

Build Robust Reactor Models

Photo credit: Applied Reactor Technologies, Inc.

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Whether scaling up a new reactor or revamping an existing one, use this proven **14-step** approach.

Although the reactor is the heart of most process plants, it usually is treated as a “black box” or a proprietary item and is not covered by commercial simulators. Each technology developer or licensor uses its own procedure to develop its reactor model. Such a procedure often is lengthy and expensive, due to ill-defined steps, many trial-and-error mistakes, and excessive pilot-plant campaigns. Finally, even if the reactor is “successfully” scaled up to commercial size, the credibility of the design and the optimum operating conditions of the reactor often is questionable.

On the other hand, a plant owner may not have the know-how or confidence to modify, revamp, or modernize the reactor or its operation. The owner needs to build an in-house model for any such effort.

This article suggests a well developed and tested procedure for building a robust reactor model/model package, and details tips and traps. It also recommends proven ways to substantially cut the cost and time for the effort. This article primarily focuses on catalytic gas/solid reactions and reactor systems.

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What is a robust model?

Such a model is a practical, reliable, and useful package for analyzing, scaling up, designing, and optimizing a given reaction and reactor system. It provides the best design for a new system, revamp, or modernization, and the optimum operating conditions for an existing reactor. The model predicts the performance for a wide variety of designs and operating conditions, including those used in the commercial reactor. It also covers conditions beyond normal operations, to predict upset, off-specification, turnaround, and unsafe situations.

Such a model should be based primarily on fundamental principles of reaction engineering and reactor hydrodynamics. It should use the minimum number of adjustable/experimental parameters and be solved by standard mathematical routines requiring minimum execution time. And, it should be easy to integrate with other in-house or commercial simulation packages.

MODEL BUILDING STEPS

There are 14 basic steps in building a robust reactor model for either revamp or scale-up. The time and effort required for a revamp model for an existing system is substantially lower, however, than that for a scale-up model for a new process — due to accumulated process know-how and data from both operating plant and various bench/pilot-plant units used in the early development of the process.

STEP 1 — DEFINE REACTION TYPE. This is the first and most basic categorization. It is based on the phases (gas, liquid, or solid) involved in the reaction system, and whether the solid phase, if involved, is catalytic or noncatalytic in nature. This definition of the reaction type — for example, homogeneous, gas/solid catalytic, gas/solid noncatalytic, or gas/liquid — immediately establishes the nature of the effort and its relative degree of difficulty.

Provided the mechanism and kinetics of the involved reaction system are known, the degree of difficulty in building a reactor model generally increases in the following, approximate order:

- homogeneous gas phase;
- homogeneous liquid phase;
- gas/solid catalytic or liquid/solid catalytic;

- gas/liquid;
- gas/solid noncatalytic or liquid/solid noncatalytic;
- gas/liquid/solid catalytic; and
- gas/liquid/solid noncatalytic.

Systems involving the liquid phase may be subdivided further into ones without phase transfer between gas and liquid, and those with it. The latter category is perhaps the most difficult, and is beyond the scope of this article.

STEP 2 — DESIGN, BUILD, AND OPERATE A TEST UNIT. A proper laboratory or process development unit (PDU) is required if the available data or knowledge on the reaction mechanism and kinetics, and the reactor hydrodynamics appear inadequate. Such a unit is mandatory for a new reaction system.

For reactions involving solids (catalytic or noncatalytic), a minimum of two stages of a PDU usually are needed for studying the reaction mechanism and kinetics. In the first stage, the solids are used in the form of a fine powder to allow generation of true or intrinsic kinetic data with minimum pore-diffusion resistance. In the second stage, the PDU should mimic as closely as possible the design, hydrodynamic conditions, and operation, including the solids' particle size, expected in the commercial unit.

Unfortunately, a close approach to a commercial system often is not possible in a lab-scale PDU. Therefore,

an extensive pilot-plant campaign usually is undertaken. A robust model, however, can minimize, if not eliminate, the cost and effort of such pilot-plant campaigns.

Additional PDUs, called “cold models,” because no reactions occur in them, may be needed to assess the hydrodynamics of a totally new reactor configuration, fluid/solid, fluid/fluid, or three-phase system. Attrition, adhesion (particle stickiness), fluidizability, and flow characteristics of a new solid catalyst are some key issues that must be studied in the cold models, as well as standard test units. Again, a robust model can keep all test units as small as practical and minimize the efforts in test campaigns.

If, for the same catalytic activity, a fluidized-bed system far outperforms a fixed-bed design, according to the model analysis (to be described later), an additional and separate development and test campaign is required for the development of the fluidized-bed catalyst.

Extensive cold-model testing and demonstration may be necessary, particularly for cases where the operation, control, and performance of a reactor or a reactor-regenerator dual system critically depends upon the solids' circulation system — to establish correlations/methodology for design, operation, and control of such units. (The modeling and design of difficult solids' circulation systems, such as ones with cross-flow and double loops, *e.g.*, as in fluid catalytic crackers, is outside the scope of this article.)

The key design criterion of a PDU is to ensure that it can cover a wide range of conditions — both higher and lower than those expected in the commercial units — for four key operating variables:

1. space velocity or throughput (of both fluids and solid in flow reactors);
2. temperature;
3. pressure; and
4. composition.

Another key feature of the PDU



should be accurate monitoring of reactor temperature profiles, if such profiles are significant. Temperature often is the most dominant and critical variable in reactor design and operation.

In addition, the PDU must have the flexibility to readily accommodate modifications, such as injection of multiple feed points, insertion of solid/gas sampling, aeration, and temperature probes, change of temperature profiles, installation or swapping of internals, and variation of feed and discharge port/plenum designs. It also should enable easy catalyst/solids loading and discharge, and product recycle.

STEP 3 — COLLECT AND ANALYZE DATA. Always keep scale-up, and commercial design and operation in mind when designing the PDUs and planning the experiments. A carefully planned test campaign is needed to collect data that adequately cover wide ranges of the four key operating variables, while minimizing the number of experiments necessary.

In the initial stage, change only one variable at a time, while, if possible, keeping all others constant. Near the final experimental campaign, study several possible and diverse combinations of these variables — say, high temperature/low pressure and low temperature/high pressure, high throughput/high temperature and low throughput/low temperature, etc. These data are useful for testing the reaction model for wide-ranging operating conditions.

Temperature usually plays the key role in the reaction kinetics of most systems; so, dedicate the maximum number of experiments to this single variable. Study various combinations of temperature with other variables. For reactions involving solids, catalytic or noncatalytic, vary both solid particle size and temperature so that the data cover conditions ranging from negligible to significant pore-diffusion resistance. The effect, if

any, of pore diffusion on reaction rate and product selectivity then can be established from these data.

For multiple reaction systems, series or parallel, to establish the kinetics of the overall reaction with better confidence, you ideally should collect data on each component reaction. Thus, for systems $A \rightarrow B \rightarrow C$ or $X \rightarrow Y, X \rightarrow Z$, each reaction $A \rightarrow B, B \rightarrow C, X \rightarrow Y$, and $X \rightarrow Z$ should be studied separately, if possible, particularly to see the temperature effect on each and to determine the reaction activation energy.

Examination of the data from both PDU and an existing commercial unit, if available, should reveal for each variable both the trends of its effect and its relative importance on the reaction system. The tabulated and graphical representation of the data also provide a consistency check — pointing to bad data points that should be eliminated and helping identify experiments that should be repeated. Data consistency and reproducibility, as well as a wide range of coverage of all key variables, are essential for building a robust model.

