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Decoupling the constraints for process simulation in large-scale flowsheet optimization

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ABSTRACT
A distinct advantage of sequential quadratic programming (SQP) is global convergence that ensures convergence from a remote starting point. When the constraints are highly nonlinear such as in flowsheet optimization, however, locally convergent Newton's method used in SQP as the equation-solving tool may deteriorate the behavior of convergence. Our recognition that this issue remains to be resolved motivated us to study a two-tier SQP approach where the constraints for process simulation consisting of nonlinear equations are decoupled from the KKT system in order to block the adverse influence of nonlinearity on global convergence. Our equation oriented (EO) process simulator (Ishii & Otto, 2011) is employed to decouple the constraints and for maintaining feasibility of the decoupled constraints. The effectiveness and potential of the two-tier SQP approach for reliably and efficiently solving large-scale flowsheet optimization problems are numerically illustrated with fully thermally coupled distillation problems.

Key Words – sequential quadratic programming, highly nonlinear constraints, reduced KKT system, flowsheet optimization, equation oriented process simulation, distillation

1. Introduction

There has been an increasing interest in the application of state-of-the-art flowsheet optimization technology to the design and operation of chemical plants. The potential impact of the application on energy savings is enormous since the chemical industry is a major energy consumer. Sequential quadratic programming (SQP) offers distinct advantages for solving flowsheet optimization problems. Its superior features include the fact that convergence of the constraints is not required at each