Integrated Process Water Networks Design Problem

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Overview

In this optimization problem we develop the superstructure and optimization model for the design of integrated process water networks (Ahmetović and Grossmann, 2010). The superstructure, which is an extension and generalization of the one given by Karuppiah and Grossmann (2006), consists of one or multiple sources of water of different quality, water-using processes, and wastewater treatment operations.The mathematical model of integrated process water networks consists of mass balance equations for water and the contaminants for every unit in the network. The model is formulated as a nonconvex nonlinear programming (NLP), and as a nonconvex mixed-integer nonlinear programming (MINLP) for the case when 0-1 variables are included to model the cost of piping and/or selection of technologies for treatment. The nonlinearities in the models appear in the mass balance equations in the form of bilinear terms (concentration times flowrate). In addition to this, nonlinearities appear in the objective function as concave terms of the cost functions for the water-treatment operations.

To effectively solve the non-convex MINLP model to global optimality we propose tight bounds on the variables which are expressed as general equations. We also incorporate the cut proposed by Karuppiah and Grossmann (2006) to significantly improve the strength of the lower bound for the global optimum. For the implementation of the proposed models, it is important to note that the derivatives become unbounded when the flows take zero values in the cost terms (investment costs of pipes and treatment units). To circumvent this problem, we add a tolerance ε (typically 0.001) in the cost function ($\text{Cost} = a\cdot(\text{Flow}+\varepsilon)^b$) for the investment cost of the pipes in the network and for treatment units. While this introduces a small error in the cost, it leads to bounded gradients for zero flows.

Two examples of different complexity are solved to illustrate the application of the proposed model. The general purpose global optimization solvers BARON and LindoGlobal are used to solve the non-convex MINLP model to global optimality.

References:

1. Karuppiah, R., Grossmann, I.E. Global optimization for the synthesis of integrated water systems in chemical processes. *Computers & Chemical Engineering*. 2006;30:650-673.
2. Ahmetović, E., Grossmann, I.E. (2010). Global superstructure optimization for the design of integrated process water networks. *AIChE J. 2010* (In press).