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Solution Strategies for the Synthesis of Heat-Integrated Process Water Networks

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This contribution describes the use of sequential and simultaneous strategies for the synthesis of heat-integrated process water networks (HIPWNs). The former strategy consists of the water network (WN) model by Ahmetović and Grossmann (2011), which determines the minimum freshwater consumption and the stage-wise model by Yee et al. (1990) for the synthesis of a heat exchanger network (HEN), both of which are performed sequentially. In the recently introduced approach by Ahmetović and Kravanja (2012) both networks are solved simultaneously by applying a combined (WN-HEN) model. This combined model is formulated as a non-convex mixed integer nonlinear programming (MINLP) problem with the objective function defined as the total annual cost (TAC). As, on the one hand, the combined model in this simultaneous approach enables the obtaining of appropriate trade-offs between freshwater, utilities, and investment, it is, on the other hand, very difficult to solve, due to its non-convex and nonlinear nature. The synthesis of HIPWNs thus still remains a big challenge. The development of efficient solution strategies is necessary in order to accomplish this task. In this paper, syntheses of HIPWNs are carried out using the above-mentioned strategies. It is worth pointing out, that in the simultaneous approach the problem can be solved directly as one system or the WN solved first to provide a good initial point followed by the overall heat-integrated process water network (HIPWN) problem after. The proposed strategies were tested on a literature Case-Study. The solutions were obtained with the minimum consumption of freshwater and utilities, and TAC was significantly improved, when compared to those reported in the literature. The solutions obtained clearly indicate that the proposed strategies can be successfully applied for the synthesis of HIPWNs.

1. Introduction

The synthesis problem of heat-integrated process water networks (HIPWNs) has only been studied within a relatively small number of published papers. In the review by Jeżowski (2010) it can be found that, until mid-to-late 2009, only eighteen papers addressed the performing of heat integration within the water network (WN) problem. Over the last decade, the synthesis of HIPWNs has become an active research field, and the main goal has been to develop efficient models and strategies for minimizing water and energy consumption within the network. Two methods have been used for the synthesizing of HIPWNs, namely, "insight-based" and "optimization-based". The first one is based on pinch analysis, and the second one on mathematical programming and superstructure optimization. The reader is referred to the review papers by Bagajevicz (2000), Furman and Sahinidis (2002), Jeżowski (2008, 2010), and books written by Biegler et al. (1997), Smith (2005), Kemp (2007), Klemeš et al. (2011), El-Halwagi (2012) for more details about insight-based and optimization-based methods. In order to synthesize HIPWNs, different *sequential* (Savulescu and Smith, 1998, Bagajewicz et al., 2002, Savulescu et al., 2005a, 2005b, Liao et al., 2008, Feng et al., 2009, Leewongtanawit and Kim,

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2009, Chen et al., 2010, Polley et al., 2010, Liao et al., 2011) and *simultaneous* (Bogataj and Bagajewicz, 2008, Leewongtanawit and Kim, 2008, Dong et al., 2008, Kim et al., 2009, Xiao et al., 2009) models and solution strategies have been used. The advantage of the sequential strategy is to hierarchically decompose the synthesis problem within a sequence of smaller sub-problems that are easier to solve. The drawback, however, is that the trade-offs between freshwater, utility, and investment cannot be appropriately established. On the other hand, the simultaneous strategy solves the problems integrally, and systematically explores any interactions between the subsystems. In this paper, we used the recently introduced approach by Ahmetović and Kravanja (2012) for the simultaneous synthesis of HIPWNs, in order to establish the appropriate trade-offs between WN and HEN by obtaining an improved solution, as presented later.

2. Problem Formulation

A set of freshwater sources, and a set of water-using units that require water of a certain quality and temperature is given. Using the sequential and simultaneous solution strategies, it is necessary to synthesize the HIPWNs with the minimum freshwater and utilities' consumptions, and the minimum TAC. In addition, the interconnections, flow rates, contaminant concentrations, and the temperatures of each stream within the network need to be determined. The standard assumptions for the synthesis problem are used, as given in the literature.