STEP 4 — ESTABLISH THE PRELIMINARY REACTION MECHANISM AND KINETICS. This is perhaps the most critical and important task in building a robust model. It also is usually the most-time-consuming effort (excepting experimental or pilot-plant campaigns), particularly for complex reactions. Without a satisfactory reaction mechanism and kinetics, though, the model may be applicable only to narrow ranges of conditions and may be dangerous to use for reactor scale-up, control, and operation, and in dynamic simulations.

Begin this step with a literature search. For most reaction systems of commercial interest, there usually is an abundance of information in the open literature. This information, however, may not exactly match your operating conditions or catalyst for-

mulation. Nevertheless, it is good enough, in most cases, to formulate or select reaction-mechanism and rate expressions that best represent your system. Carefully consider the reputation and reliability of the information source, quality of data, and experimental and analytical details before selection of the reaction mechanism. A model builder's prior experience can be particularly helpful at this stage.

For a totally new reaction system, the mechanism and rate expressions need to be established by systematic and fundamental analysis of reaction rate data, as described in the literature (1–4).

Establishing the reaction kinetics involves two steps — selection of rate expressions, and, then, determination of rate parameters. These parameters usually are found by using the selected rate expressions and matching rate data obtained from a simple and close-to-ideal experimental unit like a plug-flow reactor (PFR) or continuous stirred-tank reactor (CSTR). For a complex (multiple-reaction) system, this often involves a trial-and-error procedure for the initial estimates, followed by fine-tuning with a suitable parameter-estimation routine.

Rate expressions normally used in engineering kinetics involve four types of parameters: (1) pre-exponential factors; (2) activation energies; (3) reaction order with respect to each component involved in each rate expression; and (4) adsorption constants. For reaction systems of commercial interest, a literature search often can lead you to reasonable initial estimates for the latter three parameters. The pre-exponential factors must be determined from actual data for the catalyst or reaction conditions of interest.

For gas/solid reaction systems, Langmuir-Hinshelwood-type rate expressions that involve adsorption constants in the denominators are preferable. This type of rate expression clearly reflects the change of reaction

order with the change in gas concentration or pressure in the system. Thus, for example (5), in the following rate expression for the conversion of *n*-butane to maleic anhydride, the order of the reaction with respect to *n*-butane goes from unity to zero, as the concentration of *n*-butane increases in the reaction mixture from a very low to a very high value:

$$R = k_1 b_1 C_B C_O^{0.3} / (1 + b_1 C_B)$$

where C_B and C_O are molar concentrations of *n*-butane and oxygen in the reaction mixture, and k_1 and b_1 are the rate and adsorption constants of the reaction.

With the advent of inexpensive, high-speed computers and easily available, powerful numerical techniques, it no longer is necessary to simplify rate expressions — for instance, by treating them as zero-, first-, or second-order systems. A zero-order rate expression is not desirable, anyway, because it normally is applicable only to a limited, high concentration range of the particular component. For example, for many oxidation systems, rates are expressed either as a zero or small fractional order with respect to oxygen concentration. Yet, such a rate expression, which often indicates a pseudo (false) order of oxygen in excessive oxygen concentration, is inapplicable near complete oxygen conversion. A zero order implies that the reaction can proceed in the absence of oxygen, which is not possible.

Unless absolutely required, the reaction mechanism only should consist of a limited number of reactions involving just the significant reactants and products. A complex reaction mechanism with a very large number of reactions is both unnecessary and unacceptable for most practical applications. Many commercially significant systems can be well represented by a maximum of 5–10 reactions. Similarly, unless essential (for instance, for polymerization reactions), mechanisms involving free radicals or other difficult-to-measure intermediates should be avoided whenever possible.

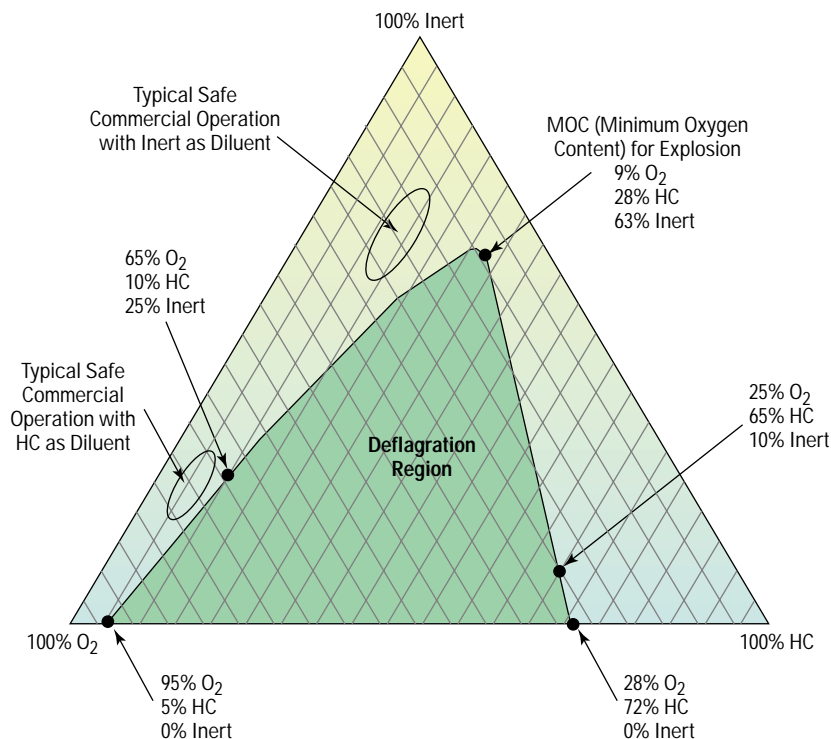


Figure 1. Typical deflagration explosion diagram for hydrocarbon/oxygen/inert mixture at a given temperature and pressure.

STEP 5 — STUDY THE SAFETY ASPECTS.

For a new, exothermic reaction system, this is a critical step to assure the safety and proper control of the commercial reactor. Lab-scale reactors and even pilot-plant units usually are made of relatively small diameter tubes that allow for heat loss to the surroundings. The diameter of a commercial reactor, on the other hand, is large enough to approach adiabatic conditions and cause heat buildup. Explosion hazards of a reaction mixture increase with the buildup of reaction heat with or without associated pressure rise.

The reaction mixture's explosion characteristics, which depend primarily upon heat source (hot spot, spark, or flame, for example), gas composition, temperature, and pressure, must be determined carefully through experimental programs carried out in a specialized laboratory. These programs usually provide combustion or flammability diagrams for the reaction system. Such a diagram, usually triangular, shows the unsafe or explosive envelope of gas mixture compositions at the particular temperature and pressure (see Figure 1). A series of such diagrams

are generated for wide ranges of temperature, pressure, and compositions of the gas mixture — so that inlet and outlet gas compositions and conditions of the commercial reactor are covered with adequate margins.

In modeling and scale-up, the operating conditions for most parts of the reactor, including its inlet and outlet, are kept outside the explosion envelopes.

The explosion characteristics, however, are also influenced by many secondary factors. For instance, in the presence of fine solids in intimate contact with reacting gases, such as in a fluidized-bed reactor, it is possible to design and operate the reactor well within the envelopes with negligible risk of explosion. This is because no hot spots are generated in such a reactor, due to vigorous mixing taking place. Caution must be exercised, though, in designing the free-board region of such a reactor, because hot spots may be created there, due to the flow of a very dilute gas/solids mixture.

