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Simultaneous Synthesis of Heat-Integrated Water Network with the Two-Step Approach

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Determining the optimal design of a Heat-Integrated Water Network (HIWN) is a complex task due to the existence of highly nonlinear relationships when considering concentrations, mass and heat balances. Due to that complexity, the solution is usually obtained by a sequential approach. In this approach, the minimum fresh water and utility consumption is firstly determined. Then, the exact design of the HIWN is synthesised with the fixed minimum fresh water and utility consumption. Another way to obtain the HIWN design is by using a simultaneous approach. However, such a model can be highly nonlinear requiring the application of a special solution strategy. In this work, a two-step approach was developed and applied. In the first step, a targeting Mixed-Integer Nonlinear Programming (MINLP) model with a high share of linearity was applied estimating also the HEN investment. In this way, the solutions are steered towards an optimal solution by establishing appropriate trade-offs between investment and operating costs during the targeting step. Based on the results of the first step, a reduced superstructure and MINLP model are used in the second design step to select promising matches for heat exchangers. By excluding the non-promising matches that previously led to an unnecessary increase in the complexity of the synthesis model, the second step MINLP model performs much better and enables synthesizing the entire HIWN simultaneously. The aim of this work was to verify whether the two-step approach is suitable for solving the HIWN problem. The obtained solution for case study considered in this work indicated the applicability of the proposed approach, which will be also applied in further research on large-scale HIWN problems.

1. Introduction

Water and energy are important resources for the process industries. They are used in large quantities and present a significant part of total cost. Accordingly, reducing water and energy consumption in various manufacturing processes, satisfying environmental constraints on streams discharged from processes to the environment and synthesizing optimal water and energy networks are continuous challenges for engineers and researchers. The main goals are to provide both economically and environmentally efficient solutions. The synthesis of Water and Energy Networks (WENs), also known in the literature as Heat-Integrated Water Networks (HIWNs), Water Allocation and Heat Exchange Networks (WAHENs) or Non-Isothermal Water Networks (NIWNs), has been a very active research field in the last decades. Systematic methods based on Pinch Analysis (PA) and Mathematical Programming (MP) or their combinations (hybrid or combined approach) have been applied to solve this synthesis problem (Ahmetović et al., 2015). Recent studies addressing this problem show an increasing trend towards the application of MP methods (Budak Duhbaci et al., 2021) and solution strategies (Kermani et al., 2018). The proposed solution strategies for the synthesis of HIWNs usually consist of several steps. The main goals of these steps are to minimize freshwater and utility consumption, find promising heat exchange matches between hot and cold streams, reduce the problem complexity, provide good initial points and tight bounds on variables, and synthesize an overall HIWN with the minimum Total Annualized Cost (TAC). In addition, several works demonstrated opportunities for using an alternative P-Graph based methodology (How et al., 2021) and a hybrid approach (Kamat and Bandyopadhyay, 2021) to address HIWN problems. The main focus of recently published works in this field was on solving various HIWN problems,

