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Process Simulation for Industrial Process Design

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Process design and optimisation are fundamental steps to ensure the economic sustainability of chemical processes. Suitable description of the performance of the various unit operations of the plant should be made and integrated, to understand the mutual interferences both under steady state conditions and under unsteady operation. Process simulation tools are helpful to compute both situations. The stationary case can be simulated with packages dealing with material and energy balances applied to each unit and extended to the whole plant. More complex is the unsteady state case, which needs dynamic modelling to describe the time-dependent evolution of the system. Separation equipment are simulated using algorithms embedded in process simulators, which may be more or less complex and adequate to represent the system with the desired approximation. A key issue in this case is the correct choice of a thermodynamic package able to cope with the system complexity in sufficient detail, in order to make reliable previsions on phase equilibria and components partition among them.

Reactors are more critical to describe, since they represent an unicum for the particular case under investigation. When introducing a reactor in a flowsheet, different options become available, as for instance the following examples from Aspen Plus®. The Stoichiometric and Yield reactors require some definition of the reactions taking place and their extent (e.g., in form of yield of different products). This is easily applied to available experimental result, but it does not allow tuning freely the process variables, since their influence on reactor performance is actually missing. *Equilibrium* or *Gibbs* reactors are useful to define the dependence on process variables, but they consider the reactor at equilibrium, so reactor sizing is not allowed. Furthermore, kinetically limited situations cannot be correctly described. Finally, the *Batch*, *Plug-Flow* (PFR, in case filled with catalyst as packed bed reactor) and *Continuously Stirred Tank* (CSTR) reactors are the most flexible options, which allow a full description of the process under variable conditions and proper sizing of the reactor. However, to perform these calculations, a suitable reaction set and the relative kinetic model are needed.

Considering transport phenomena, most process simulators allow to compute pressure drop across the reactor, e.g., through the Ergun equation. Heat transport to or from the reactor can be rather easily computed, in case defining a given temperature profile along the reactor. For catalytic reactions the effectiveness factor can also be introduced, to account for mass transfer limitations in the catalyst particles. However, the embedded models do not allow to detail the back diffusion in axial direction or to compute the radial concentration profiles. The same holds for heat transport: detailed temperature profiled in radial direction are hardly obtainable. These points may be implemented developing user-made subroutines as an embedded Fortran or Matlab codes.

Furthermore, the core of the sizing of chemical reactors remains the availability of a detailed kinetic model. Kinetics of heterogeneous catalytic reactions is a complex field, since the catalyst belongs to a different phase with respect to the reactants, thus besides the reaction step, adsorption and desorption stages should be added, increasing the complexity of modelling. All this without the effect of mass transfer limitations. The easiest model available is the power rate law model, which takes formally care of adsorption by using appropriate apparent reaction orders. Although suitable in some cases, this model is too empirical to be generalised for process simulation. The observed kinetic constant and reaction orders should include the dependence on adsorption/desorption phenomena, which can depend differently on process parameters than the intrinsic kinetic constant. For this reason, a Langmuir-Hinshelwood-Hougen-Watson (LHHW) model is preferably adopted, which more adequately computes the adsorption and desorption steps, which possibly limit the reaction rate. If more complex kinetic models are needed, also in this case the user can develop separate codes that externally compute the kinetics, possibly detailing also heat or mass transfer limitations, and these are recalled during process simulation. Some examples of process simulation on different fields are reported in the following references [1-5].

The level of detail is of course defined by the user, as a compromise between precision and computation costs. On the other hand, the versatility of the simulator insists on this key point. The best ones should be able to include in the simulation user defined models.

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