Explosion phenomena are divided into two broad types — deflagration and detonation. Most explosion dia-



grams usually cover deflagration, which is caused by sudden gas expansion by an accelerated reaction. The maximum pressure buildup due to such an explosion can be estimated from the pressure/volume relationship of the complete reaction/combustion process. The detonation process, on the other hand, is more violent, generating shock waves that travel at a speed several orders of magnitude higher than the pressure wave caused by deflagration. The local pressure buildup from this phenomenon, thus, is substantially higher — for most hydrocarbon/air mixtures, about 15–20 times the initial pressure, compared to a maximum of two times in case of deflagration. See, for example, Ref. 6 for details on these explosion phenomena.

Therefore, the detonation characteristics of the reaction mixture should be studied, along with deflagration, to address reactor safety more thoroughly.

STEP 6 — DEFINE REACTOR TYPE AND ITS HYDRODYNAMICS. The reactor type is defined by: (a) the physical configuration of the volume occupied by the reaction system; (b) the flow mode of various streams in and out of the reactor; and (c) the hydrodynamic representation of the flows within the reactor volume. Thus, for example, a CSTR usually represents a stirred vessel with continuous flow of a homogeneous fluid stream or continuous phase in and out of the vessel. The hydrodynamic representation of a CSTR assumes the fluid stream is completely mixed as soon as it enters the vessel and attains the outlet composition instantaneously. A PFR embodies the other extreme. It usually is tubular (with a high ratio of length, L , to diameter, D) in configuration. The flow in and out this reactor type is the same as that in the CSTR. The representation of the PFR hydrodynamics, however, assumes a total absence of axial mixing of the flowing streams within the reactor.

A homogeneous reactor usually is

designed using the performance equations of either the CSTR or PFR. This allows easier analysis, design, and scale-up of such reactors. But, these idealized reactors do not closely enough mirror the behavior of a real reactor. Such a reactor is better represented by a system with axial dispersion or by an axially dispersed reactor (ADR), the performance of which falls between that of a CSTR and a PFR. For a simple first-order reaction, $A \rightarrow B$, the steady-state mass-balance equation of an ADR can be described as:

$$D_a \frac{d^2 c_A}{dz^2} - u \frac{dc_A}{dz} - kc_A = 0 \quad (1)$$

where D_a is the axial dispersion coefficient.

The predicted behavior of the ADR approaches that of a PFR for no axial dispersion, *i.e.*, $D_a = 0$, and that of a CSTR for infinite dispersion (complete mixing), *i.e.*, $D_a = \infty$. For a real reactor, D_a is a finite number greater than zero.

In developing a robust model, it may be advisable to start with an ADR equation, rather than a CSTR or PFR one. For initial model development, the ADR equation can be turned into simple CSTR or PFR ones by substituting the two limiting values of D_a . But, including the D_a term allows you to fine-tune the model at a later stage to predict the reactor performance more precisely. To use this approach, however, the value of D_a needs to be determined by experiment or from one of the many correlations available in literature, for example, in Refs. 1–4 and 7–10. These correlations usually are available in the form of the dimensionless Peclet number, N_{Pe} ($= Lu/D_a$, where L and u represent tube length and fluid velocity, respectively). The Peclet number typically is expressed as a function of Reynolds number, N_{Re} , which represents the flow behavior within the reactor. $N_{Pe} > 100$ normally indicates an approach to the behavior of a PFR, while $N_{Pe} < 1$ to that of a CSTR. Qualitatively, a longer tube length or

higher fluid velocity means more PFR-like performance, and the reverse more CSTR-like.

The above discussions are for continuous flow reactors. For both homogeneous and heterogeneous reactors, however, part of the reaction mixture or one or more of the phases can be captive or in nonflow condition, while the rest can be in continuous or intermittent flow mode. Reactants can be injected along the reactor length or reactor path in the case of multiple-reactor systems. The reactor product can be recycled with the reactor feed before or after separation stages. These represent batch, semi-batch, multi-injection, and recycle reactor types. For heterogeneous reactors, the flow of the phases can be co- or counter-current.

For gas/solid reactors, the gas usually is in a continuous flow mode. The solid, however, can remain fixed in position within the reactor through which the gas percolates. Or, both solid and gas can flow continuously in co- or counter-current mode through the reactor. With the solid remaining fixed within the reactor, there are again various reactor types — for example, the nonadiabatic packed-bed tubular reactor (NAPBTR), adiabatic packed-bed multistage reactor (APBMSR), monolithic reactor, and radial flow reactor. An APBMSR can be operated with direct quench (interstage cooling or heating) by feed or recycle-gas injection or indirect quench by a heat exchanger. For continuous flow of both gas and solid, the possible reactor types include moving bed (co- and counter-current), bubbling and turbulent fluidized beds, circulating and fast fluidized beds, and entrained beds.

For gas/liquid systems, the reactor generally used is either a stirred tank or a bubble column. The bubble column can be vertically or horizontally sparged, vertical or horizontal flow, gas-lifted (internally or externally), and with or without a forced liquid-circulation loop. The bubble columns also can be categorized according to

Reactor Modeling

mixing modes of the liquid and gas stream, which can be CSTR, PFR or ADR, depending upon the design and operating conditions. The mode of each phase, to be used in model building, is determined from observations of the flow behavior in a reactor prototype or from previous knowledge of the behavior from similar and well-defined systems.

For a liquid/solid or gas/liquid/solid reactor, the solid can be a slurry or fluidized, or a stationary packed bed or a monolith. In the continuous-flow mode, it can enter and exit the reactor with the continuous liquid-flow stream. As indicated above, many other designs and operating modes of the liquid/solid and three-phase reactors are possible.

A combination of the reactor types also can be employed — for example, a CSTR followed by a PFR, or a circulating fluidized bed (CFB) followed by a bubbling fluidized bed (BFB). The latter typifies some fluidized catalytic cracking (FCC) reactors, where the riser section can be simulated by a CFB and the disengagement zone at the top of the riser by a BFB.

Reactors of very complex geometry, unusual shape, or with internals that modify the flow patterns in an unpredictable manner cannot be modeled according to the procedure described in this article. Use of suitable computational fluid dynamics (CFD) codes, together with good reaction kinetics, may be a viable option for these difficult reactors. Due to their high complexity and long computation time, however, such CFD-based models may not find easy or routine applications in plant operation and control.

STEP 7 — DETERMINE DETAILS TO BE INCLUDED IN THE MODELS. Model building should proceed in steps starting with a relatively simple preliminary model. This approach is used for two important reasons. First, it enables you to easily obtain and

verify approximate values of many model parameters (for example, the key rate parameters) needed as starting or initial guesses in numerical solution of more complex models during the final stages. Second, it provides a framework for relatively easily developing and debugging the basic structure and computer code for the final model. Details to be included in both the initial and final models need to be accounted for at this step, however, to allow a smooth transition.

As an example of this step-wise progression, a reactor that is expected to behave close to a PFR first can be modeled by simplifying Eq. 1 to:

$$u \frac{dc_A}{dz} + kc_A = 0 \quad (2)$$

where $k = k_0 \exp(-E/RT)$.

Equation 2 is obtained by dropping the second-order derivative term containing the axial-dispersion-coefficient term, D_a , from Eq. 1. Equation 2 is much easier to solve and eliminates the need for the unknown parameter, D_a . Furthermore, the results obtained can be verified by another simple, stepwise calculation procedure, for example, with a spreadsheet. Once a numerical solution procedure for Eq. 2 is established and approximate rate parameters are determined, Eq. 1 can be quickly solved by using the same procedure to obtain the value of D_a and refined rate param-

eters. In both steps, the same experimental data are used for evaluation of parameters.

For this example and in another example to follow, the equations are shown for only one reaction and for up to two reactants. Most reactions are more complex, involving multiple reactions and many more reactants. A similar equation, therefore, has to be written for material balance on each reactant. Also, for each reaction, at least two rate parameters, k_0 and E , must be estimated by data simulation. Thus, a significant number of model parameters need to be evaluated for most reaction systems.