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including large-scale problems and considering water-using and wastewater treatment units. Accordingly, Hong et al. (2018) proposed a three-step solution strategy for synthesizing of HIWNs. The first step of the strategy used an NLP model to provide initial values for nonlinear terms in an MINLP model solved in the second step minimizing the relaxed TAC and roughly considering the trade-offs between capital and operating costs. The results of the second step were used as an initial point for an MINLP model solved in the third step minimizing the TAC. Ibrić et al. (2021) proposed an MINLP model and an iterative three-step solution strategy for HIWNs. The main goals of the first two steps were to find a good initialization point for variables, good bounds for utilities, and promising heat exchange matches between hot and cold streams. This information was used in the third step to solve the combined WN and HEN minimizing TAC. Also, a simplified heat integration block was proposed for enabling non-isothermal mixing and indirect heat transfers based on a convex hull formulation (Ahmetović and Kravanja, 2013) for identifying the roles of water streams in HEN. Yan et al. (2021) proposed an NLP model for solving HIWNs. In their formulation, integer variables for identifying stream roles and denoting the existence of heat exchange matches were replaced with non-linear equations. How et al. (2021) proposed a superstructure and an NLP model which was iteratively solved for different number of heat exchangers. The possibilities for direct heat transfers were fully explored in the proposed superstructure and an alternative formulation for HEN was used instead of the traditional HEN model (Yee and Grossmann, 1990). Over the last two decades, significant progress has been made in the synthesis of HIWN and combined water and energy integration in manufacturing processes. The proposed superstructures include water-using and wastewater treatment units, various options for splitting and mixing, heating and cooling of water streams, heat transfer (direct and indirect) as well as different configurations of heat exchangers (parallel, series, and combined). It has been demonstrated in the literature that the proposed superstructures and corresponding models have been successfully applied for solving HIWN problems. However, there is still a gap in developing superstructures and models that take into account all the above-mentioned aspects and proposing solution strategies that can be successfully used to solve large-scale HIWN problems in a reasonable computational time and provide global or very good local optimal solutions. This paper addresses the previously mentioned gap by considering trade-offs between investment and operating costs in the targeting step which is a very important step before synthesizing HIWNs. This step provides an accurate enough estimate of the trade-offs between investment and operating cost for selecting promising heat exchange matches before solving the design step by an MINLP model. The results obtained for the considered case study using the proposed approach are in good agreement with the literature results. For a given number of process water-using units, optimal HIWN targets should be obtained before designing an overall HIWN with minimal TAC. In this case, process constraints include operating temperatures, maximum inlet and outlet concentrations, and the mass load of contaminants transferred to water within process water-using units, and environmental constraints include the temperature of the wastewater stream discharged to the environment.

2. Superstructure of water network with identified hot and cold streams

The initial superstructure shown in Figure 1 contains options for identifying hot and cold streams within the HIWN for the considered case study with two water-using units. This superstructure consists of freshwater preheating stages with the splitting of water after each heating stage as well as wastewater cooling stages with gradual mixing and cooling (Ahmetović and Kravanja, 2013). In addition, streams entering and leaving water-using units and streams between water-using units serve as streams for heat integration within this superstructure. It should be noted that superstructure consist of streams for water network no additional process stream is considered. The water-using units are ordered in the superstructure with increasing operating temperature - PU1 is the process unit with the lowest temperature. The streams entering/leaving the process water-using units can be hot or cold. Steams between process units ($p \rightarrow p'$) are identified as hot if the operating temperature of unit p is greater than the operating temperature of p'. Otherwise, the stream is cold.

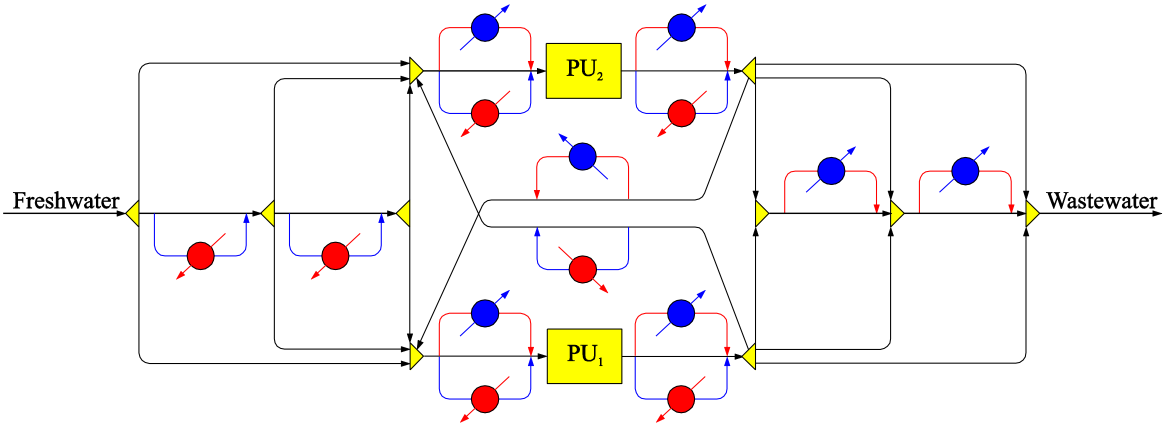

Figure 1: Superstructure of WN with identified hot and cold streams for the case study considered in this work

