106e Simultaneous Large-Scale Parameter Estimation in Tubular Polymerization Reactors

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Several kinetic and transport parameters are required for the development and on-line update of tubular polymerization reactors first-principles models. The associated complexity of these models coupled to the limited availability of plant measurements and the large sets of parameters required for off-line and on-line tasks make the parameter estimation problem particularly difficult. Multiple feed injections along the reactor are encountered in common reactor designs. This requires the reactor to be split into a number of reaction and heating/cooling zones giving rise to a complex and distributed differential-algebraic equations (DAE) system which is usually solved by the sequential integration of the DAE system associated to each zone. Under this approach, the parameter estimation problem formulation requires the repeated and expensive solution of the system by means of a DAE solver coupled to a nonlinear programming solver. Furthermore, the optimization task can become computationally highly expensive when large sets of parameters are to be estimated and, commonly, heuristic-based strategies must be devised to reduce the dimension of the large-scale problem.

In this work, a nonlinear programming (NLP) simultaneous approach is proposed for the large-scale parameter estimation in tubular polymerization reactors. Under this approach, both differential and algebraic variables in the DAE system are fully discretized leading to a large-scale nonlinear programming problem that can be solved with state-of-the art NLP solvers. With this, a more systematic parameter estimation strategy is obtained. As a result, larger and better sets of parameters can be obtained for the prediction of final product properties and the reactor operating conditions. The proposed methodology was used to obtain several sets of parameters for a first-principles model enabling the accurate prediction of operating conditions and final product properties on actual polymerization reactors. The methodology is robust and reliable and can be used for off-line and on-line applications.