For a bubble-column reactor in which a flowing gas A reacts with liquid B, $A + \nu B \rightarrow \text{Products}$, the coupled heat- and mass-balance equations (adapted from Ref. 8) are shown in the box, and represent the target equations of the final model:

Balance of A in gas phase: Eq. 3;

Balance of A in liquid phase: Eq. 4;

Balance of B in liquid phase: Eq. 5;

Heat balance (liquid phase): Eq. 6.

The recommended procedure is to start with a preliminary model for the system at steady state to avoid the complexity of time-derivative terms. Assume that the system is isothermal (with an average temperature between inlet and outlet values) and is PFR in performance. For the preliminary model, the reactor equations then become:

$$\varepsilon_G D_{aG} \frac{\partial^2 c_{AG}}{\partial z^2} - \frac{\partial}{\partial z} (u_G c_{AG}) - K_L a (c_{AL}^* - c_{AL}) = \frac{\partial c_{AG}}{\partial t} \quad (3)$$

$$\varepsilon_L D_{aL} \frac{\partial^2 c_{AL}}{\partial z^2} + a^* u_L \frac{\partial c_{AL}}{\partial z} + K_L a (c_{AL}^* - c_{AL}) - \varepsilon_L k_2 c_{AL} c_B = \frac{\partial c_{AL}}{\partial t} \quad (4)$$

$$\varepsilon_L D_{aL} \frac{\partial^2 c_B}{\partial z^2} + a^* u_L \frac{\partial c_B}{\partial z} - \nu \varepsilon_L k_2 c_{AL} c_B = \frac{\partial c_B}{\partial t} \quad (5)$$

$$\varepsilon_L \lambda_{eff} \frac{\partial^2 T}{\partial z^2} + a^* \rho_L c_p u_L \frac{\partial T}{\partial z} - k_w a_w (T - T_w) + \varepsilon_L (-\Delta H_R) k_2 c_{AL} c_B = \frac{\partial T}{\partial t} \quad (6)$$

$$a^* u_L \frac{dc_{AL}}{dz} + K_L a (c_{AL}^* - c_{AL}) - \varepsilon_L k_2 c_{AL} c_B = 0 \quad (8)$$



$$-\frac{d}{dz}(u_G c_{AG}) - K_L a(c_{AL}^* - c_{AL}) = 0 \quad (7)$$

see box for Eq. 8

$$a^* u_L \frac{dc_B}{dz} - \nu \epsilon_L k_2 c_{AL} c_B = 0 \quad (9)$$

Equations 7–9 do not require the parameters D_{aG} , D_{aL} , λ_{eff} , ρ_L , c_{pL} , k_w , ΔH_R , or the heat-balance equation. Once Eqs. 7–9 are solved satisfactorily and the rate parameters of the reaction system are determined, introduce the second-order terms containing the axial dispersion coefficients, D_{aG} and D_{aL} , and then the steady-state heat-balance equation (Eq. 6 minus the time derivative term). After the steady-state model is found to run

satisfactorily with all established model parameters, add the time-derivative terms of Eqs. 3–6 to develop the final unsteady-state reactor model.

Model complexity and the number of required model parameters grow with details that account for various phenomena that may be important to the specific reactor type and reaction system involved. Table 1 provides a list of some of these phenomena and their relevance to various reactor types. This table also points out details that may or may not be important for the various reactor types. Exclude the unimportant details to minimize model-building effort.

STEP 8 — CHOOSE THE RIGHT BALANCE EQUATIONS. You now should select the governing mass-, heat-, and pressure-balance equations, including those describing the solids' circulation system design and control (if necessary), that adequately describe the reactor performance and are consistent with Steps 6 and 7 (e.g., Eqs. 3–6 for our example). Such equations already have been developed for most reactor types of commercial interest and are available in the open literature (for example, Refs. 1–4 and 7–13). Experience and judgment are required, however, in choosing the equations for a specific need or reactor type, particularly when several alternatives

Table 1. Relative importance of major phenomena that may affect reactor models.

Phenomenon	Where It Usually Is More Important	Where It Usually Is Less Important	Where It Must Be Considered [Comment]
Pore-diffusion resistance	(a) Reactions involving solid particle size >1/16 in. (b) All fast, noncatalytic gas/solid (G/S) reactions like combustion and gasification	Catalytic bubbling fluidized-bed (BFB) and circulating fluidized-bed (CFB) reactors with particle size <100 microns	Fixed- and moving-bed G/S reactor models and fast reaction systems
Film-diffusion (interphase mass-transfer) resistance	(a) All bubbling reactors like BFB and gas/liquid (G/L) and three-phase (3-P) reactors (b) All fast, noncatalytic gas/solid reactions like combustion and gasification	Catalytic fixed-bed G/S reactors	All bubbling systems like BFB and G/L and 3-P reactors, and fast reaction systems
Pressure drop	Fixed-, moving-bed, and deep BFB G/S reactors, and liquid-phase reactors	CFB and entrained-bed reactors	G/S fixed- and moving-bed reactor models and all deep beds
Heat-transfer resistance	(a) Across two-phase interface in fast reactions (b) Gas side of tube wall in liquid-cooled gas-phase or G/S reactors	Within solid particles in solid/fluid reactions	Gas side of tube wall in liquid-cooled gas-phase or G/S reactors
Heat loss to atmosphere	Small-diameter laboratory and pilot-plant units	Commercial reactors	
Axial dispersion	(a) Low L/D and low Reynolds number (N_{Re}) flow conditions (b) Vessel with baffles or internals obstructing flows	High L/D and high N_{Re} flow in open pipes	
Radial dispersion	Large-diameter reactors with low flow rates, and CFB reactors		[Usually ignored in preliminary models]
Wall effect	Small diameter reactors with low N_{Re} flow condition, and CFB reactors		[Usually ignored in preliminary models]
Temperature profile	Fixed- and moving-bed G/S reactors	Dense phase of BFB reactors	Fixed- and moving-bed G/S reactor models
Volume change	Gas-phase G/S and G/L reactions, particularly with no gas dilution (e.g., with N_2)	Reactions not involving gas phase	
Phase holdups	All 2-P and 3-P reactors involving liquid phase		All 2-P and 3-P reactors involving liquid phase
Bed/line voidage/voidage profile	CFB reactors and solids' circulation-systems design		CFB reactors and solids' circulation-systems design

Reactor Modeling

are proposed in the literature. In some cases, the complete set of equations needs to be developed by combining the best information from several literature sources. The equations ideally should:

- be based more on sound principles of reaction engineering and reactor hydrodynamics than empiricism;
- contain a minimum number of adjustable parameters;
- include hydrodynamic, circulation system, and other parameters via reliable correlations or values already available in the open literature, for example, $K_L a$ for a bubble-column reactor;
- have undergone successful testing and validation;
- be free of unnecessary details or complications;
- be readily solvable by standard mathematical routines; and
- be easy to use, expand, and modify.

STEP 9 — SELECT EVALUATION PROCEDURES.

Now, determine correlations, sources, or methodologies for evaluating all nonkinetic model parameters, and hydrodynamic and solids' circulation phenomena involved in the reactor equations of Step 8. The reliability of the kinetic parameters and the success of the final model depend to a large extent upon the values of these parameters, which fall into the following categories:

- thermophysical properties — like density, heat capacity, thermal conductivity, viscosity, surface tension, diffusivity, solubility, and heats of formation — of the components and the reaction mixture as a function of reactor operating conditions;
- effective diffusivities of gases within solid pores;
- effective thermal conductivities of solids;
- axial and radial dispersion coefficients;
- interphase (or interzone) heat- and mass-transfer coefficients;
- wall heat-transfer coefficients;
- various hydrodynamic proper-

ties — like bubble size, bubble velocity, and bubble fraction in a BFB reactor and bubble columns, phase holdups in two- and three-phase reactors, voidage profiles in a CFB reactor; and

- all parameters in the design and control equations of the solids' circulation systems.

