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Optimization of Water Network Integrated with Process Models

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In this paper, a novel approach for the synthesis of water network incorporated with process models is introduced. The process models are utilized to relate the process output (typically defined as internal water source) with process input (i.e. water sink). A generalized water network superstructure is developed to embed all possible process units and all the connections among resources, interceptors, process units and wastes. The problem is formulated as four optimization problems (minimum freshwater flow rate, intercepted flow rate, intercepted mass load and number of connections) and the four models are solved in sequence to locate the targets. A case study is presented to illustrate the applicability and effectiveness of the proposed approach.

1. Introduction

Recently, the stringent environmental regulations and the increasing cost of freshwater as well as wastewater treatment have motivated the manufacturing industries to emphasis on waste minimization in their daily operations. Over the past decades, massive studies have been conducted on the synthesis of water network, ranging from both conceptual and mathematical optimization approaches. The basic principles and variety of applications of water network synthesis have been reviewed in the articles(Bagajewicz, 2000; Foo, 2009; Jezowski, 2010) and described in the textbooks (Mann and Liu, 1999; Smith, 2005).

In general, water network synthesis may be classified into two main categories, (Hallale, 2002; Manan et al., 2004) i.e. Fixed Contaminant load (FC) and Fixed Flow rate (FF) problems. In the former, water-using processes (e.g., washing, scrubbing, and extraction) are characterized by mass transfer operations where a fixed amount of contaminant is transferred from contaminant-rich stream to water, which acts as a mass separating agent. In contrast, water-using processes (e.g., boilers, cooling towers, reactors) are characterized as water sinks/sources that consume/generate a fix amount of water in the FF problems. Hence the primary concern of this latter problem is the water flow rate. As pointed out by Foo (Foo, 2009), the limiting water data for FC problem and FF problem are interchangeable. However, no matter the water-using processes belong to FC type or FF types, the characteristic of water-using processes could be specified via the appropriate process models, which associate the outlet process streams with the inlet process streams. Mathematical programming approaches (Ahmetović and Grossmann, 2011; Bai et al., 2010; Faria and Bagajewicz, 2010; Gunaratnam et al., 2005; Huang et al., 1999; Karuppiah and Grossmann, 2006; Meyer and Floudas, 2006; Misener and Floudas, 2010) have been considered as powerful tools for the synthesis of water conservation network. However, the water-using processes in previous models are typically classified

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into FC or FF types. In fact, the FC or FF types of water-using processes could be generally replaced by process models.
In this paper, we introduced a novel approach for the synthesis of water network incorporated with process models. The embedded process models are used to bridge the effluent of the water-using process (typically defined as internal water source) with the feed of the process (e.g. water sink). A generalized water network superstructure is developed to embed all possible process units and all the connections among resources, interceptors, process units and wastes. The proposed model is formulated as a sequential optimization problem. The applicability and effectiveness of the proposed approach is illustrated via solving a case study.

2. Problem Statement

The problem can be expressed as follows. Given a set of process unit with the constraints for the inlet flow rates and allowed concentrations. The outlet variables (such as flow rate and concentration) are the function of the corresponding inlet variables (i.e. outlet flow rate and outlet concentration). Also, a set of interceptors can intercept certain outlet streams from the process units and improve their qualities for reuse/recycle. The fresh sources may be necessity to supplement the use of process sources or upgraded streams through interceptors (typically so-called pre-treatment system). Each source has the known flow rate and concentration. In addition, the residual effluents of process units and interceptors have to be mixed before being discharged according to the environmental regulations. The objective is to identify an optimal water conservation network incorporated with process model and minimize the freshwater consumption, intercepted flow rate and the connections.

3. Mathematical programming models

3.1 Mathematical formulations

The superstructure of the problem embedding potential configurations of interest is shown in Figure 1. The mathematical formulations for the superstructure are presented as follows.

