Research topics

Design and Optimisation of Chemical Reactors

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Abstract

In most processes, the type of chemical reactor and its operation have a critical influence on the flowsheet structure and the overall performance of the process. This project has developed systematic methods to target for the maximum selectivity and yield of chemical reactors. For continuous reactors, targets are provided for the ideal mixing patterns, catalyst distribution and heat transfer arrangements required to achieve the target in design. Novel reactor designs are identified with significant advantages over conventional designs. For batch reactors, feed addition, product take-off, recycling, temperature, pressure and cycle time are all optimised simultaneously.

Project description

For the design and scale-up of reactors, the most appropriate choice of configuration and mixing pattern, arrangements for feed and recycling of raw materials, catalyst distribution and arrangements for handling the energy effects in the reaction system (and in batch reactions, cycle time also) have not only a critical effect on the performance of the reactor but that of the process as a whole. Yet, design choices are made on the basis of past experience and trial and error using laboratory tests and repeated simulation.

Methodologies have been developed for the systematic design of chemical reactors which set performance targets, predicting the maximum yield and selectivity for a given reaction system with its catalyst. Even the most complex systems can be analysed, involving multi-phase reactors and complex heat transfer arrangements. The mixing patterns and heat transfer arrangements (and cycle time for batch reactors) associated with the target provide the basis for the design to achieve the target. Optimum catalyst distribution patterns can also be predicted, accounting for the effects of catalyst aging. For new processes, the technology is capable of identifying the optimal reactor configuration and operation. For existing processes it can be used to determine the potential for modifying the design.

The application of the technology leads to the development of novel reactor schemes that would be virtually impossible to derive using an approach based on trial and error. The technology has either led to designs with very significant improvements in the yield of the process when compared with those based on conventional reactor designs, or significantly reduced capital investment.