3. Models and Steps of Solution Strategy

3.1 Targeting model – Step 1 of solution strategy

Based on the proposed superstructure, an overall MINLP model can be formulated and solved in two steps, namely the targeting and the design steps. The focus of this paper is on the targeting step in which the WN (Ahmetović and Kravanja, 2013) is combined with the TransHEN model (Nemet et al., 2019). In the previously presented TransHEN model, all inlet and outlet temperatures are considered constant. However, in the HIWN problem, the temperatures are now variables for the vast majority of the streams, for which a modified TransHEN model is developed and applied in this work. The fixed (constant) temperatures apply only to the freshwater, process units, wastewater discharged from the HIWN into the environment and hot and cold utilities. Therefore, the TransHEN model was updated to include temperatures as variables. The temperature intervals (TIs) are constructed to account for the previously mentioned fixed temperatures on a shifted scale considering the minimum temperature difference. Additional temperature boundaries/intervals are added uniformly across the temperature scale, i.e., between the highest and the lowest temperature resulting from the fixed temperatures. The higher the number of TIs, the more accurate is the estimate of the area cost. However, an increased number of TIs leads to a higher complexity of the model. The TIs are created as input data for optimization. During the optimization, binary variables are used to select the inclusion of the streams within the TIs. Two sets of binary variables are used to determine the TIs in which there is a particular stream. One is the set of y^{max} variables, which are used to identify TIs with their temperatures lower than the highest stream temperature among hot stream inlet temperatures and cold stream outlet temperatures. The other one is y^{min} variables to identify TIs with temperatures higher than the lowest stream temperature among outlet temperatures of the hot streams and inlet temperatures of the cold streams. The third variable y^{sel} is selected (value of 1), when both y^{max} and y^{min} are selected, and identifies the TIs in which the stream is presented. The heat capacity flow rate is calculated separately for each TI based on the aforementioned binary variables (Figure 2). The *fhp* presents the heat capacity flow rate of hot streams *i*, while *fcp* represents the heat capacity flow rate of cold streams *j*. It is calculated separately for each TI, which is indexed by the set *k*, in the manner shown in Eq. (1) and Eq. (2). In the TI, where the stream is fully presented, the heat capacity flow rate is determined as the mass flow rate is multiplied by the specific heat capacity of the water. In the first and last TI, where the stream is still presented, the missing fraction of the heat capacity flow rate for the portion of the stream not being presented in the TI is determined for four possible positive differences between the hot or cold inlet/outlet stream temperature and the upper and lower boundary temperature of the TI. The fraction is defined as the ratio between this positive difference and the total temperature difference of the TI. Note that for the portion of the stream not being presented in the TI, the total heat capacity flow rate is reduced proportionally to this fraction by subtracting this term from the overall one. Note also that when the difference in the binary variable y^{max} is equal to one, it identifies the TI of the highest temperature, where the stream is still presented, while the difference in y^{min} represents the TI with the lowest temperature, where the stream is still presented. It should be noted that only the principle of calculations is presented in this paper. In the MINLP model, the nonlinear equations Eq. (1) and Eq. (2) are transformed to multiple linear inequalities. The calculated heat capacity flow rates are further used in the targeting step model to allow heat integration with the area estimation, where the investment cost is also included in the objective function. The targeting step is used to make all the important decisions about flow rates, stream selection, and stream type (hot or cold).

$$fhp_{\mathrm{i,k}} = \dot{m}_{\mathrm{i}} \cdot cp \cdot y_{\mathrm{i,k}}^{\mathrm{sel}} - \dot{m}_{\mathrm{i}} \cdot cp \frac{TI_{\mathrm{k}} - TH_{\mathrm{i}}^{\mathrm{in}}}{TI_{\mathrm{k}} - TI_{\mathrm{k+1}}} \cdot \left(y_{\mathrm{i,k}}^{\max} - y_{\mathrm{i,k-1}}^{\max} \right) - \dot{m}_{\mathrm{i}} \cdot cp \frac{TH_{\mathrm{i}}^{\mathrm{out}} - TI_{\mathrm{k+1}}}{TI_{\mathrm{k}} - TI_{\mathrm{k+1}}} \cdot \left(y_{\mathrm{i,k}}^{\min} - y_{\mathrm{i,k+1}}^{\min} \right) \quad \forall i \in I, k \in K \tag{1}$$