Parameters of the first category normally are readily available, except for solid components, from many of today's commercial simulation packages. These parameters can be automatically retrieved from these packages or in-house simulators, once the model is properly integrated. Correlations or approximate values for most of the other parameters are available in the open literature. The reliability of the estimates, however, varies depending upon both the parameter and the correlation used — and, thus, demands careful evaluation. Also, once the final model is developed, a parametric sensitivity analysis may be required to determine which of the above parameters need reevaluation to improve the model.

STEP 10 — DETERMINE MODEL STRUCTURE AND SOLUTION PROCEDURES.

This step involves: (a) planning the model structure and required subroutines, and (b) selecting numerical procedures to solve the model equations and to estimate model parameters.

The model structure should provide maximum flexibility for expansion and easy modification. It should accommodate additional details or features in successive stages as the model grows. It should be built on separate subroutines dedicated to one or more key elements of the model. Such elements include effective diffusivity of gases, catalyst effectiveness factors, interphase mass transfer, phase holdups, bed voidage profile, axial and radial dispersions, bubble properties, wall heat transfer, etc. As the model grows, each of these subroutines can be improved individually as needed without disturbing the rest. The structure also can be built on

subroutines that contain governing mass- and heat-balance (or performance equations) characterizing each distinct reactor type. All these separate equation packages can share the same numerical routines, as appropriate, to generate model solutions.

A variety of highly effective numerical-solution packages, which can be easily integrated into the model, are available today. For example, Refs. 14–16 describe specific mathematical routines in detail, along with their theory and areas of application. Selected routines from these and many other available software packages can be tried with the various equation sets of the model; the best selections then can be included in the model as subroutines. (For more information on software available, see the on-line *CEP Software Directory* at www.aiche.org/CEP/software/.)

Versatility, ease of use, fast convergence time, and freedom from solution errors are among the key selection criteria. These routines, however, only can provide local solutions. A global solution of highly nonlinear equations as encountered in reaction kinetics (an integral part of most reactor-performance equations) cannot be achieved through any of the available routines. A good initial guess or initialization of each of the model parameters, therefore, is always necessary for these applications.

STEP 11 — DEVELOP A PRELIMINARY MODEL.

Now, using the design and operating conditions from Step 3 and the preliminary reaction mechanism and rate expressions obtained from Step 4, develop a model based on the procedures and equations established in Steps 8–10. After satisfactory computer code is generated, the major task of this step is to determine a preliminary set of rate parameters. This is accomplished by first considering only the major reactions and products and using an initial set of representative data. Preliminary values of activation energies, reaction orders, and

adsorption constants from a literature search or approximations are used at this stage. Keeping these values constant, the pre-exponential factors of the reaction rates are found, usually via trial-and-error by comparing key observations like conversions of major reactants and selectivities of major products with model projections. The data should be taken at approximately the same temperature, so that the effects of other variables are not masked by that of temperature.

Next, using additional data reflecting the effect of temperature, get the best values of both pre-exponential factors and reaction activation energies with a parameter-estimation routine. These parameters, along with the reaction orders and adsorption constants, are fine-tuned in Step 13 to be discussed later.

STEP 12 — INCLUDE ADDITIONAL DETAILS FOR THE FINAL MODEL. These details, as determined in Step 7, should be introduced preferably in stages, so that each's impact on the results and relative importance are established. This stagewise approach also helps in a smoother model development, due to easier debugging of modified or extended program codes.

Only major reactions, reactants, and products were considered in the development of the preliminary model. At this step, therefore, all necessary minor reactions, reactants, and products need to be incorporated, and the preliminary reaction mechanism and rate expressions expanded, as necessary.

STEP 13 — DEVELOP THE FINAL MODEL BY TUNING PARAMETERS. Once all the necessary details are incorporated, you must tune the model parameters, primarily, the kinetic ones, because the preliminary model relied on only a few sets of representative data. In this step, use all available data — ideally, these should represent a wide variation in design and operating con-

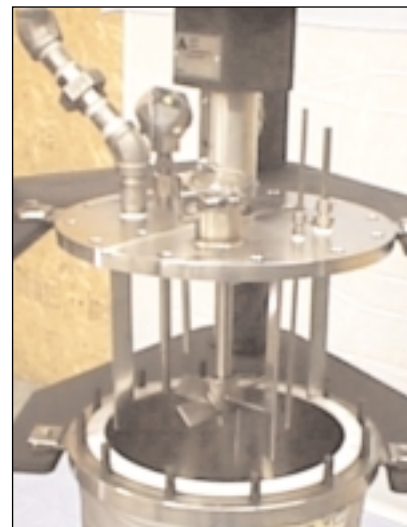


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ditions. Screen the entire data set for "bad" data, both qualitatively, via trend analyses by graphs and tabulations, and quantitatively, through parameter-estimation procedures. Eliminate data points that cannot be reproduced satisfactorily by these data reconciliation procedures.

It may be necessary at this step to carry out additional tests or experiments to fill gaps in the data and to verify observations that cannot be matched satisfactorily by a model. Additional data at this step also may be required to improve the reaction-mechanism and rate expressions. For complex systems involving many reactions, the effects of the concentration of each component of the reaction mixture on each reaction rate may need to be studied for a better estimation of the reaction orders or for better rate expressions. For a solid-catalyzed heterogeneous reaction, the impact of the concentration of each component or of pressure may have to be studied in more detail or over a wider range to satisfactorily determine the adsorption constants. Additional experiments, particularly on temperature effect, on one or more of the component reactions often are required to confirm reaction activation energies.

Now, use the parameter-estimation routine again to obtain the best possible estimates of all the rate parameters by comparing the model projections with key observations for the entire data set.

