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A Two-Step Solution Strategy for the Synthesis of Pinched and Threshold Heat-Integrated Process Water Networks

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This contribution describes a new two-step solution strategy for the synthesis of heat-integrated process water networks (HIPWNs). The proposed strategy involves the solutions of two models. The first, nonlinear programming (NLP) model consists of a water network (WN) model and a simultaneous optimisation and heat integration model. The objective function in model minimises the consumption of freshwater, heating and cooling utilities. The second, a mixed-integer nonlinear programming (MINLP) model combines the WN model from the first step using a heat exchanger network (HEN) synthesis (Yee et al., 1990) model for minimising the total annual cost (TAC) of the overall combined network. According to the proposed strategy, the first targeting NLP is solved during the first step in order to provide good initialisation for the second step, as well as to determine upper bounds for water and utility consumption, assuming a given value for the heat recovery approach temperature (HRAT). Optimal overall network structures are then obtained during the second synthesis step by solving the MINLP model, now having all the temperature driving forces in HEN as optimisation variables. The two-step procedure is repeated for a range of HRAT values. A set of good locally-optimal solutions is thus identified and the best one with minimum TAC is chosen from amongst them. The solutions obtained indicate that the proposed strategy can be successfully applied to the synthesis of HIPWNs. The results of the threshold case-studies are similar to those found in the literature. However, better solutions were achieved in pinched cases because the proposed synthesis model enables the obtaining of appropriate trade-offs between freshwater, utility consumption and investment.

1. Introduction

Water is a crucial natural resource for process industries (chemical, pharmaceutical, food industries etc.), where it is used as a mass transfer agent (extraction, absorption etc.) as well as cooling water or make-up water for hot utility (steam) generation. In order to minimise water and utility consumption within industries and obtain sustainable solutions, the synthesis problem of HIPWNs has been considered by many researchers over the past few decades. Different methods have been used to deal with these problems, namely, pinch analysis and mathematical programming. For a brief overview of these methods the reader is referred to (Klemeš, 2012) and (Jeżowski, 2010). The objective of the synthesis is to obtain HIPWN designs with the minimum freshwater and utility consumption by minimising the TAC of the overall network by the sequential or simultaneous solution approach. In the sequential approach WN and HEN are synthesised separately whilst in the simultaneous approach they are solved together in order to obtain appropriate trade-offs between freshwater, utility consumption and investment in heat exchangers (HEs). Different simultaneous solution approaches for the synthesis of HIPWNs have been used in several papers. Bogataj and Bagajewicz (2008) used a two-step solution strategy. The WN model was first solved using a local NLP solver followed by solving the combined WN-HEN model. Leewongtanawit and Kim (2008) proposed the strategy based on the decomposition of the overall MINLP problem in two sub-problems (MILP and NLP) sequentially solved with an iterative procedure. Dong et al. (2008) used a hybrid optimization strategy applying the deterministic and stochastic search techniques in order to solve the overall WN-HEN problem. Kim et al. (2009) proposed a systematic approach for solving wastewater and

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heat exchange networks and they used a specific strategy to address a MINLP problem. Ahmetović and Kravanja (2012) presented and compared sequential and simultaneous solution strategies for the synthesis of HIPWNs. In the simultaneous strategy, WN is solved first in order to provide a good initial point and after that the overall HIPWN is solved (Ahmetović and Kravanja, 2013). The abovementioned studies focused mainly on threshold problems. In this paper, a two-stage solution strategy is proposed for the simultaneous synthesis of threshold, as well as pinched HIPWNs.

2. Problem Statement

Given is a set of water sources (freshwater or secondary water) with specified temperatures and contaminant concentrations, a set of water-using units with specified temperatures and the maximum inlet and outlet contaminant concentrations, the contaminant loads in process units, and the temperature of wastewater discharged into the environment, it is necessary to determine the process parameters (flow-rates, temperatures, and contaminant concentrations) and design a pinched and threshold HIPWN minimising TAC.

