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Wastewater minimisation of industrial systems using an integrated approach

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ABSTRACT

The design of an industrial water system, which makes the most efficient use of the water resources available, is a complex problem that involves different trade-offs. If we assume that no fundamental process changes can be performed (i.e. wet cooling towers cannot be replaced by air-coolers, etc.), then we can improve the efficiency of the water system through practices as water re-use, regeneration of water prior to re-use, or regeneration and recycling. The inherent combinatorial nature of the problem calls for the development of a systematic methodology that can deal with the high dimensionality of the design problem. In this paper we propose an integrated methodology for the design of industrial water systems. This approach brings the engineering insights provided by the water-pinch analysis together with powerful mathematical programming tools. The method is based on a decomposition scheme for the optimisation of a superstructure model that includes all the possible features of a design. The proposed decomposition strategy is based on a recursive procedure. With this new approach, a network featuring minimum total annualised cost can be found where the complexity of the network structure is under the control of the designer and many practical constraints can be incorporated.

Keywords: Wastewater minimisation, mixed-integer linear programming, MILP, MINLP, network design.

INTRODUCTION

Water is probably the most widely used raw material in the process industries and it has been used in abundant quantities by chemical, petrochemical, petroleum refining, food and drink, pulp and paper and many other industries. However, increasing costs of wastewater treatment to meet environmental standards and the scarcity of good quality industrial water around the world, create a powerful economic driving force to rationalise its use. As presented by Wang and Smith (1994, 1995) there are four general approaches to water minimisation: Process changes, water re-use, regeneration re-use and regeneration recycling. In this work we exclude the possibility of making fundamental changes to the operations to reduce its water demands. Instead we present an automated method for designing a complete water system considering the remaining options above.

A number of related studies have been published where the problem is decomposed into subsystems and consequently, the interactions between all parts of the problem are not fully explored. Takama, et. al. (1980) addressed the problem of optimal water allocation in a petroleum refinery. Their approach generated a superstructure including all possible re-use and regeneration opportunities. This superstructure was then optimised using a two-level approach and uneconomic features of the design were removed. El-Halwagi and Manousiouthakis (1989) introduced the notion of Mass Exchanger Network Synthesis (MEN) for the preferential transfer of a key contaminant from a set of rich streams into a set of lean streams. Later El-Halwagi and Manousiouthakis (1990a,b) automated the approach and included regeneration opportunities. Paplexandri et. al. (1994) introduced a simultaneous approach for MEN synthesis based on a mixed-integer non-linear programming problem (MINLP) where the hyperstructure network representation of Floudas and Ciric (1989) was adapted to the problem. Many more applications and extensions to the basic MEN synthesis problem have been published since .

The specific problem of wastewater minimisation shows some particular features that make a specialised methodology more appealing than the previous general approaches. A major feature of the water system design problem lies in the fact that the largest water users in a typical site are not mass transfer operations (e.g. cooling tower, steam system, etc.). The method proposed by Wang and Smith (1992, 1994, 1995) and later improved by Kuo (1996), provides important insights on the water system design problem. Using the concept of a limiting water profile to describe all the water-using operations, allows the analysis of the complete water system on a common basis (Doyle and Smith, 1997).

PROBLEM STATEMENT

The design of a water system involves a number of freshwater sources available to satisfy the demands of each water-using operation, both in terms of volume and concentration level of certain contaminants. A set of water treatment operations is available to reduce the freshwater consumption in the site and/or to achieve the environmental limits imposed on the wastewater discharge . The design task is to find the network configuration that will minimise the overall demand for freshwater (and thus minimise wastewater generation) at minimum total annual cost.

The water system design problem can be stated as follows.

Given are:

A set of operations to be considered in the water system, this set includes all water-using operations as well as all treatment operations available for the design. Flowrate constraints may be imposed on each operation.

A set of contaminants to be analysed which may be present in the freshwater sources and/or picked up in the water-using operations.

A set of freshwater sources that are available to satisfy the water demands their supply compositions for each contaminant given. Also, an upper bound to the mass flow rate that can be used in the network, and costs associated with the consumption of each source are given.

The operations set is then separated in two subsets. (1) A subset of water-using operations, each one described by its limiting water profile for each contaminant in terms of its maximum inlet concentration, its maximum outlet concentration, and either the mass load of contaminant to be transferred, or the limiting flow rate for the operation. (2) A subset of water treatment operations, its performance for the removal of contaminants specified as a removal ratio, and which may also have an inlet concentration restriction.

The objective is to synthesise a minimum annual cost water network, in terms of investment cost, freshwater consumption, and network topology for water re-use, regeneration, recycling and treatment, that can satisfy the specifications of the problem.

The following assumptions are made:

i) All data for the limiting water profiles is available and certain.
ii) The number of water using and water treatment operations is fixed.
iii) The removal ratios for each treatment unit are independent of the inlet concentration to the particular unit.
iv) Heat integration is not allowed; isothermal network operation.
v) The network operates under constant pressure

In order to consider the investment cost of the network due to the piping required we also need to specify the length of the pipe run for each possible connection, flow velocities and also the materials of construction for each pipe.