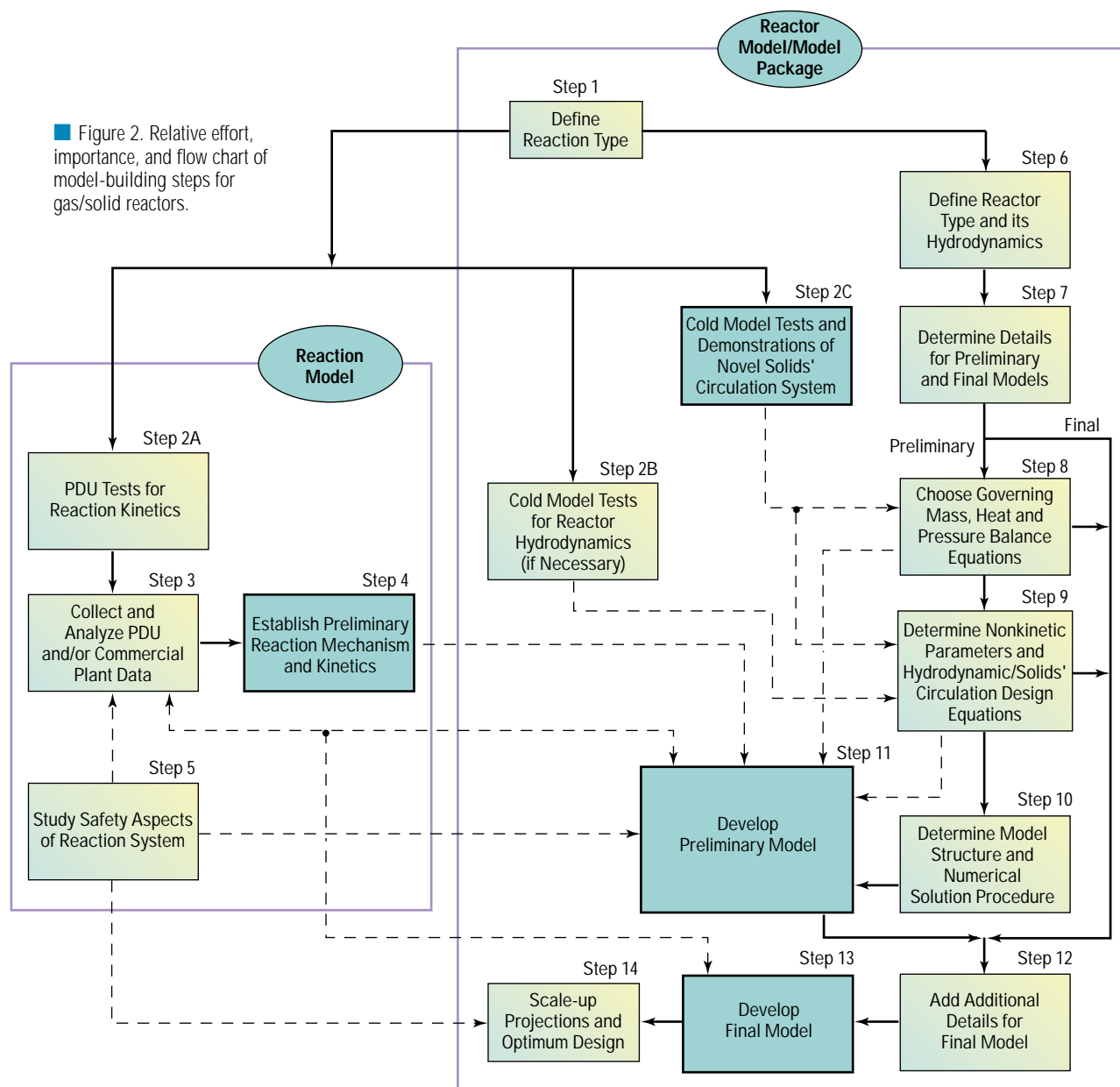


STEP 14 — MAKE SCALE-UP PROJECTIONS AND ESTABLISH THE OPTIMUM DESIGN. At this stage, consider a variety of possible combinations of design and operating variables within ranges deemed feasible from preliminary safety and mechanical considerations. Narrow down the ranges in successive projections by taking into account various other limitations, such as pressure drop, heat-transfer rate, and throughputs and holdups of various phases (gas, solid, and liquid) within the reactor. Then, evaluate the best design and operating conditions based on yield, productivity, and product quality on additional factors such as control and operational flexibilities, detailed safety and mechanical checks, and compatibility with upstream and downstream sections for an existing plant — and use economics to make the final selection.

Figure 2 shows a flow chart for the model-building steps and indicates the relative effort and importance of each of these steps. Bold solid lines highlight the major flow path, while dotted lines show the interactions between the steps. The relative effort typical of each step is depicted qualitatively by the size of each rectangle.

Reactor Modeling

■ Figure 2. Relative effort, importance, and flow chart of model-building steps for gas/solid reactors.



Deeper tints indicate the most critical steps. Step 2 is broken into three separate and parallel steps — 2A, 2B, and 2C, the latter two for hydrodynamic tests and solids' circulation-system tests and demonstration, if required. Step 2A and Steps 3–5 are unique to a new reaction system and are grouped as a reaction model block. All the remaining steps belong to a common block called a reactor model or model package — and, once developed for multiple-reactor configurations, can be shared by any new reaction system or for system revamp and modernization.

Building multiple-reactor models

A package must contain a multiplicity of reactor models if it is to determine the best configuration for plant revamp or modernization. Such a multiple-reactor model package also is necessary for developing a new reaction or catalyst system before launching major pilot-plant or new process-development campaigns. For any known reaction system or catalyst activity, the package should predict the performance of a given reactor configuration, as well as of a variety of alternative configurations.

The model must be applicable to any combination of reactions and reactor systems included in the package. It should identify optimum operating conditions to best meet a given demand from an existing reactor, and evaluate various possible new design options or modifications of an existing reactor.

For example, assuming the same catalyst activity for a catalytic gas/solid reaction system, a user can immediately determine the possible advantages of switching from an existing fixed-bed reactor to a fluidized-bed one as part of a revamp or modernization, or quickly



discriminate between a BFB and a CFB, if models for these reactor configurations are available. The package speeds quantitative comparisons of the performance and the advantages and disadvantages of various possible fixed-bed configurations, such as multitubular, multistage adiabatic quench, radial flow, or double-wall annular tubular, if such models also are included. Multistage feed injection, partial or total products recycle, and programmed temperature profiles are among the many options for minor design modifications that can be easily included in this model package, as well.

Figure 3 schematically shows how a multiple-reactor model package can help discriminate between alternative reactor concepts and decide on the best option(s) for any reaction system. This discrimination process, if carried out early in the scale-up or revamp efforts, leads you to the most competitive design promptly and avoids wasted efforts from trial and error in long experimental or pilot-plant campaigns.

To develop such a package for any given reaction system, repeat Steps 6–14, excluding Step 13, for all reactor types of possible interest. Use the kinetic parameters of the first reactor type determined in Step 13. Select the best reactor configurations for a new reaction or catalyst system by comparing the optimum designs and operating conditions determined in Step 14 for all the reactor types studied.

One of the biggest advantages of building such a model package is that, once developed, it is applicable to any other reaction or catalyst system involving the covered reactor types. At plants that include a variety of reaction systems and reactor configurations, the package can be an important asset for meeting the constant demands for reactor revamps and modernization. It also can be a valuable tool in utilizing existing reactors for new products and catalyst systems, when the demands for old products decline or an advanced catalyst formulation must be used for economic benefits.

Tips and traps

Collect adequate data on each of the four major variables. You must have a sufficient number of observations on the effect of each of the four major variables, namely, throughput(s), temperature, pressure, and feed composition. Insufficient observations on any one of these may lead to bias in the parameter estimation that will cause greater errors in model predictions.

Cover various combinations of variables. The test or experimental programs should be planned, if possible, in such a way as to provide data on a variety of variable combinations, including some extreme conditions, such as high temperature/low pressure, low temperature/high pressure, high temperature/high pressure, and low temperature/low pressure. More robust model parameters can be obtained through validation with such data.

Ensure ranges are adequate. A model is strictly applicable only to the ranges covered by the data upon which it is built. The wider the data coverage, therefore, the wider the applicability of the model. Thus, the data should cover an adequate range of each of the four major operating variables. The coverage should extend both below and above the expected operating conditions of the commercial reactor, so that the model, when needed, can satisfactorily predict off-specification and transient conditions.

Pay particular attention to the impact of temperature. Because of its exponential effect, temperature often is the most dominant variable for chemical reactions. Therefore, study the effect of temperature most thoroughly and systematically. It also is advisable to evaluate the impact of other variables at various temperature levels so as to gain an understanding of the entire possible operating domain of the reaction system. This also provides more data on temperature effect that are useful for a better estimation of the reaction acti-

vation energies and, thus, increased reliability of the model.

For most reactions, a good knowledge of reaction activation energies is essential to accurately predict reactor yields and product quality. This also is critical for the design and control of reactors with sharp temperature peaks, such as steam-cooled tubular fixed-bed reactors for exothermic reactions. These reactors, which normally have a very narrow operating window, are prone to temperature runaways without proper design and control.