$$fcp_{\mathrm{j,k}} = \dot{m}_{\mathrm{j}} \cdot cp \cdot y_{\mathrm{j,k}}^{\mathrm{sel}} - \dot{m}_{\mathrm{j}} \cdot cp \frac{TI_{\mathrm{k}} - TC_{\mathrm{j}}^{\mathrm{out}}}{TI_{\mathrm{k}} - TI_{\mathrm{k+1}}} \cdot \left(y_{\mathrm{j,k}}^{\max} - y_{\mathrm{j,k-1}}^{\max} \right) - \dot{m}_{\mathrm{j}} \cdot cp \frac{TC_{\mathrm{j}}^{\mathrm{in}} - TI_{\mathrm{k+1}}}{TI_{\mathrm{k}} - TI_{\mathrm{k+1}}} \cdot \left(y_{\mathrm{j,k}}^{\min} - y_{\mathrm{j,k+1}}^{\min} \right) \quad \forall j \in J, k \in K \tag{2}$$

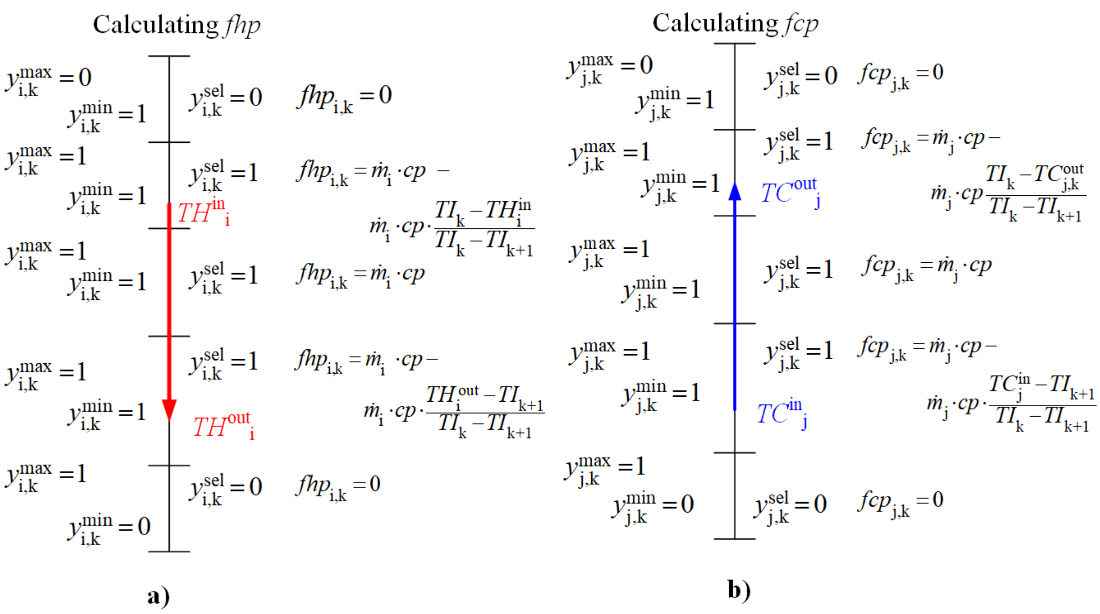

Figure 2: Building temperature intervals and determining heat capacity flowrates in the targeting step with the TransHEN model

3.2 Design model – Step 2 of solution strategy

The proposed targeting model (step) presented in this work can be used in combination with the design model (step) to address the synthesis of the overall HIWN problem. The targeting step provides important information (i.e., the selection of promising heat exchange matches between hot and cold streams, freshwater and utility consumption, good initial points and bounds on variables) for the design step to synthesize a HIWN. The design step combines WN (Ahmetović and Kravanja 2013) with stage-wise HEN superstructure (Yee et al., 1990), considering only the streams selected in the targeting step with specified flowrates and inlet/outlet temperatures. The design step serves to obtain the exact HIWN.

