17th European Symposium on Computer Aided Process Engineering – ESCAPE17
V. Plesu and P.S. Agachi (Editors)
© 2007 Elsevier B.V. All rights reserved.

Design of non-isothermal Process Water Networks

Miloš Bogataj,^a Miguel J. Bagajewicz^b

^aFaculty of Chemistry and Chemical Engineering, University of Maribor Maribor SI-2000, Slovenia, milos.bogataj@uni-mb.si
 ^bSchool of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, 73019, USA, bagajewicz@ou.edu

Abstract

Despite the fact that many methods have been developed for the optimization of process water networks, solving the problem simultaneously considering heat recovery has rarely been addressed. This paper presents a new approach for the simultaneous synthesis and optimization of heat integrated water networks. The procedure is based on mixed integer non-linear mathematical programming (MINLP). A new superstructure for heat exchanger network (HEN) synthesis capable of exploiting unique features of water networks, like non-isothermal mixing of different streams, thus providing potentially more cost-effective solutions, is proposed. An example is presented to illustrate the synthesis of heat integrated water networks using the proposed approach.

Keywords: water networks, wastewater minimization, heat integration, MINLP, HEN synthesis, process synthesis.

1. Introduction

Different methods, rooted in conceptual design or mathematical programming, have been developed for water minimization as well as for the heat exchanger network (HEN) synthesis problem. The reader is referred to Bagajewicz (2000) for a comprehensive review of technologies developed to solve the water

minimization problem and to Furman and Sahinidis (2002) for a review of the HEN synthesis technologies.

The most widely used technology in HEN synthesis field is the well-known Pinch Technology (Linnhoff et al., 1982). However, designs using the pinch methodology were shown to be in many cases non-optimal, mainly due to its sequential nature (minimize energy first, followed by strict unit number minimization), although some improvements have been noted (Supertargeting). To overcome the drawbacks of the pinch method different approaches using mathematical programming were presented over the last two decades. Of these, them as transportation-transshipment oriented can classify one and superstructure oriented. The latest model on the transportation-transshipment type is the one proposed by Barbaro and Bagajewicz (2005), which is linear and allows non-isothermal mixing as well as multiple matches between two streams. Among the superstructure-based models, the most popular method is a stagewise superstructure approach (Yee et al., 1990a, 1990b).

Simplicity of pinch methodology and some similarities between water minimization and energy minimization problem induced a development of conceptual design approaches in the field of water minimization (Wang and Smith, 1994, Majozi et al., 2006). The conceptual approach is useful for the single contaminant case, with limited applicability to multicontaminant cases.

Despite all the enabling technologies, the influence of heat integration on the solution of water allocation planning (WAP) has been rarely addressed in the past. Savelski and Bagajewicz (1997) first studied the problem pointing out the existence of a trade off. A graphical procedure was introduced (Savulescu & Smith, 1998) in attempt to solve the energy efficient WAP problem. The method was recently extended to use a two stage procedure (Savulescu et al. 2005a, 2005b). However, the approach is limited to a single contaminant case. In turn, Bagajewicz et al. (2002) solved the problem using mathematical programming. With minor modifications their approach can be extended to handle the multi-contaminant case. The model is, nonetheless, sequential.

An important realization about all these systems is that, in the absence of regeneration, systems are generally pinched at the lowest (inlet) temperature. In addition, what makes the design challenging is that mixing of streams is a part of the design, especially if it is used to achieve target temperatures, and therefore avoid the use of heat exchangers or utilities. In addition, it has been shown that clever mixing can reduce the number of exchangers in the system (Bagajewicz et al., 2002).

This paper introduces a new approach for simultaneous synthesis of energy efficient water networks. The approach is based on MINLP mathematical programming. The main feature of the formulation is mixing and splitting of streams within the HEN superstructure, thus enabling direct heat exchange in order to reduce the number of heat exchangers as well as to reduce the complexity of heat integrated process structure.

2. Problem statement

Given a set of water using/water disposing processes which require water of adequate quality and temperature, determine the optimal process structure (i.e. a network of water stream interconnections among the processes) and the corresponding heat exchanger network. Usually, the objective is related to fresh water usage, energy consumption, and investment costs. The following assumptions were used in this work:

- processes operate isothermally,
- constant heat transfer coefficients,
- counter current heat exchangers.

3. Heat integration model

Consider the following example (Table 1) which uses water network targets from Savulescu and Smith (1998). The solution obtained by Bagajewicz et al. (2002) is presented in Fig. 1.

Process No.	$q_m^{\mathrm{cont.}}$ /(kg/h)	c_{in}^{max} /ppm	c_{out}^{max} /ppm	$T_{\rm proc}./^{\circ}{ m C}$
1	2	0	100	40
2	5	50	100	100
3	30	50	800	75
4	4	400	800	50

Table 1: Example data from Savulescu and Smith (1998).

It can be seen that heat exchange takes place only between cold fresh water streams and hot discharge wastewater streams.



Figure 1: Solution from Bagajewicz et al. (2002).

