WATER NETWORK SYNTHESIS USING MUTATION-ENHANCED PARTICLE SWARM OPTIMIZATION

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Abstract: Different techniques for the synthesis of industrial water reuse/recycle networks have been developed in recent process integration research. These tools range from graphical pinch analysis approaches to mathematical programming models. The latter have the advantage of being flexible enough to incorporate various water network constraints, but in many cases these are often non-linear, thus making the identification of global optima difficult. Recent work has demonstrated the effectiveness of metaheuristic algorithms such as particle swarm optimization (PSO), for finding good solutions these problems. This work describes the use of a modified PSO for solving mixed integer non-linear programming (MINLP) models for water network synthesis. By incorporating a mutation operator for the binary variables in the model, the algorithm is able to escape sub-optimal network topologies and proceed towards better solutions than can be found with ordinary PSO. Two case studies involving water recycle/reuse are used to demonstrate the new design methodology.

Keywords: process integration; water minimization; mixed integer non-linear programming; particle swarm optimization.

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INTRODUCTION

In the recent decades, process industries have started to shift from conventional end-of-pipe waste treatment to more sustainable pollution prevention or waste minimization practices. Among some of the factors that drive this shift include environmental sustainability and stringent emission legislations, as well as increasing cost of resources and waste treatment. One of active areas for waste minimization activities has been that of in-plant material reuse/recycle; the term ‘reuse’ refers to directing a waste stream from one process to another process, while ‘recycle’ implies that a waste stream is returned directly or indirectly to the same process from which it originates. The benefits of implementing material reuse/recycle are twofold. Apart from the reduction of raw material (and its associated treatment) needed for a process, less waste is generated. Recent efforts have seen the advancement of systematic design of material reuse/recycle network for resource conservation, with the most active area being the water network synthesis. The different approaches presented for water network synthesis can broadly be categorized into two main sectors, i.e., insight-based graphical techniques and mathematical-based optimization approaches.

The seminal work for insight-based graphical techniques was initiated by Wang and Smith (1994) who presented the pinch targeting approach for fixed load problems, based on the more generalized mass exchange network synthesis problems (El-Halwagi and Manousiouthakis, 1989). More recently, various approaches have been developed to handle the fixed flowrate problems (Hallale, 2002; El-Halwagi *et al.*, 2003; Manan *et al.*, 2004; Prakash and Shenoy, 2005; Foo *et al.*, 2006; Almutlaq *et al.*, 2005). The main advantage of the graphical targeting tools is its ability to incorporate conceptual insights during network synthesis.

On the other hand, mathematical optimization approaches for water network synthesis have also received much attention from the research community. Mathematical approaches serve as good supplement tools to graphical pinch approach in addressing more complex systems, such as system with large number of water-using processes

(Savelski and Bagajewicz, 2001), multiple impurities (Takama *et al.*, 1980a; Doyle and Smith, 1997; Alva-Argáez *et al.*, 1999; Bagajewicz *et al.*, 2000; Dunn and Wencel 2001), mass load uncertainty (Tan *et al.*, 2004; Koppol and Bagajewicz, 2003) or even detailed cost estimation (Alva-Argáez *et al.*, 1998; Jödicke *et al.*, 2001; Feng and Chu, 2004). In general, the various mathematical approaches can be further classified as deterministic and stochastic approaches. Early work on deterministic approaches was reported by Takama and co-worker (Takama *et al.*, 1980a, 1980b, 1981). Alva-Argáez and co-authors (Alva-Argáez *et al.*, 1998, 1999) as well as Jacob *et al.* (2002) combined the use of deterministic approaches with insight from graphical pinch approach to address the network synthesis problem. The algorithmic procedures developed by Bagajewicz and co-workers (Bagajewicz and Savelski, 2001; Savelski and Bagajewicz, 2000a, 2000b, 2001, 2003; Gómez *et al.*, 2001; Bagajewicz *et al.*, 2000) are of good examples of deterministic approaches. Among the many deterministic algorithms, linear programming (LP) that is used for simple water network problem and its optimality is guaranteed. However, when other considerations such as network topology are considered in the model, the result is a mixed integer nonlinear programming (MINLP) problem due to the additional of binary variables. The difficulty in solving a MINLP problem is that global optimum cannot be guaranteed by conventional gradient-based search algorithms. Global optimization strategies for non-convex problems have been developed, based on decomposition or convex relaxation techniques (Floudas, 1995; Adjiman *et al.*, 2000); for example, Karuppiah and Grossmann (2006) apply such procedures for designing integrated water reuse, recycle and treatment networks.