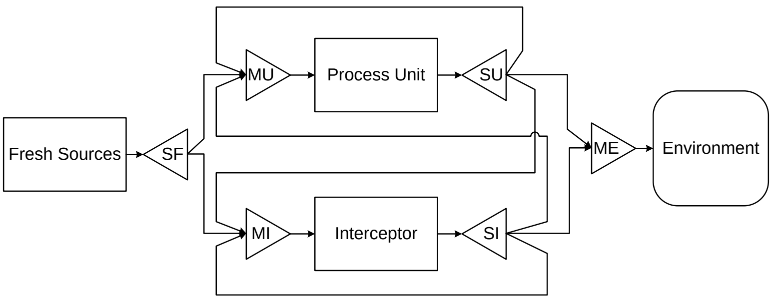

Figure 1: Superstructure of water conservation network

Mass balance on the splitting node after the *s*th fresh sources,

$$F_s = \sum_{u \in NPU} F_{s,u} + \sum_{i \in NIU} F_{s,i} \qquad \forall s \in NFS \tag{1}$$

where $F_{s,i}$ implies the flow rate assigned from the fresh sources to the interceptors for pre-treatment. Typically, the fresh sources are not sent to the interceptor for treatment. However, practically in the manufacturing plant, the pre-treatment sections are compulsory involved and the interceptors are necessary to upgrade the fresh sources for fulfilling the requirement of the downstream processes.
Mass balance for the mixing node before *u*th process unit:

$$F_u^{in} = \sum_{s \in NFS} F_{s,u} + \sum_{u' \in NPU} F_{u',u} + \sum_{i \in NIU} F_{i,u} \qquad \forall u \in NPU \tag{2}$$

If u'=u, then the local recycle is allowed for process unit u.
Component material balance for cth component in the mixing node before the u-th process unit:

$$F_u^{in} z_{u,c}^{in} = \sum_{s \in NFS} F_{s,u} z_{s,c} + \sum_{u' \in NPU} F_{u',u} z_{u',c}^{out} + \sum_{i \in NIU} F_{i,u} z_{i,c}^{out} \qquad \forall u \in NPU, c \in NCOMP \tag{3}$$

Process model is integrated and it relates the outlet variables (outlet flow rate, outlet concentration, etc) and the inlet variables (inlet flow rate and inlet concentration, etc) of process unit *u*, such as,

$$(F_u^{out}, z_{u,c}^{out}) = f_u(F_u^{in}, z_{u,c}^{in}) \qquad \forall u \in NPU, c \in NCOMP \tag{4}$$

Flow rate balance for the splitting node after the *u*th process unit:

$$F_u^{out} = \sum_{u' \in NPU} F_{u,u'} + \sum_{i \in NIU} F_{u,i} + F_{u,e} \qquad \forall u \in NPU \tag{5}$$

If u'=u, then the local recycle is allowed for process unit *u*.

Component mass balance for the splitting node after the *u*th process unit:

$$F_u^{out} z_{u,c}^{out} = (\sum_{u' \in NPU} F_{u,u'} + \sum_{i \in NIU} F_{u,i} + F_{u,e}) z_{u,c}^{out} \qquad \forall u \in NPU, c \in NCOMP \tag{6}$$

The constraints for the *c*th component concentration for the inlet and outlet of *u*th process unit:

$$z_{u,c}^{in,\min} \le z_{u,c}^{in} \le z_{u,c}^{in,\max} \qquad u \in NPU, c \in NCOMP \tag{7}$$

$$z_{u,c}^{out,\min} \le z_{u,c}^{out} \le z_{u,c}^{out,\max} \qquad u \in NPU, c \in NCOMP \tag{8}$$

Flow rate balance for the mixing node before *i*th stream interceptor,

$$F_i^{in} = \sum_{s \in NFS} F_{s,i} + \sum_{u \in NPU} F_{u,i} + \sum_{i' \in NIU} F_{i',i} \qquad \forall i \in NIU \tag{9}$$

If i'=i, then the local recycle is allowed for *i*th stream interceptor.

