Dynamic Chemical Process Optimization

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Chemical process optimization has become a well developed and widely used and appreciated tool in the chemical industries. Nonlinear programming algorithms have become important tools in the design of new processes, control of highly interacting and nonlinear processes, process identification and parameter estimation and the evaluation of uncertainty in design and operation. Nevertheless, as process applications increase in size and complexity, and processes interact more strongly with each other, several challenges need to be overcome in the formulation of optimization problems and the development of specialized NLP algorithms. In particular, the integration of design, operations and planning leads to an important but difficult large-scale optimization problem.

Chemical process engineering optimization problems have a number of unique characteristics. Unlike many other design optimization problems, process models form a sparse set of nonlinear equations with no regular, scalable structure. Optimization problems are often highly constrained but consist of relatively few decision variables. Stategies for the optimization of steady state processes are well developed for design and operation. On the other hand, dynamic process models described by Differential Algebraic Equations are being considered more frequently in industry with the goal of solving dynamic optimization problems.

This talk surveys some recent advances in dynamic process optimization. Modeling tools for process dynamics have relied on powerful state of the art DAE solvers. For optimization, these have been embedded within black box NLP strategies. These often work well but they have similar stability properties as single shooting applied to BVPs. In addition, inequality path constraints can also be difficulty to enforce with these approaches. Instead we explore simultaneous approaches such as multiple shooting or collocation on finite elements.

For process optimization, the resulting NLP can be addressed efficiently with a reduced space strategy to solve Karush Kuhn Tucker system. This approach is useful if few decisions are present. Moreover we review a number of advances including: a globally convergent barrier approach for inequality constraints, a novel line search globalization based on filter concepts due to Fletcher, and a preconditioned finite difference CG method to provide a cheap approach to incorporate second derivatives.

Finally, the talk presents some open problems for dynamic process optimization. Included are high index path constraints and their impact on the NLP solution, formulation of optimization problems with moving finite elements and the exploitation of parallelism for very large process problems. Some preliminary work is also sketched to address some of these questions.