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Stochastic optimization based approach for designing cost optimal water networks

G. Poplewski, J. M. Jezowski*

Rzeszów University of Technology, Department of Chemical and Process Engineering, Al. Powstanców Warszawy 6, 35-959 Rzeszów, Poland

Abstract

This work addresses a design of water network (WN), i.e. a subsystem consisting of water using processes and regenerators. A systematic approach was developed for synthesis and retrofit of WN. The method is based on superstructure optimization. To solve the problem adaptive random search optimization (ARS) technique was applied. The method accounts for water reuse, regeneration processes within WN and, also, for various optimization criteria as well as industrial requirements as water losses and gains, fixed flow-rates and so on.

Keywords: water network, design, simultaneous approach, stochastic optimization

1. Introduction

Stringent ecological regulations effect in a growing interest in minimization of freshwater usage in industrial processes (Bagajewicz, 2000). Water reuse among water using processes and application of regenerators (i.e. application of distributed treatment subsystem) are the means to reach the aim. A problem of designing a network consisting of water using processes is referred here to as Water Network (WN) problem. The approaches developed to date can be roughly divided into two broad classes:

1. insight-based (thermodynamic / conceptual) approaches
2. optimization-based (mathematical / superstructure optimization) approaches

These from the first group often follow Pinch Technology concepts (e.g. Wang and Smith, 1994, Wang and Smith, 1995). They provide deep insights into the problem but don't give a designer systematic tools for solving the problem, particularly if a cost performance index and multiple contaminant cases have to be accounted for.
Optimization approaches are most often based on superstructure concept (e.g. Huang et al., 1999, Bagajewicz, 2000, Tsai and Chang, 2001). In order to account for cost goal function a MINLP (mixed-integer nonlinear programming) model has to be solved while to minimize only freshwater cost NLP optimization model is usually sufficient. Despite the significant progress in last years (e.g. Lee and Grossmann, 2001, Lee and Grosssmann, 2003) deterministic optimization approaches aren't robust techniques for solving MINLP problems, particularly if general-purpose solver is applied. Hence,

* Corresponding author: E-mail address: ichjj@prz.rzeszow.pl (J.M. Jezowski)

genetic algorithms (GA) were tried (e.g. Tsai and Chang, 2001). The alternative way is to use some conditions on outlet concentrations, which allowed problem linearization (Savelski and Bagajewicz, 2000, Savelski and Bagajewicz, 2003). However, such conditions were proved sufficient to minimize freshwater usage but not the cost of WN. The analysis of WN design problem and of the approaches developed to date shows that simultaneous approach by superstructure optimization provides systematic and general framework. However, MINLP model is difficult to solve to global optimum. In order to deal with such the model we applied adaptive random search (ARS) technique. To date such optimization method hadn't been applied to designing process systems. The optimization algorithm is based on the so-called Luus-Jaakola (LJ) method (Luus and Jaakola, 1973). The original approach was modified and extended and the exhausted tests proved the efficacy of the modified version, particularly for NLP problems with limited number of equality constraints (Jezowski and Bochenek, 2002, Jezowski and Jezowska, 2003). In order to deal with large number of equations in the WN superstructure model we developed an efficient and robust solution scheme.

2. Problem formulation, superstructure optimization model

2.1. Mathematical models of processes, optimization criterion

Water network consists of freshwater sources of various qualities and costs, water using processes, regenerators, mixers and splitters. Similarly to other works on water networks it is assumed here that water using processes are modeled as counter-current mass exchangers. Mass load of contaminants to be removed from each process are known as well as the values of maximum limiting concentration of contaminants at each process outlet and inlet. To model regenerators two types of design equations were used: regeneration efficiency and fixed outlet concentrations.