The solution considers the fact that fresh water is coming from a unique source, and can be progressively heated up through a series of heat exchangers. Furthermore, discharge wastewater streams can freely mix as long as the maximum sink inlet concentration constraint is satisfied. The design presented in Fig. 1 was obtained by means of a non-systematic merging procedure. Recently the same example was solved by Savulescu et al. (2005a, 2005b). The

authors used a two stage design strategy (based on the generation of separate systems and non-isothermal mixing) to reduce the number of heat transfer units. Neither of these approaches gives a directly cost-driven solution/design.

In order to exploit the possibilities of direct heat transfer by mixing the superstructure of the Synheat model presented by Yee et al. (1990b) was modified. The main feature of the proposed superstructure is that mixing and splitting of hot and cold streams is enabled in each stage of the superstructure before heat exchange takes place. For this reason additional variables and equations were added. The majority of the original equations were reformulated. Note that splitting and mixing should be allowed only for those streams for which the outlet contaminant concentration is not important or it equals zero as in case of fresh water streams. By allowing mixing and splitting of streams additional nonlinearities (bilinearities in mixing points) are introduced into the model. The MINLP model consists of a nonlinear objective function (Investment + heating/cooling utilities + fresh water costs), constraints describing the proposed the HEN superstructure and a set of linear and nonlinear equations describing the WAP superstructure presented in Fig. 2. The WAP superstructure in Fig. 2 was modeled as a NLP, and the costs of processto-process connections were not considered in the objective function.

3.1. Results

The model was solved using GAMS software. DICOPT was used with BARON as a NLP solver for the first (relaxed) NLP and CONOPT for subsequent NLPs. The model consists of 658 equations, 562 continuous variables and 55 discrete variables. Total CPU time needed to find optimal solution was 15 s. In Fig. 3 only the HEN is presented, since the WAP structure is identical to the one reported by Bagajewicz et al. (2002). In Table 2, a comparison of results obtained with the SYNHEAT model (no mixing of streams) and those obtained with the proposed method are presented. It is evident that fresh water and hot utility consumption is equal in both cases. However, the number of heat exchangers obtained by the proposed approach is noticeably smaller and the area is slightly higher.

4. Conclusions

A superstructure model was presented that addresses the simultaneous water and heat recovery problem. Even though the solutions are not global, comparison of the results using the SYNHEAT model without direct heat transfer (mixing of streams) and the results using the proposed approach shows the latter to be superior. Fresh water is delivered to the corresponding processes as a split from a main fresh water stream, and wastewater is discharged to the

sink as a single stream, the target temperatures being met using heat exchangers and mixing.



Figure 2: Schematic representation of combined WAP and HEN superstructures.

Table 2: Comparison of the results.

Model	Fresh water	No. of heat exchangers	Total heat exchanger	Investment costs/\$	Utility costs/(\$/a)
	/(t/h)		area/m ²		
SYNHEAT	90	10	996.7	96,400	83,700
Proposed superstructure	90	5	1004	61,900	83,700

References

- 1. M. J. Bagajewicz, A review of recent design procedures for water networks in refineries and process plants, Computers and Chemical Engineering, 24 (2000) 2113.
- 2. K. C. Furman, N. V. Sahinidis, A critical review and annotated bibliography for heat exchanger network synthesis in the 20th century, IECR, 41 (2002) 2370.
- 3. B. Linnhoff et al., User guide on process integration for the efficient use of energy, Institute of chemical engineers, UK, 1982.
- 4. A. Barbaro, M. J. Bagajewicz, New rigorous one-step MILP formulation for heat exchanger network synthesis, Computers and Chemical Engineering, 29 (2005) 1976.

- 5. T. F. Yee, I. E. Grossmann, Z. Kravanja, Simultaneous optimization models for heat integration I, Computers and Chemical Engineering, 10 (1990) 1164.
- 6. T. F. Yee, I. E. Grossmann, Z. Kravanja, Simultaneous optimization models for heat integration III, Computers and Chemical Engineering, 11 (1990) 1200.
- 7. Y. P. Wang, R. Smith, Wastewater minimisation, Chem. Eng. Science, 49 (1994) 1006.
- 8. T. Majozi, C. J. Brouckaert, C. A. Buckley, A graphical procedure for wastewater minimisation in batch processes, J. of Environmental Management, 78 (2006) 329.
- 9. M. J. Savelski, M. J. Bagajewicz, Design and retrofit of water utilization systems in refineries and process plants, Annual national AIChE Meeting, 1997 paper 188g.
- 10. L. E. Savulescu, R. Smith, Simultaneous energy and water minimisation. AIChE Annual meeting, 1998.
- 11. L. Savulescu, J-K. Kim, R. Smith, Studies on simultaneous energy and water minimisation I, Chemical Engineering Science 60 (2005) 3290.
- 12. L. Savulescu, J-K. Kim, R. Smith, Studies on simultaneous energy and water minimisation II, Chemical Engineering Science 60 (2005) 3308.
- 13. M. J. Bagajewicz, H. Rodera, M. Savelski, Energy efficient water utilization systems in process plants, Computers and chemical engineering, 26 (2002) 79.



Figure 3: HEN for the example data obtained using proposed approach.