In the following sections the water system synthesis without decomposition will be presented based on the superstructure developed for water systems. The problem is formulated as an MINLP model that is then decomposed for its solution in a sequence of MILP problems. A case study from a petroleum refinery will then be used to illustrate the capabilities of the method.

SUPERSTRUCTURE MODEL FOR WATER NETWORKS

The automated method relies on the optimisation of a superstructure All possibilities for water re-use, regeneration, recycling and treatment are included in the mathematical formulation. Here, the number of units in the water network is fixed and a "match" in this context refers to a pipe connecting a source and a sink of water. The following basic features of the model can be highlighted:

- Each freshwater stream entering the network is split towards all operations, including water-using and treatment operations.
- All the effluent streams generated from each operation are mixed in a final discharge point, where the environmental limitations must hold.
- Prior to each operation a mixer is considered, where the flow from the freshwater splitters and re-use flows from all other operations are merged into a flow towards the operation.
- After each operation a splitter is considered, from which potential flows are driven towards the final mixer and the other operations in the system.

The model includes mass balances for every contaminant around each mixing and splitting point, as well as mass balances around every operation. In order to control the structural features of the design, we introduce binary variables associated with each possible connection. The solution to this problem will result in the minimum freshwater consumption and the topology of the network. Also, all flow rates and concentrations for each contaminant in each stream are identified. In order to calculate the capital investment due to the pipework we need to add restrictions relating the flow rate of water with the cross sectional area of the pipe required. We assume a flow velocity for each connection and based on this estimate, a pipe diameter is calculated.

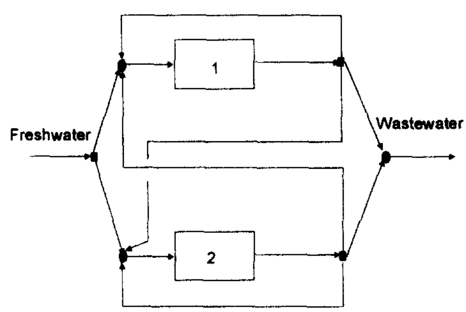

Figure 1. Superstructure

Some problems related with the automated method can be dealt with by introducing logic constraints in the formulation; namely, small flowrates in the solution are avoided by specifying tolerance parameters. To preclude water recycling in the final design (e.g. closed paths in the network) the grouping strategy from water pinch analysis proposed by Kuo (1996) is applied within the optimization framework.

Finally, in the objective function we include terms for the operating cost of the network (freshwater costs on an annual basis) and capital costs due to the cost of piping and the investment required for the treatment units.

Objective function:

Operating cost:

$$OC = AF * \sum_{j}\sum_{i}\left(FFW_{j,i} * FWC_j\right)$$

Capital cost:

$$CC = AFC * \begin{bmatrix} \sum_{j}\sum_{i} CC1_{ji} + \sum_{i}\sum_{i'} CC2_{ii'} + \\ \sum_{i} CC3_i + \sum_{it} CT_{it} \end{bmatrix}$$

$$\min Z = OC + CC$$

where $FFW_{j,i}$ is the flow rate of freshwater source j into operation i,
FWC_j is the cost per unit of freshwater source j,
CC1-3 is the capital investment required for the pipes in the network
CT_{it} is the cost of the treatment units, and
AF and AFC are the appropriate annualisation factors for each term.

SOLUTION PROCEDURE

The complexities associated with the solution of nonconvex MINLP problems are well documented in the literature (Floudas, 1995) and a number of different algorithms for their solution have been developed. However, in the mathematical formulation of the superstructure presented, the nonlinearities in the model are created only in the mass balance equations around every operation in the form of bilinear terms (concentration times flow rate). Clearly, fixing the vector of exit concentrations from all the operations and for all the contaminants results in a linear problem.

From water pinch analysis we know that for all water-using operations, in the optimal solution, at least one of the contaminants will reach its maximum permissible value (Doyle and Smith, 1997). With this information we can then set all outlet concentrations to their maximum levels for all water-using operations and obtain a set of linear mass balance equations for these operations. In the case of the water treatment operations however, we do not have any information of the exit concentrations as these will depend on the inlet to each operation, removal ratios for each contaminant, the sequence of treatment units and the environmental limits specified in the final mixer.

Here, we propose a decomposition of the original MINLP problem into a sequence of MILP problems to approximate the optimal solution. In a first instance we fix all outlet concentrations to their maximum levels for water-using operations, and to zero for treatment operations. In the water-using operations not all contaminants will be able to reach their maximum level for a given mass load and flow rate. Those contaminants, which do achieve their maximum level will be denoted "limiting contaminants" and these define the water demand for the operation. "Non limiting contaminants" will exit the unit at a lower concentration than their maximum level and these do not affect the water consumption in the operation.

Similarly, for the water treatment operations, setting the outlet concentrations to zero for all units and all contaminants will result in a linear formulation. To cope with this difference we need to introduce artificial variables in the mass balance equations. In a similar approach to the one proposed by Takama et. al, (1980), we then introduce the summation of all artificial variables in the objective function and, within an iterative procedure, a sequence of infeasible points is generated until, in the final solution, all these variables are driven to zero and a near-optimal solution is found. The revised objective function is:

$$\min Z = OC + CC + \lambda * \sum \text{artificial\_variables}$$

The weighting factor λ is modified in each iteration so as to force the sum of infeasibilities term to zero.

