Chapter 2. The development process

The development of reactor design models is just one portion of the process needed to develop a new chemical process. This chapter discusses the overall outline of the development process. The integration of reactor modeling into the development process is more likely to succeed when the entire design team have a common understanding regarding the purposes for each step of the development process.

In one sense, there are two methods of process development, scale up and scale down. The first method starts with the initial discovery, usually a catalyst with a desired productivity, and incrementally increases the reactor size through pilot plant, demonstration plant, to commercial plant. The second method also starts with the initial catalyst discovery, but then switches to a focus on the end objective, the commercial plant. Subsequent development works "backward" from that commercial design goal. The typical outline of the two methods are shown below.

2.1 Scale Up Method

- Catalyst screening and development using a small, laboratory reactor.
- Development of a conceptual process sequence without an economic analysis.
- Scale up of the laboratory reactor to a pilot plant size with the addition of other process steps for study of recycle effects.
- Scale up of the pilot plant to commercial size (sometimes a demonstration plant is an intermediate step).

2.1 Scale Down Method

- Catalyst screening and development as above.
- Development of a conceptual process design and simulation of the commercial scale process to explore economic sensitivity.
- Development of a kinetic model using possibly another type of laboratory reactor.
- Development of a reactor model using the kinetic model.
- Scale down of the commercial scale to the smallest possible pilot plant size.
- Determination or verification of design parameters using the pilot plant data.
- Final design of the commercial plant using the validated or updated parameters from the pilot plant program.

2.3 Dangers of the Scale Up Method

The first drawback to this method is that the pilot plant dimensions, primarily those of the reactor, may not be appropriate for the commercial process. By selecting the pilot plant dimensions without regard to the needs of the commercial unit (e.g. pressure drop or heat transfer), the scaling relationships, such as length/diameter, are set at a non commercial value. When these dimensions are changed for the commercial design, the "scale up" lacks the desired similarity, and therefore the commercial reactor will perform differently than the pilot plant reactor.

An even greater error can be made when using the Scale Up method. Notice that the Scale Up method doesn't include the development of a kinetic model, nor does it include simulation of the commercial scale process. By skipping those steps, the wrong reactor type may be chosen for the process. Often, when the Scale Up method is followed, the reactor used to develop the catalyst (or reactions) is assumed to be the best reactor. However, high heat exchange or high recycle requirements, or a need to regenerate or resupply a catalyst may mean that another type of reactor would be a better choice. Without full simulation of the commercial process, these demands might be overlooked in the second step of the Scale Up sequence.

2.4 Advantages of the Scale Down Method

In the Scale Down method, the process simulation program is used to develop the conceptual process design before the reactor model has been developed. The reactor will be modeled as a stoichiometric or equilibrium reactor at this stage. A study of the effects of conversion and selectivity on the process economics yields targets for the reactor design engineer. With these targets, the design engineer selects the reactor, determines reactor configuration and size for the commercial reactor, and determines the reactor operating conditions that produce the desired target performance. The reactor is then scaled down for the pilot plant. After the pilot plant program has been used to update the reactor model parameters, it can be used "off line" to provide to the process simulation program the performance for a given feed condition. If possible, the reactor model can be fully integrated into the process simulation program, but that integration is not an absolute necessity.

Two kinds of parameters are used to design processes...scale dependent and scale independent parameters. Examples of the latter are physical properties of fluids and their components, and properties of other materials. The scale dependent parameters usually arise due to the use of a simplified model for a complex, often stochastic process. Examples of scale dependent parameters are axial and radial heat and mass dispersion coefficients, and gas fraction in a bubble column. The scale independent parameters are often well known or can be obtained by a laboratory that specializes in physical properties. The uncertainty in the commercial design usually concerns the scale dependent parameters. (Scale dependent is not the same as extensive. A reaction rate constant is an extensive parameter that is not scale dependent.)

Correlations for the common scale dependent parameters have been developed and are found in the literature. The examples include a set of recommended correlations. Usually, these correlations are developed for a certain range of parameters such as Reynolds number, superficial velocity, ratio of catalyst diameter to reactor diameter. When scaling down the commercial reactor, these constraints for the correlations may limit the minimum size of the pilot plant reactor. For example, many of the reactor parameter correlations used in the examples are for reactors longer than 5 ft. If the pilot plant reactor is greater than this length, then the correlation for wall heat transfer may be compared to the measured value. If not in agreement, then the same correlation may be used with some adjustment. If the pilot reactor is less than 5 ft., then a discrepancy between the correlation and the measured value may be due to an entrance effect that is not included in the correlation. Without a length term, there is no link between the data and the correlation to be used for the commercial design. Both scenarios still have risk for the scale up, but the risk is probably higher with the second scenario.

Although "eureka" discoveries can be part of the invention process, for project development, setting project and commercial goals first and then "working backward" from the goal, as outlined above, is a more productive process than other alternatives.