Abstract

The field of chemical process estimation and control has been intensively explored in the last decades. However, novel applications, the demands required by strict safety regulations, tightening environmental standards, operating constraints and product quality specifications, generate more difficult and challenging situations.

This stimulates the need of more sophisticated solutions than the ones that can be provided by traditional techniques alone. *(i)* Exploiting the process model structure along with *(ii)* methods to deal efficiently with estimation and control problems are of paramount importance to reduce the computational load that new techniques often demand. This dissertation explores these two aspects for a particular class of first principles dynamic models. On the one hand, structure exploitation is studied through a widely used input-affine chemical process, namely distillation. A rigorousmodel is developed for a packed distillation column, leading to large scale differential-algebraic equations (DAEs). It is shown that these DAEs can be reduced by constraints differentiation and algebraic manipulation,preserving the physical meaning of the states in the representation. This kind of models exhibits high differentiation index, making its simulation impossible with off-the-shelf solvers. Hence, a simple procedure, based on the model Jacobian structural properties, is proposed in order to reduce the index of the model.

Moreover, the reduced index DAEs are cast such that sparse structures are obtained for simulation tasks, alleviating the computational load when solving the model. On the other hand, input/parameter-affine models are analyzed in the formulation of dynamic optimization problems (DOP). It is shown that a DOP using this kind of models, with convex cost and convex inequality constraints, can be approximated by a convex formulation. This approximation is performed by proposing a parametric optimization problem whose extremes correspond to the original nonconvex DOP and to a convex one. The method is used in the context of optimal control and parameter estimation, such that a simple 2-step approach is proposed as an alternative to the solution of the original nonconvex problem.

In this form, the computational load involved in solving a parameterized DOP exactly, is reduced by a simple 2-step convex optimization method that leads to a nearly optimal solution.