3. Superstructure and Model

The superstructure of HIPWN (Figure 1) consists of freshwater sources with corresponding heating and cooling stages in order to provide water of different temperature levels, process units with mixers and splitters, wastewater discharge mixers with corresponding cooling and heating stages to satisfy temperature constraint for the effluent discharged into the environment.

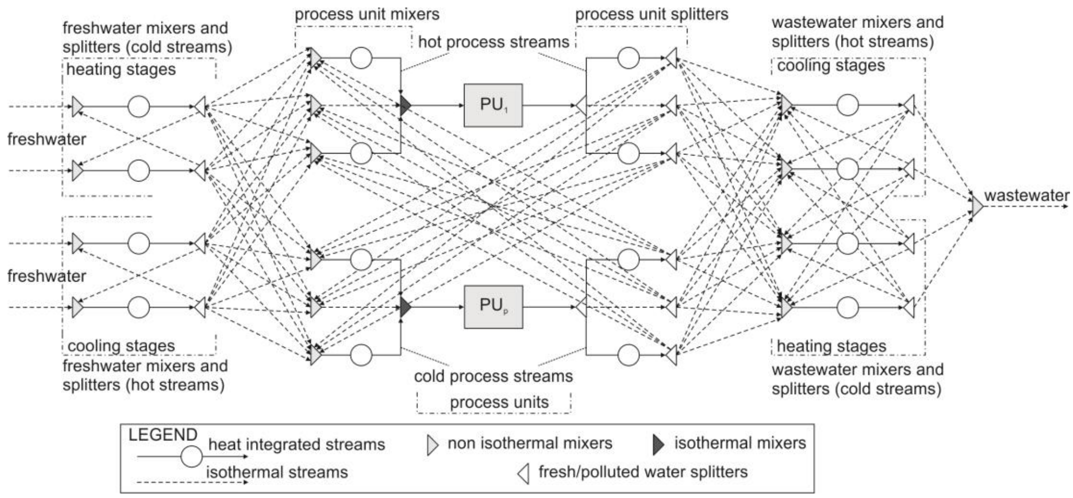

Figure 1: Superstructure of HIPWN.

The proposed superstructure is used for creating a WN model consisting of mass balance equations for splitters and mixers, contaminant mass balance and heat balance equations for mixers, and a cut proposed by Karuppiah and Grossmann (2006) in order to improve the strength of the lower bound for the optimum. The NLP model used during the first initialisation step of the proposed strategy consist of the WN model and the simultaneous optimisation and heat integration model (Duran and Grossmann, 1986). The objective of this model is to minimise freshwater, hot and cold utilities consumption. Note that a similar freshwater and utility targeting model using a different superstructure and linearisation techniques was developed by Yang and Grossmann (2012). The MINLP model of the overall network used in the second synthesis step of the proposed strategy, consists of the WN model and HEN synthesis model (Yee et al., 1990). The objective function of this model is to simultaneously minimise freshwater, utilities and the investment costs of the HIPWN.

4. Two-Step Solution Strategy

In the first step of the proposed two-step solution strategy (Figure 2) the NLP model, briefly described in the previous section, is solved in order to minimise freshwater and utility consumption. The solution of this model, i.e. a water network with minimum freshwater and utility consumption, flow-rates, temperatures, and contaminant concentrations, is used as an initialisation point during the second synthesis step. In addition, the values for freshwater and utility consumption obtained during the first step for a given value of HRAT would be set as rigorous upper bounds for solving the MINLP model during the second step. The objective of the MINLP model is to minimise the TAC of the overall network now with all the temperature driving forces in HEN as optimisation variables. A set of good locally optimal solutions would thus be obtained and the best one with minimum TAC chosen from amongst them. The problem was modelled in GAMS (Rosenthal, 2012), and NLP sub-problems solved by local solvers. AlphaECP, in combination with CONOPT as NLP and XPRESS as MIP solvers, were used for solving the NLP during the first step and SBB with SNOPT as NLP solver during the second step for solving the MINLP model. In principle, GAMS/AlphaECP can handle NLP models, especially in combination with an NLP solver for finding solutions that the NLP solver could not find by itself. In this case it acts as a good starting point generator. In order to solve NLPs with GAMS/AlphaECP you need to trick the GAMS system by solving NLP as an MINLP (GAMS Solvers, 2012).

