496g Managing Technological Risk in Process Design Using Detailed Models

Rodrigo F. Blanco Gutierrez, Claire Adjiman, and Constantinos C. Pantelides

In today's business environment, technology development can bring a competitive advantage with new products or new processes. As with any other innovative process, uncertainty is likely to be present, resulting in increased risk with respect to safety and/or productivity. In process design this technological risk is typically related to new process technology and/or new process chemistry which can be used in new designs or to retrofit existing processes.

As time, money and resources are invested in R&D activities, the new technology can be further developed and understood, reducing the associated uncertainty and increasing the confidence in the designs generated. However, the increased initial cost and delays incurred in reaching full-volume production can reduce the probability of achieving a leading market position. Therefore, in developing an R&D strategy, the potential risk implications have to be weighted against the potential competitive advantage that may be realised by the deployment of new technology.

Process modelling plays a key role in quantifying the risk associated with decisions under uncertainty. While simple models can be acceptable for simple units, such as heat exchangers, it is the details, such as reaction microkinetics, the spatial variations of properties, and the finite rates of mass transfer, that often distinguish new technology from existing ones. Thus, it is important to use models which capture these details to arrive at a reliable quantification of risk.

This work considers the problem of process design under technological risk where the risk arises from limitations in the available understanding of the dynamic and steady-state behaviour of the new technology. A methodology is proposed to manage the technological risk in process design. The approach consists of a series of steps from model building to robust design.

In the first step, we start by building and validating a detailed process model which is a key element in the risk evaluation of new technologies. The model is expressed in the form of a mixed system of partial differential and algebraic equations (PDAEs). A model of the unit based on the new technology may be considered on its own or, more realistically, in the wider context of a process model with some well-established unit operations. In such cases, the uncertainty arising from the new technology can be reduced by the design and operation of downstream units. A key outcome of model validation is a set of confidence intervals on the uncertain model parameters.

In the second step, we identify a deterministic optimal design and control strategy for the process, using the nominal values of the uncertain parameters. In the third step, a global sensitivity analysis is used to identify uncertain parameters which have an important effect on key performance indicators, on the basis of the confidence intervals. The Sobol' sensitivity indices (I.M. Sobol', 2001, Mathematics and Computers in Simulation, 55, 271-280) are calculated using a Monte Carlo technique. The calculation of the sensitivities requires the objective function to be evaluated at different values of the uncertain parameters. In sensitivity analysis, the control variables are usually fixed at their nominal values. Here, an alternative approach is proposed: every sampled point is treated as an optimisation problem. The approach allows to find the optimal operating conditions for the given sampled point, while making use of the control variables. A parallel implementation of this step has been developed using gPROMS (Process Systems Enterprise Ltd.). First order and higher order sensitivity indices are calculated to identify individual parameters or groups of parameters affecting the process performance. The sensitivity of the process to the design variables is also quantified in this step. This information provides an initial assessment of the feasibility of different designs in the presence of uncertainty.

In the fourth step, once the subset of critical uncertain parameters has been identified, a series of scenarios is generated to solve a robust design problem using dynamic optimisation. The information obtained from the sensitivity analysis is used to reduce the number of parameters to be sampled and to generate specific sample points aimed at obtaining an optimal design with a minimum number of scenarios. The different scenarios are treated as uncertain parameter disturbances over the “pseudo-time” domain, which facilitates the initialisation of complex models.

The methodology is applied to a case study involving the design of a catalytic tubular reactor. The process is described by a set of PDAEs with 8 uncertain parameters. The sensitivity analysis shows that only half of the parameters have an important effect on the performance of the reactor. This allows computational effort to be focussed on the key uncertainties. A robust design is obtained by sampling the subset of uncertain parameters and optimising the expected reactor performance. A large sample size is used, giving confidence in the validity of the robust optimisation.