

# THE STATE OF THE ART IN REACTION ENGINEERING

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## *Summary*

A survey of textbooks on reaction engineering and on transport reveals the presence of many obsolete concepts and the absence of a number of important advances. Chemical engineers are apt to cling, throughout their careers, to the concepts they acquire in school. Hence it is essential that such shortcomings be identified and corrected by their teachers. The simplest and perhaps most effective corrective is the regular distribution of electronic supplements by the teacher or the book-writer.

## *Keywords*

Reaction Path Analysis, Process intensification, Complex reacting flows, Deployable software and databases for reaction engineering,

## **Introduction**

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For many decades chemical engineering, including separations, was limited to physical processes, but once reaction engineering emerged it rapidly became one of the key elements and glories of the profession. Experimental, theoretical, and computational advances have continued apace with those in other aspects of processing, but progress in education and practice have begun to falter because of the persistence of obsolete concepts and the associated neglect of new ones. In all arts, sciences, and technologies the practitioners, including teachers, are prone to resist change and to cling to familiar concepts long after they have become outworn or superseded, but that does not excuse such practices in reaction engineering.

The depth of understanding of reactive processes is comparable to that of non-reactive processes such as fluid flow, heat transfer, and mass transfer, but the execution of experimental measurements is more difficult, and the formulation and numerical solution of mathematical models are greater challenges because of the inclusion of reaction-rate expressions in the equations of conservation for atoms and energy, as well as because of the coupling of the latter with those for momentum. The greater complexity and greater number of variables has also

impeded the development of generalized correlative and predictive expressions.

A number of obsolete concepts are to be found in the textbooks and computer packages on reaction engineering, and thereby infect industrial practice. Some are a carry-over from physical chemistry, and in particular from the expression of reaction-kinetics and Lagrangian terms, but most are a consequence of idealizations made in order to obtain closed-form solutions.

The objective of this presentation is to identify some of the avoidable and unavoidable complexities, some of the explicit and implicit idealizations, and some of the advances that permit discarding obsolete concepts and models. In the interests of brevity, attention is focused primarily on homogeneous chemical conversions in tubular flow. Students graduating in chemical engineering are apt to cling, throughout their careers, to the simplifying concepts and idealizations in their textbooks. Hence it is essential that their shortcomings as well as their merit be identified by teachers and experienced practitioners.

### **Idealizations utilized in transport**

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Common idealizations in the textbooks for fluid flow, heat transfer, and mass transfer in tubes include full development, time-averaging, invariant physical properties, the boundary layer concept, the log-mean temperature difference, a uniform heat flux density or a uniform temperature at the wall, the expression of rate data in terms of transfer coefficients, mixed-means, correlating equations in the form of products of powers, analogies between momentum and energy transfer and between heat and mass transfer, eddy diffusion, mixing lengths, the  $k$ - $\epsilon$  model, direct numerical simulation, and large-eddy simulation. Advances that have not yet appeared in most textbooks include predictive expressions based on the power-mean of asymptotes, the use of the fraction of transport due to turbulence as a variable, greatly improved experimental data for turbulent flow, essentially exact analogies, and predictive expressions for the enhancement of heat and mass transfer coefficients by energetic reactions.

## **Idealizations utilized in reaction engineering**

The illustrative idealizations to be discussed herein for reacting systems include most of those for flow, heat transfer, and mass transfer, but in addition include plug flow, space-velocity, space-time, the expression of rate mechanisms in terms of concentrations, global kinetic models, the pseudo-stationary-state hypothesis, fully developed reaction, and invariant physical properties. Often-neglected items to be discussed include stiffness, the use of sensitivity analyses, the use of computer packages to solve atomic balances, and the use of heat transfer to control the temperature of gas-phase reactions.

## **Conclusions and recommendations**

The primary conclusion from this analysis of the state of the art in reaction engineering is that many textbooks, despite their overall merits, propagate obsolete concepts and, perhaps understandably, fail to include important recent advances. The primary recommendation is that teachers should regularly prepare and distribute electronic supplements that correct and up-date the textbook(s) that they assign. Because this analysis is illustrative rather than comprehensive, it is proposed that those with expertise in particular aspects of reaction engineering should extend it.