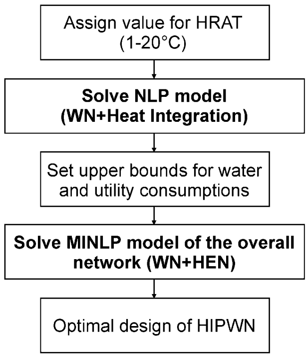

Figure 2: Two-step solution strategy for the synthesis of pinched and threshold HIPWNs.

5. Examples and Results

Two examples were solved in order to demonstrate the applicability of the proposed solution strategy for threshold and pinched problems. In Example 1 the water source was freshwater free of contaminants at a temperature of 20 °C, with wastewater discharged into the environment at a temperature of 30 °C. In Example 2 a secondary free of contaminants water source at a temperature of 80 °C was used with wastewater discharged into the environment at a temperature 60 °C. The hot utility was low pressure steam at a temperature of 120 °C. The inlet and outlet temperatures of the cold utility were 10 °C and 20 °C. The freshwater and secondary water prices were assumed to be 0.375 $/t and 0.45 $/t, and the ones for the hot and cold utilities 377 $/(kW y) and 189 $/(kW y). The total heat transfer coefficient was assumed to be 0.5 kW/ (m^2K). The annual investment costs for the shell and tube HEs were estimated by the equation: $8{,}000 + 1{,}200 \cdot A^{0.6}$. The plant operated continuously at 8,000 h/y. The specific heat-capacity of the water streams was 4.2 kJ/ (kg °C). The operating parameters (Table 1) for Example 1 were taken from Savulescu et al. (2005), and for Example 2 from Dong et al. (2008).

5.1 Example 1

This example considered a single contaminant problem with four water-using process units. Note that this example belongs to a class of threshold problems requiring hot utility only when the temperature of the discharged wastewater is greater than that of the freshwater. This problem has been studied by several authors using different methods and solution approaches, and here we present and compare some of the best results reported in the literature, all with minimum freshwater consumption (90 kg/s) and hot (3,780 kW) and cold (0 kW) utility consumption. Bagajewicz et al. (2002) used a state space representation of the problem and Bogataj and Bagajewicz (2008) proposed a two-step solution procedure in order to synthesise HIPWN with a TAC of 2,711,555 $/y, where the investment cost for the HE was 324,495 $/y. The network consisted of three HEs and one heater. Dong et al. (2008) presented a water network with a TAC of 2,738,107.4 $/y, and an investment cost for HEs of 341,047 $/y. The network consisted of four HEs and one heater. Leewongtanawit and Kim (2009) used a graphic-based approach and obtained a solution consisting of three HEs and one heater with a TAC of 2,707,353 $/y. Ahmetović and Kravanja (2013) presented optimal solutions with different numbers of HEs and the best solution reported in the literature with a TAC of 2,652,959 $/y, and investment cost of 255,899 $/y for a network with two HEs and one heater. Using the model and solution strategy proposed in this paper, we obtained a set of good locally optimal solutions (Table 2) for a range of values for HRAT (1 - 20 °C).

Table 1 Process units' data for Examples 1 and 2.

Examples	Process Unit	Contaminant(s)	Contaminant(s) mass load (g/s)	Maximum inlet concentration (ppm)	Maximum outlet concentration (ppm)	Temperature (°C)
Example 1	1	A	2	0	100	40
	2		5	50	100	100
	3		30	50	800	75
	4		4	400	800	50
Example 2	1	A	3.0	0	100	100
		B	2.4	0	80	
		C	1.8	0	60	
	2	A	4.0	50	150	75
		B	3.0	40	115	
		C	3.6	15	105	
	3	A	1.5	50	125	35
		B	0.6	50	80	
		C	2.0	30	130	

Table 2: Investment cost, TAC, and number of HEs for Example 1.