ILLUSTRATIVE EXAMPLE

An example from a petroleum refinery will now be used to illustrate the capabilities of the proposed method. This case was adapted from an earlier application of the water pinch method. Consider an existing water system where there are seven water-using operations, namely, an hydrodesulphurization operation (HDS), crude distillation unit (CDU), vacuum distillation unit (VDU), boiler house

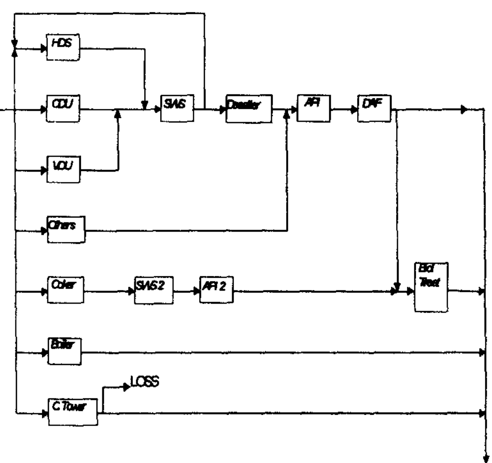

Figure 2. Conventional design.

(Boiler), cooling tower (C. Tower), desalter and other operations grouped together (Other). There is a water loss in the evaporative cooling tower.

There are three water treatment operations in place, working at maximum capacity. As it can be seen from the flowsheet, the steam stripper (SWS) is operating as a water regenerator as its output is used as a feed to both the desalter and HDS (both water-using operations). An API separator (API)and a dissolved air flotation unit operating in series deal with the effluent stream so as to achieve the discharge limits required. Then, a delayed coker unit operation is installed and new and more stringent environmental regulations are imposed on the plant effluent. Besides the three treatment operations already in place, there are five other units to be considered for the retrofit flowsheet. Three similar units (SWS2, API2 and DAF2), a biological treatment unit and an hydrocyclone. All of these are specified in terms of removal ratios for each one of the contaminants. A conventional approach to solve this problem would probably leave the existing treatment units operating as before, and would add a new treatment train to cope with the new effluent stream from the delayed coker. In this example, a second steam stripper (SWS2) and a second API separator (API2) were chosen to perform this duty (see figure 2). Finally, a biological treatment unit is added at the end of the treatment train to achieve the new environmental requirements.

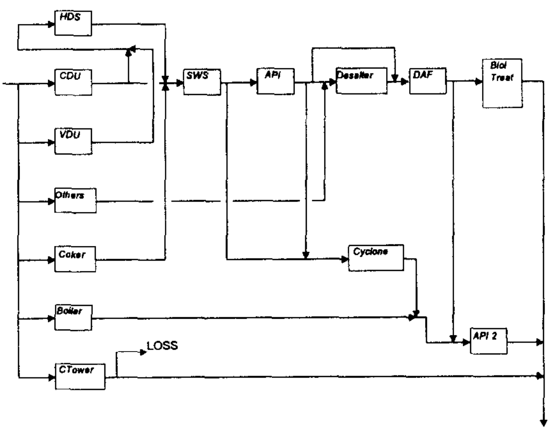

Figure 3. Minimum total cost design.

Applying the automated method outlined above to this problem results in the design shown in figure 3. As it can be seen the flowsheet structure is far from trivial and a different set of treatment units is selected. Here the second API separator and the biological treatment unit are also chosen, but the hydrocyclone is introduced in the minimum total cost design. An interesting observation on the new design can be made on the existing SWS and API treatment units. In previous approaches where a decomposition strategy was used, an arbitrary decision had to be made regarding the mode of operation of a treatment unit, i.e. either as a regenerator or as a treatment unit. Here both units are operating both as regenerators and as treatment units. Clearly, a decomposition-based approach could not generate a similar flowsheet. The new design features total annual savings of $554,408 as compared with the conventional solution. The problem was solved by performing five major iterations (MILP problems) using a 100 MHz pentium PC.

CONCLUSIONS

An automated method has been developed for the synthesis of industrial water systems. The designs generated feature minimum total annualised cost and it is possible to control the complexity of the emerging flow pattern. Many practical constraints can be included, e.g. compulsory/ forbidden connections, geographical, control or safety constraints. Water recycling in the network can be avoided through the inclusion of logic constraints.

With the proposed solution strategy, the method generates a sequence of infeasible points in the course of the optimisation. By increasing the weighting factor of the sum of infeasibilities in each iteration we force the term to zero in the final solution. A branch and bound algorithm is used to find each optimal point in the search procedure. A case study from petroleum refinery was solved to illustrate the capabilities of the proposed approach. It was also shown that previous approaches based on a decomposition strategy could result in topology traps due to arbitrary decisions made. This new approach avoids these drawbacks by performing a simultaneous optimisation of the overall system.

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