HANDLING UNCERTAINTY IN THE DEVELOPMENT AND DESIGN OF CHEMICAL PROCESSES

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In the development of new chemical manufacturing processes, particularly in the pharmaceutical industry, there is a large element of process uncertainty since detailed knowledge of the chemical reaction mechanisms and of the power and effectiveness of separation devices (to purify the product and recover raw materials) is often limited. Data is obtained from the laboratory during the identification stage of a new product (for example a new drug) and this is used during the manufacturing process development stage. Much data is generated but often not useful for the development of the large scale manufacturing process. In some cases large amounts of data are available but often single data points with confidents limits are obtainable in the form of interval bounds. Using a structured approach with the computational process design tools, which are used extensively, the uncertainty can be managed and improved process performance may be obtained. Methodologies can be based either on a stochastic formulation or by using interval bounds.

The paper will present a stochastic methodology for process development in a general framework for batch and continuous process models, consisting of two main parts. The first combines systematic modelling procedures with Hammersley sampling based uncertainty analysis and a range of sample-based sensitivity analysis techniques, used to quantify predicted performance uncertainty and identify key uncertainty contributions. In the second, a stochastic optimisation approach is employed to solve different problems under uncertainty. The methodology was implemented on a batch reactor process. Some undesirable performance characteristics were observed when the published nominal optimal isothermal operating policy was implemented in the uncertain system. It was found that a robust operating policy significantly improved the total process time characteristic.

If the data required to base design decisions is insufficient to derive a meaningful statistical distribution an alternative approach is to use instead the error bars as intervals and employ the machinery of interval analysis to determine the best ‘worst-case’ design which allows for the range of uncertainty given by the laboratory data. An approach using interval based methods with modular systems which employ ‘grey-box models’ will be outlined. Modular systems are the preferred type of system for chemical process design by most major process design and development companies.