) exhibit increased freshwater consumption (37.589 kg/s vs. 27.778 kg/s) as well as decreased utility consumption when compared to the base case (1,820.26 kW of hot and 117.19 kW of cold utility). Increased freshwater consumption due to its lower cost increases heat load within heat exchangers and thus HEN investment. Also, when freshwater consumption increases less water is recycled and thus wastewater flowrate through wastewater treatment unit decreases (33.656 kg/s vs. 41.667 kg/s). The optimisation results for the case with high freshwater cost (+ 50 %) and low utility cost (-50 %) exhibit the same network design as for the base case cost. The solution with decreased freshwater consumption compared to base case is not forced. The solution with lower freshwater consumption would require additional amount of recycled wastewater and thus wastewater operating, and investment cost would increase. This is the case for high freshwater cost (+ 50 %) and high utility cost (+ 50 %) with freshwater consumption of 27.329 kg/s at the expense of wastewater treatment operating and investment cost. On the other hand, with the freshwater decrease heat load within heat exchangers also decreases and thus HEN investment on the expense of utility consumption. This case study shows how close interactions exist between freshwater and utility consumption on the one side and HEN and wastewater treatment on the other side. The optimisation results are not straightforward as many trade-offs exist. The future research can be directed towards developing multi-period HIWN considering future changes in freshwater and utility cost. An impact of investment cost can also be analysed considering different depreciation periods. Different types of heat exchangers can be considered with different investment and equipment constraints regarding the maximum heat exchange area and the exchanger minimum approach temperature.

Nomenclature

CU – Cold utility
EMAT – Exchanger Minimum Approach Temperature
FW – Freshwater
HEN – Heat Exchanger Network
HRAT – Heat Recovery Approach Temperature
HU – Hot utility
OC – Operating cost
TAC – Total Annual Cost
TU – Treatment unit

Acknowledgements

The authors gratefully acknowledge the support from the internal call for financing/co-financing projects important for the Federation of Bosnia and Herzegovina (Project No: 01-6211-1-IV/19). Also, the authors gratefully acknowledge the program for Scientific and Technological Cooperation between the Republic of Slovenia and Bosnia and Herzegovina in the period 2019-2020 (Project: “SISUMP”, No: 01-1282-1/20) and Cost Action CA18224 entitled Green Chemical Engineering Network towards upscaling sustainable processes – GREENERING.

References

Bogataj, M., Bagajewicz, M. J., 2008, Synthesis of non-isothermal heat integrated water networks in chemical processes, Computers & Chemical Engineering 32(12), 3130-3142.
Budak Duhbacı, T., Özel, S., Bulkan, S., 2021, Water and energy minimization in industrial processes through mathematical programming: A literature review, Journal of Cleaner Production 284, 124752.
Duran, M. A., Grossmann, I. E., 1986, Simultaneous optimization and heat integration of chemical processes, AIChE Journal 32(1), 123-138.
Ghazouani, S., Zoughaib, A., Bourdiec, S. L., 2017, An MILP model for simultaneous mass allocation and heat exchange networks design, Chemical Engineering Science 158, 411-428.
Ghazouani, S., Zoughaib, A., Pelloux-Prayer, S., 2015, Simultaneous heat integrated resource allocation network targeting for total annual cost considering non-isothermal mixing, Chemical Engineering Science 134, 385-398.
Hong, X., Liao, Z., Sun, J., Jiang, B., Wang, J., Yang, Y., 2018, Energy and Water Management for Industrial Large-Scale Water Networks: A Systematic Simultaneous Optimization Approach, ACS Sustainable Chemistry & Engineering 6(2), 2269-2282.
Ibrić, N., Ahmetović, E., Kravanja, Z., 2013, A Two-Step Solution Strategy for the Synthesis of Pinched and Threshold Heat-Integrated Process Water Networks, Chemical Engineering Transactions 35, 43-48.
Ibrić, N., Ahmetović, E., Kravanja, Z., Grossmann, I. E., 2021, Simultaneous optimization of large-scale problems of heat-integrated water networks, Energy, 121354.
Kermani, M., Kantor, I. D., Maréchal, F., 2018, Synthesis of Heat-Integrated Water Allocation Networks: A Meta-Analysis of Solution Strategies and Network Features, Energies 11(5).
Sujak, S., Handani, Z. B., Wan Alwi, S. R., Manan, Z. A., Hashim, H., Lim Jeng, S., 2017, A holistic approach for design of Cost-Optimal Water Networks, Journal of Cleaner Production 146, 194-207.
Yee, T. F., Grossmann, I. E., 1990, Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis, Computers & Chemical Engineering 14(10), 1165-1184.