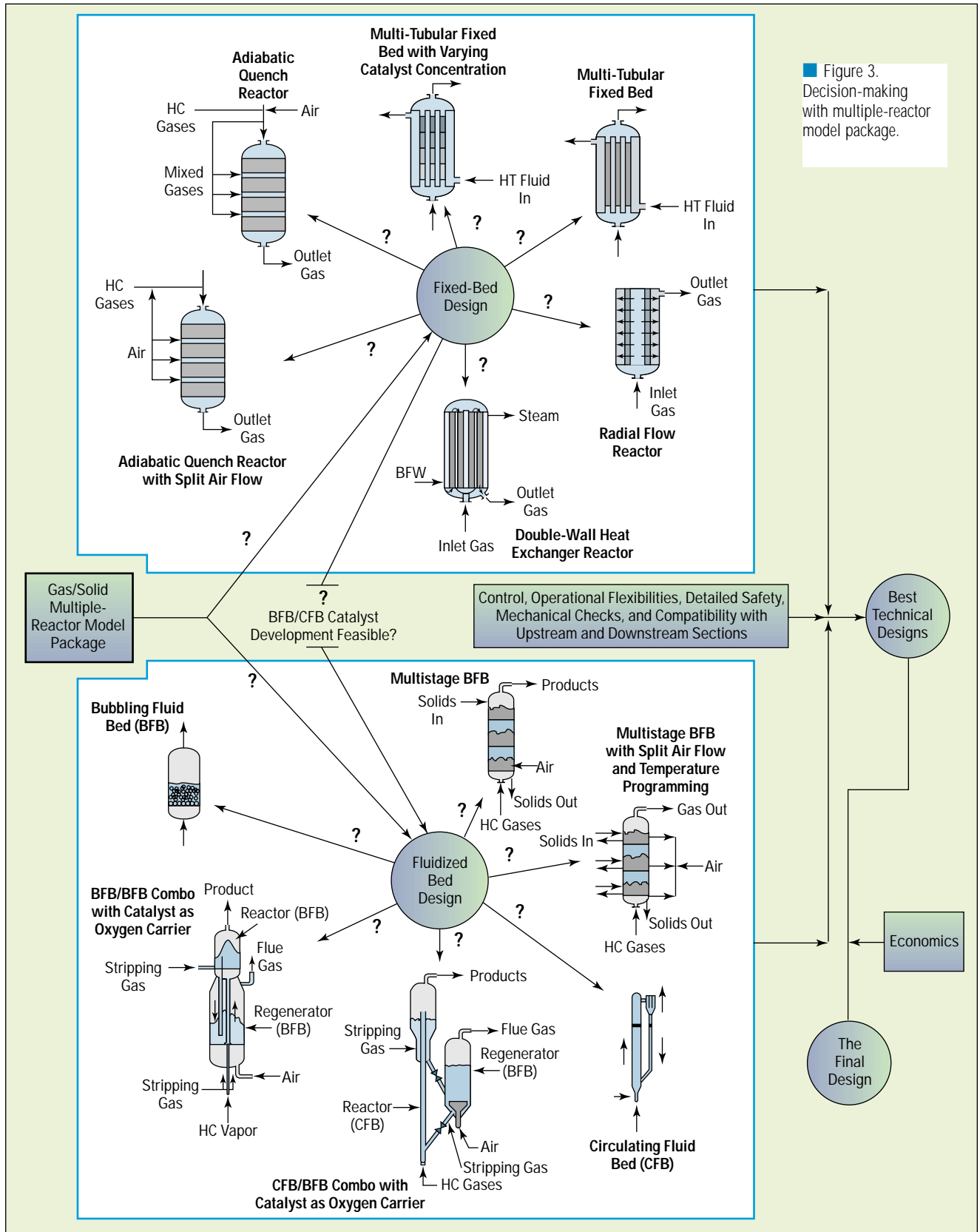
Assess the effect of residence time. This is important because, for many complex reactions, the final products are generated through intermediates formed early in the reaction.

An example is the liquid-phase oxidation of *p*-xylene to *p*-toluic acid in the commercial production of dimethyl terephthalate (DMT). The *p*-toluic acid is generated via two intermediates, *p*-toluol alcohol and *p*-toluol aldehyde, which are formed very early in the reactions. As time progresses, these intermediates get oxidized to the final product. Concentrations of these products in the reaction mixture, therefore, are very high early in the process, and negligible at the end. Data covering a wide range of reaction times starting from a very low value, thus, are necessary to reveal this fact and the true reaction mechanism for the process. Only a careful evaluation of the residence-time effect on this reaction system would disclose that the reaction products *p*-toluic acid and *p*-toluic ester accelerate the *p*-xylene oxidation. This rate-acceleration effect must be accounted for by the rate expressions of this reaction system.

Get rate data on each component reaction. As indicated earlier, such rate data should be collected, if possible, particularly to confirm the activation energy of that reaction.

Perfect the reaction model first. Reaction mechanism and kinetics generally are the most dominant fac-

Reactor Modeling





tors in determining reactor performance and design. (Exceptions, however, include systems involving novel or difficult solids' circulation systems, and some very fast reactions like combustion and gasification or instantaneous absorption with reaction in a liquid phase, where the chemical conversion rates essentially are diffusion controlled.) The following words of caution, therefore, are in order for building a robust model for most chemical reactors.

- Don't attempt to model a reactor before perfecting the reaction model. Otherwise, the reliability of the overall model invariably is questionable. Efforts spent on a reliable reaction model are always justified, because they save effort and trial-and-error downstream during design, scale-up, and operation of the reactor.

- Don't concentrate on reactor hydrodynamics. A great deal of effort often is focused on the study of reactor hydrodynamics like bubble properties in a BFB reactor, or cluster behaviors in a CFB reactor, while ignoring the importance of a reliable reaction model. A reactor model combines the reaction and hydrodynamic models of the reactor. We cannot overemphasize that, in most cases, an inadequate reaction model affects the reliability of the reactor model far more than an inadequate hydrodynamic model.

- Don't rush to extensive PDU and pilot-plant campaigns. With the exception of some systems as indicated above, place more emphasis on careful data collection and analysis to build a solid reaction model rather than on extensive PDU or pilot-plant campaigns.

Don't downplay the regeneration model in reactor-regenerator dual system. In such systems, such as a FCC, a solid catalyst typically is in continuous circulation between the reactor and the regenerator. The design and performance of each of these units, as well as the solids' circulation loop design and control, in-

timately depend upon both reaction and regeneration kinetics. So, the reaction model for each system must be developed with equal care. This is particularly true for some processes involving partial oxidation reactions, where the catalyst itself acts as the carrier for oxygen. Oxygen is fed in the regenerator to oxidize the catalyst, which then moves to the reactor to be reduced.

Adequately address the solids' circulation system. For reactor-regenerator dual systems, the inability to properly scale up and design the solids' circulation loop could be the worst bottleneck. The circulation lines connecting these two units must be sized and equipped with solids' flow control devices in such a way that the operational flexibility or limitations of solids' flow rate do not compromise the optimum operation of either the reactor or the regenerator. This may be particularly critical for a system, as cited above, where the catalyst itself has to act as an oxygen carrier for the reactor, and, thus, which demands an unusually high solids' circulation rate.