The following basic data are required to solve the typical WN design problem:

- number of water using processes
- number of freshwater sources and contaminant concentrations for each source
- mass load of each contaminant to be transferred in each water using process
- maximum permissible concentrations of each contaminant at inlet and outlet of each water using process
- design parameters of each regenerator

However, our approach allows solving the WN design for several constraints important in industry:

- forbidden and must-be connections among processes and regenerators,
- lower and upper limits on flow-rates through connections (pipe segments)
- fixed, required flow-rates through water using processes
- gains and losses in each water using process
- upper limit on contaminants concentration at each regenerator inlet
- upper limit on flow-rate through each regenerator

It is worth noting that the above conditions allow designing WN in both grass-root and retrofit scenarios. Also, various water using processes can be accounted for due to the fact that fixed flow-rates and water gains and losses can be included into the optimization model. Hence, the design problem that can be solved with developed approach is very general in regards to models of processes and technological conditions. Most often usage of freshwater or cost of freshwater is employed as WN performance index. However, this can increase cost of piping and regenerators significantly (Koppol et al., 2003, Lee and Grossmann, 2003). Hence, cost performance index should be applied. The developed approach is not limited to freshwater minimization but several various indices can be applied such as total cost of the network.

2.2 Superstructure

The notion of the superstructure for water networks was presented in several papers (e.g. Huang et al., 1999, Bagajewicz, 2000, Savelski and Bagajewicz, 2001a, Tsai and Chang, 2001, Lee and Grossman, 2003). In general the superstructure consists of two basic building arrangements: mixer - water using process -splitter (Fig.1) and mixer - regenerator - splitter (of structure similar to that in Fig.1). There exist all possible connections from a splitter attached to a process to any process mixer/regenerator mixer and from splitter of a regenerator to any process mixer/ another regenerator mixer. All available freshwater sources can supply any process. It is worth noting the so-called self-recycles are embedded in our superstructure i.e. connections from a splitter of a process to a mixer of the same process. Such the self-recycle can be used to minimize freshwater usage if there exists fixed given flow-rate through a process (Wang and Smith, 1995). It is worth noting that self-recycles were not included in superstructures used in other optimization-based approaches. The superstructure applied embeds all possible and structurally feasible water networks relevant to the problem.

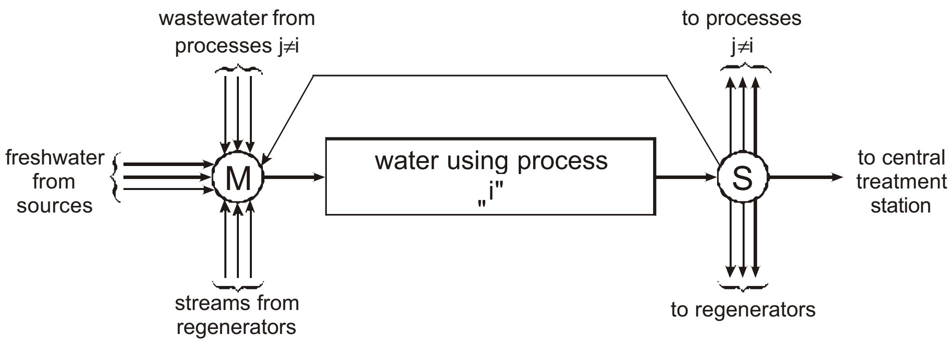

Figure 1. Illustration of the arrangement: mixer (M) – water using process – splitter (S)

Due to space limitations we present here only very general optimization model for WN superstructure optimization

min (freshwater usage/ freshwater cost/ cost of WN)

s.t.

- general mass balances for the arrangements: mixer-process-splitter and mixer - regenerator - splitter
- mass balances of each contaminant for the arrangements: mixer-process-splitter and mixer - regenerator - splitter
- mass balances of contaminants for mixers in both arrangements
- design equation of regenerators
- limits on variables

- additional conditions (e. g. forbidden connections, fixed flow-rates)

Notice, that if goal function accounts for cost of connections (piping) and regenerators the model will contain binaries and proper logical conditions, i.e. it will become MINLP type.

3. Optimization algorithm overview

To solve WN superstructure optimization problem adaptive random search strategy was applied. The method is based on LJ algorithm (Luus and Jaakola, 1973), which can be briefly summarized as follows: starting with initial point decrease gradually search region size of variables around currently best solution. It is important that currently best solution is chosen from among a number of points, hence, the method has some resemblance to population-based approaches. The trial points are generated using uniform probability density distribution (i.e. by Monte Carlo generator). The modifications of the original LJ method used in solving WN problem are described in Jezowski and Bochenek, (2002), Jezowski and Jezowska, (2003).