More recent works have also seen the advancement of various stochastic approaches for water network synthesis as an alternative to the use of deterministic techniques. While the latter may be used to find guaranteed global optima for models that meet certain structural criteria, stochastic computing techniques are more robust in the sense that they are able to handle a broader variety of problems; on the other hand, this advantage comes at the expense of added computing time and the inability to converge deterministically to true optima. Stochastic (or metaheuristic) algorithms are used mainly to find good solutions to design problems, but do not provide a guarantee of locating globally optimal solutions. They include genetic algorithm (GA) (Tsai and Chang, 2001; Li *et al.*, 2003; Wu and Chang, 2003; Prakotpol and Srinophakun, 2004; Shafiei *et al.*, 2004; Lavric *et al.*, 2005), adaptive random search (Poplewski *et al.*, 2002; Jeżowski *et al.*, 2003; Poplewski and Jeżowski, 2005) and particle swarm optimization approaches (PSO) (Luo *et al.*, 2006; Hul *et al.*, 2007). Among the various evolutionary algorithms (EAs), GA is the most established technique. However GA has some limitations in terms of success rate, computational efficiency and solution quality (Elbeltagi *et al.*, 2005; Abido, 2002; Luo *et al.*, 2006; Hul *et al.*, 2006).

In this work, a recent developed PSO technique (Hul *et al.*, 2007) is utilized to solve the MINLP model in a water network. The objective is to find the minimum fresh water and wastewater flow rates for each network for a given set of topology constraints. For example, networks may have a large number of reuse/recycle streams, with correspondingly high fixed capital costs. Process designers and plant management will be interested in achieving water savings with the simplest possible networks, which will be less expensive to implement and may entail lower total (life cycle) impacts (Ku-Pineda and Tan, 2005). In addition, simpler networks will be more robust, safer and easier to control. There may also be forbidden matches in the plant due to stream incompatibilities, plant layout considerations (as when a source is located at a great distance from its potential sink), or compulsory matches (as when alkaline and acidic water streams need to be mixed in order to neutralize each other).

PROCESS MODEL

This section describes MINLP models for the design of simplified water reuse/recycle networks based on the water source/sink allocation concept (Hul *et al.*, 2006). Similar models have been developed for mass-exchange based formulations (Bagajewicz and Savelski, 2001).

MINLP Model

The objective function is to minimize the total amount of freshwater used in the system:

$$\min \Sigma_j F_{FW,j} \tag{1}$$

The problem is subject to several constraints. The water balance for each source is given by

$$F_{WW,i} + \Sigma_j \cdot B_{i,j} F_{i,j} = F_i \quad \forall i \tag{2}$$

The water balance for each sink is given by

$$F_{FW,j} + \Sigma_i \cdot B_{i,j} F_{i,j} = F_j \quad \forall j \tag{3}$$

The impurity load limit of each water sink must be met at the maximum load by the mixed stream supplied to it:

$$\Sigma_i F_{i,j} C_i B_{i,j} \leq F_j C_j \quad \forall j \tag{4}$$

The model is based on the linear programming formulation of El-Halwagi *et al.* (2003) except for the insertion of the binary variables $B_{i,j}$. This modification makes the model nonlinear, but is necessary to be able to consider topological constraints on the water network. Such constraints may arise out of various plant-specific design considerations. Examples of such constraints are given in Table 1. Finally, all variables in the system are non-negative:

$$F_{FW,j}, F_{WW,j}, B_{i,j}, F_{i,j} \geq 0 \quad \forall i, j \tag{5}$$

This model thus allows the smallest water consumption to be found for a network of given topological constraints.

PARTICLE SWARM OPTIMIZATION

Solving the MINLP model described in the previous section presents significant computational difficulties. There is a considerable risk that conventional deterministic algorithms will converge towards local optima. Metaheuristic algorithms can be used to find good solutions to such problems, although without a guarantee of convergence to the global optimum. In practice, lack of true convergence is not a major problem for as long as it the resulting solutions are