Component material balance for *c*th component in the mixing node before *i*th interceptor,

$$F_i^{in} z_{i,c}^{in} = \sum_{s \in NFS} F_{s,i} z_{s,c} + \sum_{u \in NPU} F_{u,i} z_{u,c}^{out} + \sum_{u' \in NIU} F_{i',i} z_{i',c}^{out} \qquad \forall i \in NIU, c \in NCOMP \tag{10}$$

Process model for each interceptor is incorporated and it relates the outlet variables (outlet flow rate, outlet concentration, etc) and the inlet variables (inlet flow rate, inlet concentration, etc), such as,

$$(F_i^{out}, z_{i,c}^{out}) = f_i(F_i^{in}, z_{i,c}^{in}) \qquad \forall i \in NIU, c \in NCOMP \tag{11}$$

Flow rate balance for the splitting node after the *i*th stream interceptor,

$$F_i^{out} = \sum_{u \in NPU} F_{i,u} + \sum_{i' \in NIU} F_{i,i'} + F_{u,e} \qquad \forall i \in NIU \tag{12}$$

If *i'*=*i*, then the local recycle is allowed for the *i*th stream interceptor.

Component mass balance for the splitting node after the *i*th stream interceptor,

$$F_i^{out} z_{i,c}^{out} = (\sum_{u \in NPU} F_{i,u} + \sum_{i' \in NIU} F_{i,i'} + F_{u,e}) z_{i,c}^{out} \qquad \forall i \in NIU, c \in NCOMP \tag{13}$$

Flow rate balance on the mixing node before the environment,

$$F_e = \sum_{u \in NPU} F_{u,e} + \sum_{i \in NIU} F_{i,e} \tag{14}$$

Component mass balance on the mixing node before the environment,

$$F_e z_{e,c} = \sum_{u \in NPU} F_{u,e} z_{u,c}^{out} + \sum_{i \in NIU} F_{i,e} z_{i,c}^{out} \qquad c \in NCOMP \tag{15}$$

3.2 Objective functions:

Model 1: the first objective function can be simply formulated to minimize the freshwater consumption.

$$\min FS = \sum_{s \in NFS} F_s \tag{16}$$

Subjected to Eqs.(1)-(15).

Model 2: the second objective function aims to minimize the total intercepted (so-called regenerated) water flow rate with the constraint of minimized freshwater flow rate as presented by Eq.(18).

$$\min FI = \sum_{i \in NIU} F_i^{in} \tag{17}$$

Subjected to Eqs.(1)-(15) and (18).

$$\sum_{s\in NFS} F_s \le FS^{\min}(1+\lambda_1) \tag{18}$$

where λ_1 denotes the slack parameter for the freshwater flow rate.

Model 3: the third objective function aims to minimize the total intercepted (so-called regenerated) component mass load with the constraint of minimized freshwater and intercepted water flow rate as presented by Eq.(20).

$$\min MFI = \sum_{i\in NIU} (F_i^{in} z_i^{in} - F_i^{out} z_i^{out}) \tag{19}$$

Subjected to Eqs.(1)-(15) and (18)(20).

$$\sum_{i\in NIU} F_i^{in} \le FI^{\min}(1+\lambda_2) \tag{20}$$

where λ_2 denotes the slack parameter for the intercepted water flow rate.