Parameter	HRAT (°C)					
	1	5	**9**	12	15	20
Investment cost ($/y)	270,974.6	280,786.6	**255,899.3**	270,974.6	270,974.6	408,825.2
TAC ($/y)	2,668,034.6	2,677,846.6	**2,652,959.3**	2,668,034.6	2,668,034.6	2,805,885.2
Number of HEs	2	3	**3**	2	2	2

The freshwater consumption (90 kg/s), as well as the hot (3,780 kW) and cold (0 kW) utility consumption were the same for all HRAT values. Table 2 shows that we can obtain different solution networks in terms of investment cost, TAC, and the number of HEs. The best solution network was obtained with HRAT=9 °C. The obtained investment cost for HEs of 255,899.3 $/y, and TAC of 2,652,959 $/y were the same as given by Ahmetović and Kravanja (2013), and present the best result reported so far in the literature for this example. The obtained HIPWN design (Figure 3) was practically the same as in Ahmetović and Kravanja (2013), with slightly different distribution of HEs and wastewater mixing within the network.

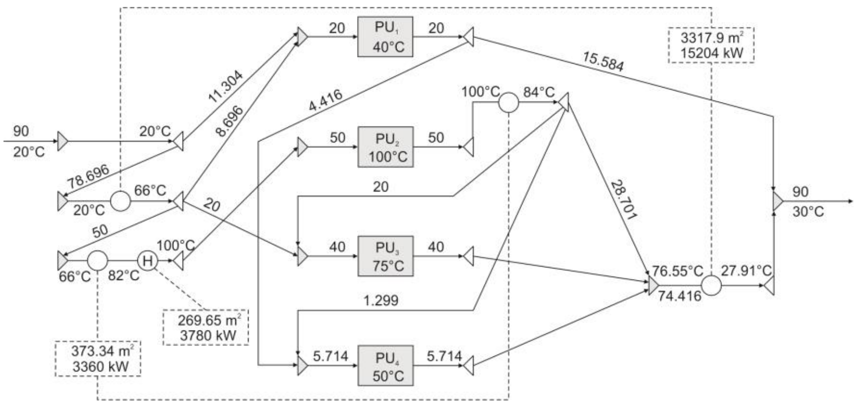

Figure 3: Optimal network design for Example 1

5.2 Example 2

This example studied a multiple contaminant problem with three contaminants and three water-using units. The temperature of the water source (80 °C) was greater than the temperature of the wastewater (60 °C) and, consequently, required the external cold utility. Note also that the temperature of the water source was lower than the maximum temperature of the water-using units (100 °C) and, consequently, also needed the external hot utility. The problem was thus pinched as it required both hot and cold utilities. Dong et al. (2008) solved their MINLP model using the state-space superstructure and obtained an optimal solution with a TAC of 2,905,307.4 $/y. Their network design consisted of two HEs, three coolers and one heater with an investment cost of 173,627.4 $/y. The freshwater consumption was 70 kg/s whilst the consumption of hot and cold utilities was 1,260 kW and 7,140 kW. Note that the correct investment cost for the HEs and TAC of their network design should be 200,893.9 $/y and 2,932,573.96 $/y, since the investment cost for the heater was neglected. The minimum approach temperature (EMAT) for their HEs was set at 10 °C, whist in our approach at 1°C in order to obtain HEN with optimal temperature- driven forces, allowing for obtaining appropriate trade-offs between investment, freshwater and utility costs of the overall HIPWN. The optimal design obtained using our approach consisted of one HE, one heater and three coolers. The freshwater consumption was the same (70 kg/s) as given by Dong et al. (2008). However, the consumption of the hot utility was reduced by 86.29 % (172.7 vs. 1,260 kW) and for the cold utility by 15.23 % (6,052.7 vs. 7,140 kW). However, in this design (Figure 4) the temperature approach for the HE (3,425.71 m^2) was 1.37 °C at both sides of HE, and could be impractical for the shell and tube HEs. On the other hand this temperature approach could be suitable for plate and frame HEs. The TAC of our network design was 2,371,364 $/y, which was an approximately 18 % lower than the TAC obtained by Dong et al. (2008) and the investment cost was 255,110.6 $/y. This problem was also solved for EMAT=10 °C and Figure 5 shows the obtained optimal network design.