3. Superstructure and Optimization Model

In the sequential strategy, the WN superstructure and the model recently proposed by Ahmetović and Grossmann (2011) are used in order to determine the minimum freshwater consumption, identify hot and cold streams, and define their inlet/outlet temperatures and heat capacity flow rates. The HEN superstructure and the model proposed by Yee et al. (1990) are used for the synthesis of HIPWNs. In order to perform simultaneous optimization, the above-mentioned WN superstructure is combined with that of HEN. The combined WN-HEN superstructure and the optimization model for the simultaneous synthesis of process water and heat exchanger networks recently developed by Ahmetović and Kravanja (2012) are used to perform and illustrate the simultaneous solution strategy. The combined superstructure involves direct and indirect heat-exchanges, the splitting and mixing of freshwater and wastewater, and additional opportunities for heat integration within the network. A non-convex MINLP problem is formulated for the combined network superstructure, in order to minimize TAC, consisting of annual freshwater and utilities costs, and annualized investment for heat exchangers. A new convex-hull formulation is used for identifying the hot and cold streams within the network (i.e. the outlet streams of the mixers and splitters of the water-using units), as well as the connecting equations for HEN. The synthesis problem is solved using the sequential and simultaneous solution strategy, as explained in the next section.

4. Solution Strategies

The sequential strategy consists of two steps. The first one represents the synthesis of WN, and the second one the synthesis of HEN. In this strategy, the synthesis problem is thus hierarchically decomposed within a sequence of two smaller problems that are easier to solve. During the first step, the WN model proposed by Ahmetović and Grossmann (2011) is used to synthesize WN and to minimize the freshwater consumption. The temperature of the outlet streams from the mixer and splitter process units is assumed to be the same as the temperature of the water-using operations. Under an assumption of the isothermal mixing of the streams, the best energy performances at the targeting stage can be ensured (Kemp, 2007). From the obtained WN solution, the hot and cold streams can then be identified, as well as their heat capacity flow rates, and inlet and outlet temperatures. During the second step, the HEN superstructure introduced by Yee et al. (1990) is used to synthesize the HIPWNs minimizing TAC. The simultaneous solution strategy is used to take into account the trade-offs between the annual freshwater and utility costs, and the annualized investment, and explores the interactions between WN and HEN. This simultaneous strategy can be successfully used for obtaining improved solutions for HIPWNs with reduced TAC, and minimum freshwater and utilities consumption. In this strategy, WN is solved first in order to provide a good initialization point, followed by a simultaneous solution of the combined WN-HEN model. The synthesis problem is implemented in GAMS (Brooke et al., 1998) and solved on a Toshiba Notebook PC with an 8 GB RAM memory, and Intel i5 processor. A BARON solver was used in both the above-mentioned strategies for solving WN, and an SBB solver for solving HEN and the combined WN-HEN. The network solutions are obtained within reasonable computational times. By applying the simultaneous strategy given in this paper to the Case-Study, a new network design with the freshwater and utilities targets is obtained, with a TAC smaller than any one reported in the literature so far.

5. Case-Study

Table 1 shows the process data for a Case-Study taken from Bagajewicz et al. (2002). In order to calculate the TAC involving freshwater and utilities costs, and the capital cost for heat exchangers, the cost and operating parameters (Table 1) were used as given by Dong et al. (2008). The freshwater cost was assumed to be 0.375 \$/y; the cooling utility cost 189 \$/(kW y); the heating utility (low pressure steam, 120 °C) cost 377 \$/(kW y); the fixed charge, the area cost coefficient, and the cost exponent for the heat exchangers were assumed to be 8,000 \$, 1,200 \$/m^2, and 0.6, respectively; the overall heat transfer coefficient 0.5 kW/(m^2 °C) (individual heat transfer coefficients for water streams and utilities were assumed to be 1 kW/(m^2 °C)); the working hours of the network per year 8,000 h; the inlet and outlet temperatures of cooling water 10 °C and 20°C, respectively; the temperatures of freshwater and wastewater, 20°C and 30°C, respectively, and the specific heat capacity of water 4.2 kJ/(kg °C).

Table 1: Water-using operation data for a Case-Study.