4. Case study

This work considers a case study with two process water-using units, which is simple enough that the global solution could be obtained by the simultaneous approach (Ahmetović and Kravanja, 2012) with the simultaneous HEN model by Yee et al. (1990). The objective is to compare the solution of the proposed two-step approach for HIWN synthesis with the global solution of that simultaneous approach. Also, another objective is to demonstrate that the proposed approach can provide solution close to the global optimum, and be recognized as suitable for solving large-scale HIWN problems. Table 1 shows operating data for this case study. The temperature of freshwater without contaminants is 20 °C and the temperature of wastewater discharged into the environment is 30 °C. The temperature of hot utility is 120 °C, and the inlet and outlet temperatures of the cold utility are 10 °C and 20 °C. The freshwater price is 0.375 $/t, the price of hot utility 377 $/(kW·y) and the price of cold utility 189 $/(kW·y). The total heat transfer coefficient is assumed to be 0.5 kW/(m^2·K).

Table 1: Operating data for the case study

Process unit	Mass load (g/s)	Maximum inlet concentration (ppm)	Maximum outlet concentration (ppm)	Limiting water flowrate (kg/s)	Temperature (°C)
1	30	50	800	40	75
2	5	50	100	100	100

Table 2: Key performance indicators of HIWNs and comparison of the results

Parameter	Ahmetović and Kravanja (2012)	This paper Targeting step	This paper Design step
Freshwater consumption (kg/s)	70	70	70
Hot utility consumption (kW)	2,940	2,940	2,940
Cold utility consumption (kW)	0	0	0
Operating cost ($/y)	1,864,380	1,864,380	1,864,380
HEN investment ($/y)	248,189	299,540	247,781
TAC ($/y)	2,112,569	2,163,920	2,112,161

The annualized investment costs for the shell and tube HEs are given by the equation 8,000+1,200·(Area)0.6. The plant operates continuously 8,000 h/y. The specific heat capacity of the water streams is assumed to be constant (4.2 kJ/(kg·°C)). Table 2 presents key performance indicators of two solutions. As can be seen, the TAC with the proposed new approach was 2,112,161 $/y, which can be considered as the same result as the global optimal result presented as the best result for this case study (Ahmetović and Kravanja 2012). It is a good indication that the procedure developed can be claimed as successful. It is interesting to note that TACs obtained by the targeting step (2,163,920 $/y) and the design step (2,112,161 $/y) of the two-step procedure proposed in this paper present only 2.5 % difference. It can also be seen that freshwater and utility consumption and, consequently, also the operating cost are identical in both steps and are in accordance with the best results. There is some noticeable difference in the investment calculation; however, the results obtained still represent an acceptable estimate. It should be noted that in first step supertargeting is needed by applying different ΔTmin. Based on these results, it can be concluded that the two-step approach proposed in this paper has the potential to achieve near-globally optimal solutions. This verification is crucial before proceeding with the application of the two-step approach to medium and large-scale problems, as sometimes it is not even possible to obtain locally optimal solutions, let alone global solutions, at this scale of problems.

5. Conclusions

This paper has addressed the simultaneous synthesis of HIWN considering WN and HEN at the same time. The main focus was on the targeting step considering trade-offs between investment and operating costs while keeping the model as linear as possible. Also, the aim was to enable precise enough decision-making about flows, type of streams (hot/cold), estimated heat transfer and required heat exchanger area and selection of promising matches for the design step. The proposed approach was applied to solve a simple case study to verify the capability of obtaining satisfactory results by using the proposed approach. The case study indicated that the solution obtained by the proposed two-step approach was the same as the global optimum solution. It is expected that by applying the proposed two-step approach in future research, medium and large-scale problems will become solvable and near-global optima can be achieved.

Nomenclature

i – set of hot streams
j – set of cold streams
k – set for temperature intervals
fhp – heat capacity flowrate of hot stream, W/°C
fcp – heat capacity flowrate of cold stream, W/°C
$\dot{m}$ – mass flowrate, kg/s
cp – specific heat, J/(kg·°C)

TI_k – temperature at boundary of temperature interval, °C
TH^{in} – inlet temperature of hot stream, °C
TH^{out} – outlet temperature of hot stream, °C
TC^{in} – inlet temperature of cold stream, °C
TC^{out} – outlet temperature of cold stream, °C
ΔT_{min} – minimum temperature difference, °C

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