Model 4: the fourth objective function is utilized to minimize the total number of connections of the water network.

$$\begin{aligned}\min NC = &\sum_s \sum_u y_{s,u} + \sum_s \sum_i y_{s,i} \\ &+\sum_{u'} \sum_u y_{u',u} + \sum_u \sum_i y_{u,i} + \sum_i \sum_u y_{i,u} \\ &+\sum_u \sum_e y_{u,e} + \sum_i \sum_e y_{i,e}\end{aligned} \tag{21}$$

Subjected to Eqs.(1)-(15), (18)(20) and (22).

$$\begin{aligned}&F_{s,u}^{LB} y_{s,u} \le F_{s,u} \le F_{s,u}^{UB} y_{s,u} \\ &F_{s,i}^{LB} y_{s,i} \le F_{s,i} \le F_{s,i}^{UB} y_{s,i} \\ &F_{u',u}^{LB} y_{u',u} \le F_{u',u} \le F_{u',u}^{UB} y_{u',u} \\ &F_{u,i}^{LB} y_{u,i} \le F_{u,i} \le F_{u,i}^{UB} y_{u,i} \\ &F_{i,u}^{LB} y_{i,u} \le F_{i,u} \le F_{i,u}^{UB} y_{i,u} \\ &F_{u,e}^{LB} y_{u,e} \le F_{u,e} \le F_{u,e}^{UB} y_{u,e} \\ &F_{i,e}^{LB} y_{i,e} \le F_{i,e} \le F_{i,e}^{UB} y_{i,e}\end{aligned} \tag{22}$$

where all the *y*-s are introduced binary variables to denotes the existence of the connection.

Note that, the objective functions can be easily modified to minimize the total cost by adding the cost coefficient for different fresh sources, treatment cost, fixed cost for treatment processes (interceptors) and piping network. If the environment influence is taken into consideration, the problem can be improved to be multiple objectives optimization problem.

Typically, Models 1, 2 and 3 are NLP problems and Model 4 is MINLP problems. Those four models are solved sequentially to achieve the minimum freshwater consumption, intercepted flow rate, interpreted mass load and number of connections. Global optimization techniques for the four models are ongoing by introduce the relaxation techniques (i.e. piecewise linearization).

4. Case study

The limiting data for five water-using processes with single contaminant is shown in Table 1, which is slightly modified compared with the original data from the literature(Wang and Smith, 1995). Note that the outlet flow rate for the water-using processes (F_u^{out}) is replace by ΔF_u, which denotes the flow rate difference between the outlet and inlet flow rates. It is assumed that a single pure freshwater supply (0 ppm) is available in service. The interceptor of the fixed outlet concentration (z_i^{out}) is considered and z_i^{out} is set to be 200 ppm.

Table 1: Limiting Data

Operation	F_u^{in} (t/h)	ΔF_u (t/h)	$z_u^{in,\max}$ (ppm)	$z_u^{out,\max}$ (ppm)
Reactor	80	-60	100	1000
Cyclone	50	0	200	700
Filtration	10	30	0	100
Steam System	10	0	0	10
Cooling System	15	-10	10	100

For simplicity and comparison, the inlet flow rates for water-using processes are set to be fixed value as shown in Table 1 and the maximum outlet concentration for each process is achieved.
The process model for *u*th process unit can be expressed by Eq.(23),

$$F_u^{out} = f(F_u^{in}) = F_u^{in} - \Delta F_u \tag{23}$$

Therefore the constraint Eq.(4) in the three models should be replaced by Eq.(23). That means the outlet flow rates for processes are fixed variables. Thus, for this example, Models 1, 2 and 3 are transferred to be LP problem and Model 4 is changed to be MILP problem. The optimization solver CPLEX is applied to solve the four models sequentially. The minimum freshwater flow rate is located at 42.25 t/h, intercepted water flow rate is 67.75 t/h, minimum intercepted mass load is 39.2 kg/h and the minimum number of connections is 12. One optimal water network is shown as Figure 2.