Don't use a too complex or too simple reaction model. An overly complex model is undesirable, because of the extra effort of handling such a system and the difficulty of parameter estimation. It also is unnecessary, as, for most practical applications, it won't improve performance much, if at all. An over-simplified model (such as one with pseudo-first order or zero-order kinetics or without some important intermediate reactions) also is unacceptable, as it is applicable to a limited range of operating conditions. For example, it does not apply at very low contact times, when primary intermediates may be at very high concentrations, or at very high contact times, when some components attain near-complete conversion.

Use alternative methods to check results. During model building and, particularly, during expansion from simpler to more advanced models, it

is advisable to check the model's results against those from alternative methods. Such methods may include spreadsheet calculations or analytical solutions of simplified kinetics. For example, the conversions predicted by an advanced model for a single reaction of first- or second-order kinetics of a fixed- or fluidized-bed reactor should be the same as those obtained from analytical solutions available in the literature for these systems. Such checks assure that, in spite of continued expansion and increasing complexity, the model can reproduce results for known simple systems.

Take extra care in defining reactor hydrodynamics. A model should be based as closely as possible on the actual hydrodynamics of the system. For example, a tubular reactor with high aspect (length to diameter, L/D) ratio, operating with a high fluid velocity, should be represented by a close-to-PFR model. An ADR model should represent the same reactor with internal baffles that create local turbulence and mixing. Misrepresentation of hydrodynamics leads to false models of limited application.

Don't make the hydrodynamic model too complex or too simple. The hydrodynamic model should not include, for example, local or micro-phenomenon that likely have negligible impact on the overall reactor behavior. For most practical applications, a very detailed hydrodynamic model may not contribute to an overall improvement of reactor model predictions. On the other hand, though, the hydrodynamic model should not ignore major phenomena occurring within the reactor volume. Thus, if there are distinct zones of totally different hydrodynamic behaviors (for example, PFR, mixed, dead zones, etc.), each occupying a significant reactor volume, the impact of each zone on the reactor performance needs to be evaluated.

Examine entrance and exit effects. Many reactor-design models are fo-

cused only on the main body of the reaction zone, for example, the packed-bed section of a fixed-bed reactor or the dense bed of a BFB reactor. Reactions may continue, however, beyond such sections into the plenums or free-board regions of these reactors, due to

gas-phase or dilute-phase reactions. For exothermic reactions, this may lead to temperature buildup in these regions, causing product degradation and, in extreme cases, possible explosion by temperature runaway. Be particularly careful about the mixing zone

and injection procedure for hydrocarbons and oxidants in the entrance section of partial oxidation reactors, due to explosion possibilities of the reaction mixture. Attention to entrance and exit effects also is very important in a CFB reactor, because the design of these sections may significantly affect the hydrodynamic behavior of the entire reactor.

In many cases, a significant fraction of the total conversion occurs very close to the reactor entrance. This conversion may depend to a large extent upon the design of the entrance region or fluid- or fluid/solid-distributor device at the entrance. The model, therefore,

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Nomenclature

a	= specific interfacial area based on dispersion volume
a^*	= constant = +1 for counter-current, -1 for co-current flow
a_w	= specific heat-transfer area
c_A, c_{AG}	= molar concentration of A, in gas, and in liquid, respectively
c_{AL}	= molar concentration of A in liquid in equilibrium with gas at gas/liquid interface
c^*_{AL}	= molar concentration of A in liquid phase
c_B	= molar concentration of B in liquid phase
c_{pL}	= specific heat capacity of liquid
D_a, D_{aG}	= axial dispersion coefficient of A, in gas, and liquid, respectively
D_{aL}	= axial dispersion coefficient of A, in liquid, respectively
E	= reaction activation energy
$-\Delta H_R$	= heat of reaction
k, k_2	= reaction rate constants
k_w	= wall heat-transfer coefficient
k_0	= reaction pre-exponential factor
K_L	= liquid-side mass-transfer coefficient
R	= gas constant
t	= reaction time
T	= reaction temperature
T_w	= wall temperature of heat-transfer surface
u, u_G	= linear velocity, of gas, and of liquid, respectively
u_L	= liquid velocity
z	= axial coordinate

Greek letters

ϵ_G, ϵ_L	= gas- and liquid-phase holdups
λ_{eff}	= effective thermal conductivity of liquid
ρ_L	= liquid density
ν	= reaction stoichiometric coefficient



should account for this phenomenon.

Include sufficient flexibility in the test unit. The design of the PDU or the final model-validation or demonstration unit should allow test runs to be carried out over a wide range of operating conditions, as discussed earlier.

Consider alternative designs early on. In developing new technology or modernizing a plant, use the package to assess alternative reactor concepts before a particular reactor type is selected. Typically, industry has chosen a reactor type or design option without a quantitative evaluation of alternative concepts. This often leads to an inferior choice or wasted efforts in following a wrong development path.

Don't attempt a dynamic model before perfecting the steady-state model. The availability of various commercial process simulators and control and optimization tools has led to a tendency in industry to rush to build dynamic reactor models. It often is not realized, however, that a dynamic model is of little value until a robust steady-state model for the same system has been perfected. A dynamic reactor model is meant to predict the transient behavior during startups, shutdowns, or emergencies, when operating conditions may be far from those of the normal operation at steady state. But, before such predictions can be realistically attempted, the model first must successfully forecast the behavior at steady state at various operating conditions. Many commercial reactor models built only to apply around the steady-state operations in the plant, therefore, are totally inappropriate for dynamic model development. These dynamic models would fail to predict reactor behavior at startups, shutdowns, and in emergencies, when the reactors operate far from design or normal conditions.

A proven approach

We know these steps and our recommendations work, because we have used them to develop a general modeling package that has proven it-

self for reaction and reactor systems of various kinds in the real world. The currently available package applies to both catalytic and noncatalytic gas/solid reactions of just about any complexity and kinetics, and reactor systems of virtually any type, including those with a fixed bed, fluidized bed (bubbling, turbulent, circulating, or entrained), or moving bed, singly or in combination. The model currently is being extended to include liquid-phase reactions.

The package handles many design modifications like product recycle, multiple-feed injections, multistaging, and temperature programming, as well as various design options for each reactor type. It includes all necessary correlations and methodologies for heat- and mass-transfer, and hydrodynamic calculations, performance equations for each reactor configuration, and a parameter-estimation routine. Customizing and incorporating additional correlations, design features, and phenomena is easy.

Details on the development and application of this package are provided elsewhere (5, 17–26). The four most-recent publications (17, 24–26), in particular, provide background on the use of the package, and a summary of its features and applications.

With this package, it is possible to extract kinetic and other parameters from data obtained from virtually any type of reactor and scale of operation — given a suitably wide range of operating conditions. It is not necessary that such data be generated exclusively in idealized reactors, like integral or differential as in conventional practice. Such reactors, however, may be needed to provide supplementary data for improved parameters.

An early version was a key to the successful scale-up of world's first fluidized-bed catalytic process (the ALMA process) for production of maleic anhydride from *n*-butane — directly from bench to commercial scale without going through a pilot plant. The model has been the basis

for successful development of another fixed-bed catalytic process planned for commercialization next year.

The package also has been used to screen alternative reactor-design concepts for a variety of other commercial reaction systems, including propylene to acrylonitrile, naphthalene to phthalic anhydride, oxidative coupling or methane, hot-gas desulfurization by zinc titanate, and partial oxidation of paraffins. It has served to simulate lab, pilot-plant, and commercial data for a wide range of other reaction and reactor systems, such as FCC catalyst regeneration in a CFB reactor, FCC riser, methanol synthesis, ammonia synthesis in multistage adiabatic quench reactor, and hydrocracking/isomerization of naphtha (an example of an application for nonstoichiometric reactions of refineries).

Use of such a model package should substantially reduce the model/model-package building effort for most new and existing reaction and reactor systems. CEP

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