Process unit	Contaminant mass load (g/s)	C_{in} (ppm)	C_{out} (ppm)	Limiting water flow rate (kg/s)	Temperature (°C)
1	5	50	100	100	100
2	30	50	800	40	75
3	50	800	1,100	166.7	100

Bagajewicz et al. (2002) only presented the solution of the WN design for this problem, with a minimum freshwater consumption (77.273 kg/s), whilst the HIPWN design was not given. Later, in order to solve this problem as HIPWN, and minimize TAC, Dong et al. (2008) used the state-space superstructure, and a MINLP model. They presented two solutions for HIPWNs designs. The first one was obtained by the sequential solution procedure, as suggested by Bagajewicz et al. (2002). The resulting network produced consisted of four heat exchangers, two heaters, and one cooler. The freshwater consumption was 77.27 kg/s, whilst the consumptions of cold and hot utilities were 491 kW and 3,763.2 kW, respectively. Note, that the hot utility consumption (3,763.2 kW) was larger than the minimum hot utility target (3,245.5 kW). The TAC of the network was 2,742,198.4 \$/y, whilst the capital investment was 406,290.8 \$/y. Their second HIPWN design was obtained by a simultaneous strategy, where a single state-space MINLP was solved for obtaining a design with the minimum TAC. The network design consisted of two heat exchangers and two heaters. In this case, TAC (2,631,805.4 \$/y) and the capital investment (305,913.3 \$/y) were reduced compared to the equivalent solution obtained by the sequential procedure. However, in this network the freshwater (87.2 kg/s) and hot utility (3,671.4 kW) consumptions were greater than the freshwater (77.273 kg/s) and hot utility (3,245.5 kW) target for this Case-Study.

6. Results and Discussions

We solved this case study using both the sequential and simultaneous strategies, and compared the results with those reported in the literature. During the sequential strategy, WN was solved in the first step, and a minimum freshwater consumption (77.273 kg/s) was obtained, which was the same as given by Bagajewicz et al. (2002) and Dong et al. (2008). On the basis of the resulting WN design, two hot and three cold streams with their heat-capacity flow rates, and inlet and outlet temperatures, were identified. During the second step, the HEN superstructure was solved and a network was obtained with five heat exchangers and two heaters. The solutions from both steps were then combined into an overall HIPWN solution. It is worth pointing out that the TAC thus obtained was in this case (2,494,716.5 $/y) significantly reduced (by about 10 %), compared to the TAC (2,742,198.4 $/y) of the network proposed by Dong et al. (2008). In addition, by using the sequential strategy, a network was obtained with the minimum freshwater (77.273 kg/s), hot (3,245.5 kW) and cold (0 kW) utilities consumption. The results for this case-study using the proposed sequential solution strategy, and their comparison with the reported results in the literature are summarized in Table 2.

Table 2: A comparison of the results obtained using the sequential solution strategies.

	The method proposed by Dong et al. (2008)	The method proposed in this paper
TAC ($/y)	2,742,198.4	2,494,716.5
Investment costs ($/y)	406,290.8	436,627.43
Freshwater consumption (kg/s)	77.3	77.273
Cold utility consumption (kW)	491	0
Hot utility consumption (kW)	3,736.2	3,245.5
Equipment requirements (/)	2 heaters, 1 cooler, 4 heat exchangers	2 heaters, 0 coolers, 5 heat exchangers

The resulting HIPWN design obtained by the proposed simultaneous solution strategy is given in Figure 1. Its HEN consists of three heat exchangers and two heaters. As can be seen from Figure 1, the outlet streams of process units PU_2 and PU_3, and the freshwater and wastewater play an important role during heat integration. In order to achieve a target temperature for process units PU_1 and PU_3 (100°C), two heat exchangers and one heater were placed on the freshwater stream and one heat exchanger and one heater on the outlet stream of the process unit PU_2. The connections between the process units and their corresponding flow rates selected by the sequential and simultaneous solution strategies were the same, whilst there was a difference in the selected matches for heat integration.