Equality constraints cause difficulties in stochastic optimization approaches. The use of penalty terms and/or relaxation to inequalities is possible but in this problem there exist a more efficient solution by direct solution of equations. The nonlinearities in constraints of WN optimization model are caused by bi-linear terms in mass balances of processes. These terms are products of mass flow-rates and concentrations. Let divide the total set of optimization variables into two groups: decision and dependent (state) variables. These from the first group are generated by ARS algorithm. Notice also that ARS approach can be organized in sequential manner, i.e. equalities can be solved sequentially and inequalities can also be checked in sequence. Hence, decision variables are applied as data for solving equalities. Mass flow-rates in bi-linear terms are fixed and mass balances become linear equations in regards to state variables. They can be solved easily in seriatim fashion or as a sequence of small sets of simultaneous linear equations. In consequence, it was possible to develop novel and efficient scheme of solving equality constraints in stochastic optimization which was coded in modelling system of program OPTI-STO (Jezowski and Bochenek, 2002) applied to solve WN design problem.

The optimization algorithm in program OPTI-STO is efficient in solving NLP problems (though it can be applied also to MINLP of small scale (Bochenek et al., 1999)). To deal with binaries defining connections in the superstructure we applied logical conditions and also proper penalty terms in goal function. Hence, binary variables were not decision variables in optimization routine.

4. Example

To illustrate application of the method for designing cost optimal WN we present here the example – data in Table 1. The problem has 6 water using processes. Regeneration is not considered, i.e. freshwater usage is minimized by reuse only. There is single contaminant and single freshwater source with contaminant concentration equal to naught. The example was solved in many papers (e.g. Olesen and Polley, 1997, Savelski and Bagajewicz, 2001b) applying freshwater consumption as the goal function. The minimum obtained was 157.14 tonnes/hr. We calculated the same solution.

Table 1. Data for the example

Process number	Contaminant mass load [kg/h]	Max. inlet concentration [ppm]	Max. outlet concentration [ppm]
1	2.0	25	80
2	5.0	25	100
3	4.0	25	200
4	5.0	50	100
5	30.0	50	800
6	4.0	400	800

Lee and Grossman (2003) solved this problem for the same data but using cost function which is the sum of freshwater cost and cost of all interconnections. They used fixed cost coefficient of 10 for each interconnection and unit cost of freshwater equals to 1.0. The cost goal function is given by:
(freshwater cost) + (10 y_i)
where: $y_i = 1$ if connection "i" is in the WN; $y_i = 0$ if not

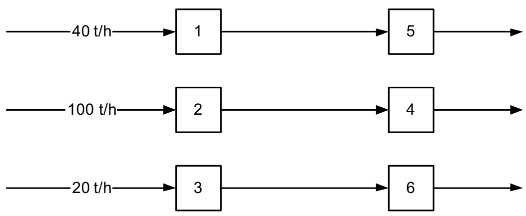

Figure 2. Cost optimal WN for the example - 1st optimal solution

Applying the advanced disjunctive programming Lee and Grossman (2003) reached the global optimum shown in Fig.2: WN with nine connections and freshwater usage of 160 tonnes/hr. Notice, that due to the costly interconnections the freshwater usage is larger than the minimum value (157,15 tonnes/hr).We were able, applying the same cost goal function, to calculate the same solution, and, also the second optimum shown in Fig.3. The network has the same goal function (freshwater consumption and number of pipes) but different structure.

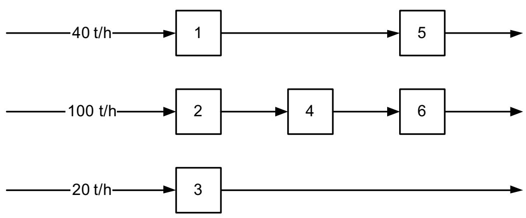

Figure 3. Cost optimal WN for the example – 2nd optimal solution

The approach was applied to solve many WN design problems from the literature. In all cases we reached the results identical to optimal networks from the literature. In some cases better solutions were obtained.

5. Conclusions

A method for synthesizing and retrofitting water network has been developed. The approach is flexible and general. It accounts for water reuse, regenerators and multiple contaminants. Various goal functions can be applied, including total cost of WN. Specific industrial scenarios are accounted for, e.g. forbidden connections, fixed flow-rates, water gains and losses and so on. The examples solved to date proved that the approach calculates optimum solutions. It is also easy to use and does not require advanced optimization solvers.

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