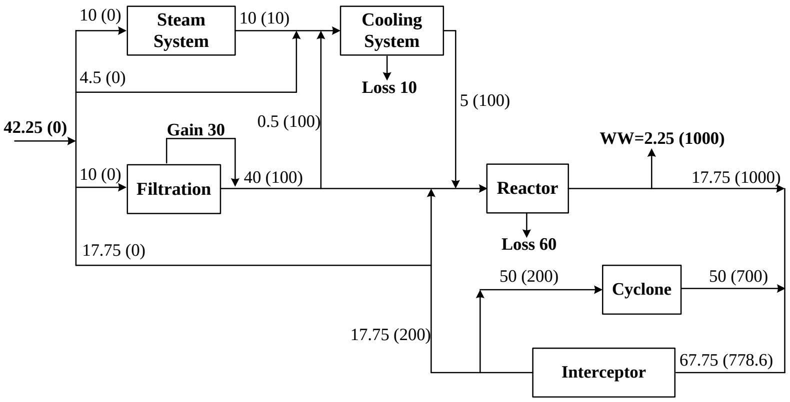

Figure 2: An optimal water network with one interceptor with fixed outlet concentration model (unit for flow rate, t/h; unit for concentration in bracket, ppm)

5. Conclusions

A novel approach for the synthesis of water network incorporated with process models is developed in this paper. The effluent of the water-using process (typically defined as internal water source) is related with the feed of the process (e.g. water sink) by introducing process model equations. The proposed water network superstructure then is formulated as four optimization problems in sequence. A simple case study is solved to show the applicability of the proposed approach. The ongoing work is to deduce the empirical process model equations on the basis of simulation via certain simulation tools (such as Aspen Plus, UniSim, etc) and they would be incorporated into the developed models.

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References

Ahmetović E., Grossmann I.E., 2011, Global superstructure optimization for the design of integrated process water networks. AIChE J. 57, 434-457.

Bagajewicz M., 2000, A review of recent design procedures for water networks in refineries and process plants. Comput. Chem. Eng. 24, 2093-2113.

Bai J., Feng X., Deng C., 2010, Optimal design of single-contaminant regeneration reuse water networks with process decomposition. AIChE J. 56, 915-929.

Faria D.C., Bagajewicz M.J., 2010, On the Appropriate Modeling of Process Plant Water Systems. AIChE J. 56, 668-689.

Foo D.C.Y., 2009, State-of-the-Art Review of Pinch Analysis Techniques for Water Network Synthesis. Ind. Eng. Chem. Res. 48, 5125-5159.

Gunaratnam M., Alva-Argaez A., Kokossis A., Kim J.K., Smith R., 2005, Automated design of total water systems. Ind. Eng. Chem. Res. 44, 588-599.

Hallale N., 2002, A new graphical targeting method for water minimisation. Adv. Environ. Res. 6, 377-390.

Huang C.H., Chang C.T., Ling H.C., Chang C.C., 1999, A mathematical programming model for water usage and treatment network design. Ind. Eng. Chem. Res. 38, 2666-2679.

Jezowski J., 2010, Review of Water Network Design Methods with Literature Annotations. Ind. Eng. Chem. Res. 49, 4475-4516.

Karuppiah R., Grossmann I.E., 2006, Global optimization for the synthesis of integrated water systems in chemical processes. Comput. Chem. Eng. 30, 650-673.

Manan Z.A., Tan Y.L., Foo D.C.Y., 2004, Targeting the minimum water flow rate using water cascade analysis technique. AIChE J. 50, 3169-3183.

Mann J.G., Liu Y.A., 1999, Industrial water reuse and wastewater minimization. McGraw-Hill Professional, New York, United States.

Meyer C.A., Floudas C.A., 2006, Global optimization of a combinatorially complex generalized pooling problem. AIChE J. 52, 1027-1037.

Misener R., Floudas C.A., 2010, Global Optimization of Large-Scale Generalized Pooling Problems: Quadratically Constrained MINLP Models. Ind. Eng. Chem. Res. 49, 5424-5438.

Smith R., 2005, Chemical process design and integration, 2nd ed. John Wiley & Sons Ltd, Chichester, England.

Wang Y.P., Smith R., 1995, Wastewater minimization with flowrate constraints. Chem. Eng. Res. Des. 73, 885 - 900.