The freshwater, hot and cold utility consumption was the same as reported by Dong et al. (2008). However, our network design had lower investment cost (145,784.2 vs. 173,627.4 $/y) for HEs due to their smaller number and, consequently TAC was decreased (2,877,464 vs. 2,905,307.4 $/y).

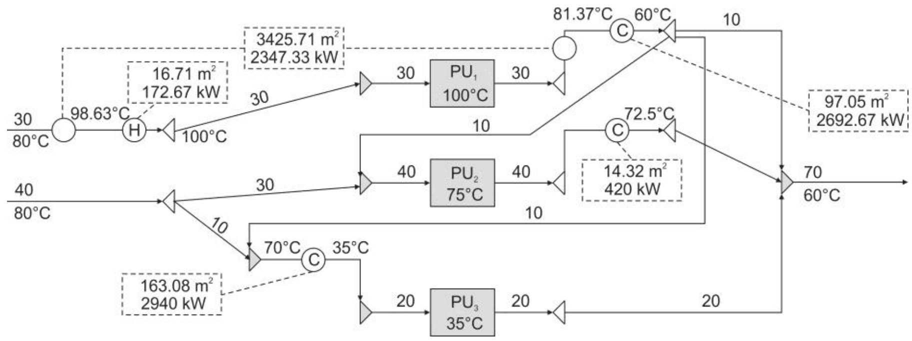

Figure 4: Optimal network design for EMAT=1 °C

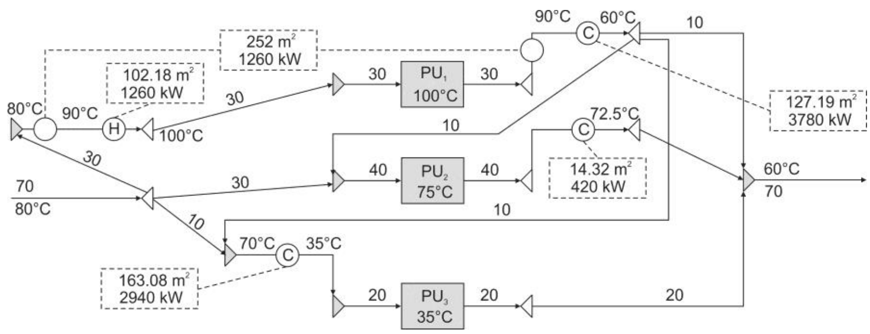

Figure 5: Optimal network design for EMAT=10 °C

6. Conclusions

This paper presented a two-step solution strategy for the simultaneous synthesis of pinched and threshold HIPWNs. The overall strategy consists of the subsequent solution of two models, NLP and MINLP. The NLP is solved during the first step in order to provide an initialisation point and rigorous upper- bounds on utility consumption for solving the MINLP in the second step. Two examples were used to demonstrate that the proposed model and solution strategy could be used for solving threshold and pinched HIPWNs. The threshold problem solution proposed for Example 1 was the same as obtained by Ahmetović and Kravanja (2013). The pinched problem solution of Example 2 was better than the one reported by Dong et al. (2008) since the appropriate trade-offs were obtained between the freshwater cold and hot utility consumption. It is clear that the proposed strategy can be successfully applied for the synthesis of pinched and threshold HIPWNs.

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