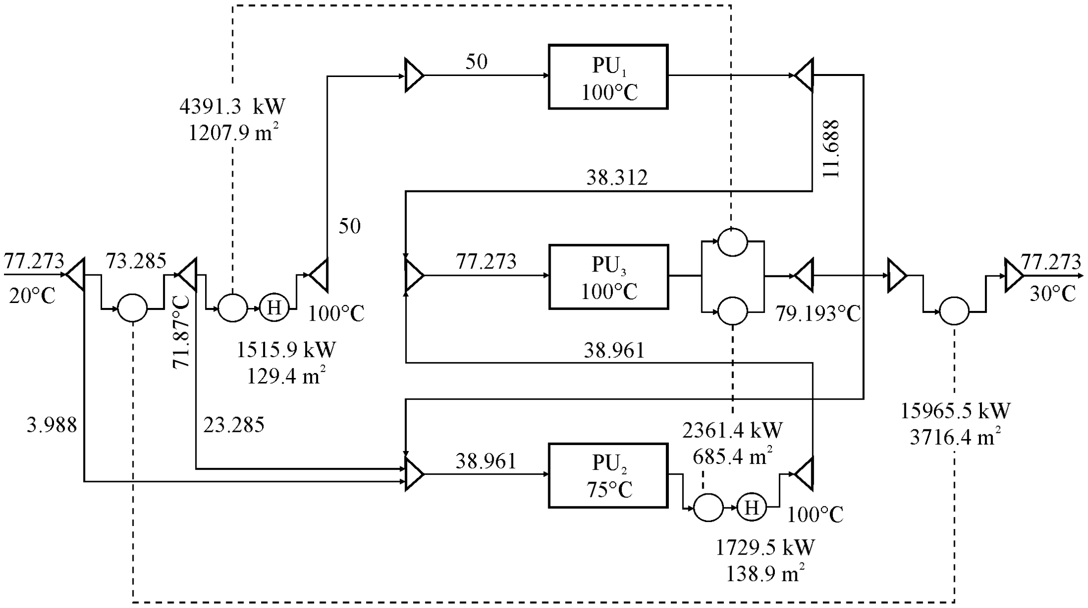

Figure 1: Optimal design of a heat-integrated water network obtained by a simultaneous solution strategy.

The network design obtained by our simultaneous solution strategy exhibited the minimum freshwater consumption (77.273 kg/s), the minimum hot (3,245.5 kW) and cold (0 kW) utilities consumptions, which was not the case for the design obtained by the simultaneous solution strategy proposed by Dong et al. (2008). In the network solution by (Dong et al., 2008), the freshwater consumption and hot utility consumption were 87.2 kg/s and 3,671.4 kW, respectively. In addition, the TAC of the presented network design (2,455,048.09 \$/y) was significantly lower (7.2 %) than that obtained by Dong at al. (2008). This decrease was mainly achieved due to the reduction of freshwater (77.723 kg/s vs. 87.2 kg/s) and hot utility consumption (3,245.5 kW vs. 3,671.4 kW). The results of this case study using the proposed simultaneous solution strategy, and their comparison with the reported results in the literature are summarized in Table 3. These results clearly indicate that the simultaneous solution strategy proposed in this paper can be successfully used for the synthesis of HIPWNs with reduced TACs compared to those reported in the literature.

Table 3: A comparison of the results obtained using the simultaneous solution strategies.

	The method proposed by Dong et al. (2008)	The method proposed in this paper
TAC (\$/y)	2,631,805.4	2,455,048.09
Investment costs (\$/y)	305,913.3	396,966.28
Freshwater consumption (kg/s)	87,2	77.273
Cold utility consumption (kW)	0	0
Hot utility consumption (kW)	3,671.4	3,245.5
Equipment requirements (/)	2 heaters, 0 coolers, 2 heat exchangers	2 heaters, 0 coolers, 3 heat exchangers

7. Conclusions

This paper presented new sequential and simultaneous solution strategies for the synthesis of HIPWNs. A literature Case-Study has been solved, in order to demonstrate the efficiency of the proposed strategies. Optimal water network designs with the minimum freshwater and utility consumption were synthesized by both strategies. In particular, by the use of the proposed sequential approach, the TAC was significantly reduced (by about 10 %) compared to that given by Dong et al. (2008) (2,494,716 \$/yr vs. 2,742,198 \$/yr). In the case of the proposed simultaneous strategy, the TAC of the network was reduced even further to 2,455,048 \$/yr, which represented a reduction of about 7 %, when compared to the simultaneous TAC by Dong et al. (2008) (2,455,048 \$/yr vs. 2,631,805 \$/yr). These better solutions are obtained due to a reduction in the freshwater (77.723 kg/s vs. 87.2 kg/s) and hot utility consumption (3,245.5 kW vs. 3,671.4 kW) for the simultaneous approach, and due to the reduction of hot (3,245.5 kW vs. 3,736.2 kW) and cold (0 kW vs. 491 kW) utilities consumptions for the sequential approach. From the results it is clear that the proposed strategies can be used successfully for solving HIPWNs. Using the simultaneous strategy, appropriate trade-offs between WN and HEN were established, an improved solution obtained, and the TAC of the network significantly reduced, when compared to the reported results in the literature.

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