# Three Phases of Chemical Reaction Engineering
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## Abstract

Chemical Reaction Engineering has evolved in the last century, and can be divided into three phases. The first phase of Empirical Craft is exemplified by textbooks of descriptive industrial chemistry for different industries, to codify decades of empirical experiences. When the influence of unit operations began to be felt, a series of textbooks in chemical reaction engineering emerged in the second Science-Based phase, and written to be much more useful for process improvements and innovations, as well as for operations. Complex kinetics and reactor problems had to be simplified so that they can be solved by analytical and graphical methods. When computers became more powerful and available, much more complex and realistic aspects can be considered, which led to the third Computer-Based phase of textbooks. The dominance of Commodity chemicals has to make way for newer Specialty industries that have smaller volumes and shorter product life cycles, which pose new challenges to reaction engineers.

Chemical Reaction Engineering has gone through many phases, which is reflected in the dominant textbooks of that phase. The construction and operation of chemical reactors are as old as the first hearth for heat and light, and the first fermenter to make beer and wine, which developed over the ages and improved over generations. The development of modern chemical reactors were accelerated by the large scale production of chemicals such as the LeBlanc process for making soda ash in 1791, the introduction of nitroglycerin by Sobrero in 1846, and the invention of synthetic dye by Perkin in 1856. Books are needed to instruct a newcomer how to design and build appropriate chemical reactors, and how to operate them successfully. For an author to master the most interesting and proprietor aspects of an industry and the reactors, it would be necessary to have the insider knowledge of an employee, or a regular consultant and collaborator. It is more manageable when a chief editor brings a team of experts from different industries to produce a book.

## Phase I. Empirical Craft: Descriptive Industrial Chemistry

In this early phase that began before the founding of the AIChE in 1908, the textbooks described the successful industrial technologies which were evolved over several generations of development and empiricism. Some of the leading textbooks of this genre and their descendants were:

1898 F. H. Thorpe, "Outline of Industrial Chemistry"
1928 E. R. Riegel, "Industrial Chemistry"

1935 P. H. Groggins, "Unit Processes in Organic Synthesis"
1945 R. N. Shreve, "Chemical Process Industries"

These books mainly tell you how things are done, without elaborations on scientific explanation on why they are done this way, and why other ways would not work. The starting point may be a verbal or a drawn flowchart of the various streams in the manufacturing of a product such as sulfuric acid, which contains reactors among various auxiliary equipments. There is description of the raw material sources and feedstock preparation, the operating conditions such as temperature, pressure, and residence time, the product distribution from the reactor, and finally the market for the product.

If you are entering employment in a sulfuric acid plant, this type of book can serve as orientation of the establishment that you have joined. However this book is short on the factors that compel you to design and operate the reactor this way, and how you may make contributions by taking incremental improvements in efficiency and yield, to say nothing of radical breakthroughs in innovations. If you are an engineer at a developing nation who has just received an order to build a sulfuric acid plant, this book can suggest ideas on what to do as a start, but without the details necessary to design, build and operate an efficient plant. What can this book do for students of chemical engineers who are planning to work for another branch of the chemical industry, such as petroleum refining? Can the lessons learned here be applied to manufacture other products under current production, or brand new discoveries and inventions. This mode of teaching is appropriate in a static environment when you are asked to do the same thing as your predecessors in the same way, but it suffers in a dynamic environment as it cannot be easily generalized to a different or a new industry. It does not provide you with knowledge and skills that are generally useful in many other applications, and to deal with dynamic new developments.

Progress was very slow in this period. It took many pioneers over the course of many decades to consolidate these isolated cottage technologies into the learned discipline of reaction engineering, which is a paradigm of recognized and systematic body of knowledge in the university curriculum, accredited by professional societies, recognized topics of research, presented in learned society meetings, and published in archival journals.

## Phase II. Science-based Reaction Engineering: petroleum and petrochemicals

The coming of Unit Operations made a profound change in the way our profession looked at research and teaching as sources of innovation and improvement in chemical engineering. This paradigm shift looked for common threads among various branches of the chemical industries for knowledge that are generally useful, and led to Unit Operations in the book "Principles of Chemical Engineering" by Walker-Lewis-McAdams in 1923. The subjects of inquiry were no longer the individual industries, but were the principal physical operations that take place in all chemical plants, such as pumping fluids, heating and cooling, distillation and absorption. Once the design and operation of individual equipments are understood, any chemical plant can be designed as an orderly synthesis of well understood constellation of parts. However this revolution has left out a most important component - the chemical reactor which is the heart of making useful things.

We see in the next generation textbooks in reaction engineering, which adopted the same unifying approach, and were organized around different types of kinetics and reactors, instead of around different industries:
1947 O. Hougen and K. Watson, "Chemical Process Principles, part 3, Kinetics and Catalysis"
1956 J. M. Smith, "Chemical Engineering Kinetics"
1962 O. Levenspiel, "Chemical Reaction Engineering"
1963 H. Kramers and K. R. Westerterp, "Elements of Chemical Reactor Design and Operation"
1966 K. Denbigh, "Chemical Reactor Theory"
The topics in Hougen and Watson started with individual and networks of chemical reaction kinetics, with considerations of reaction order and Arrhenius relations to temperature, and of thermodynamics and equilibrium. Two chapters have the titles of "Mass and Heat Transfer in Catalytic Beds" and "Catalytic Reactor Design". We find here concepts that have become staples: the Thiele modulus of diffusion in catalyst pellets, longitudinal diffusion in flow reactors, graphical calculation of reactor sizes, pressure drops in granular beds, and optimum reaction temperatures.

The most dynamic industries at that period in rapid development and growth were petroleum refining and petrochemicals, where catalytic reactions held the center place, so that most of the classic examples and homework problems were taken from that industry. This is not surprising since many leading professors were also consultants to these companies, drawn by the challenge of unsolved and important problems of feasibility, efficiency, scale-up, and safety. The commodity chemical industries have good problems for chemical engineers to solve, as the scales are enormous so that even one percent improvement in efficiency and yield would mean millions of dollars, and the product cycles are long enough so that process improvements are worth doing. In this phase, chemical reaction engineers concentrated in analyzing critical steps, in quantitative problems of optimal design and operation, and of stability, which can be solved by analytical methods, approximation methods, and simple graphic methods. Chemical engineers have also developed a number of textbooks in applied mathematics to solve their more complex problems:
1923 Hitchcock and Robinson "Differential Equations in Applied Chemistry"
1939 T. K. Sherwood and C. E. Reed "Applied Mathematics in Chemical Engineering"
1947 W. R. Marshall and R. L. Pigford "The Application of Differential Equations to Chemical Engineering Problems"
1962 L. Lapidus "Digital Computation for Chemical Engineers"
1966 N. R. Amundson "Mathematical Methods in Chemical Engineering: Matrices and Their Applications"
The first nine chapters of Sherwood and Reed are about treatment of data, mathematical formulation of physical problems, and analytical solutions to ordinary and partial differential equations. When the problem is too non-linear or too complex, so that

analytical solutions are not available, chapter 10 is devoted to numerical solution of partial differential equations. This is a very slow and tedious process by slide rules or hand calculators, and will be taken up by reaction engineers only if the problem is very important and cannot be done any other way.

This method of teaching gives the students the knowledge and skill to enter any industry where a chemical reactor is employed, to understand how it works and to consider improvements in operations, and to consider design improvements for the more ambitious. When a new product is introduced without any previous history of manufacture, the chemical engineer has the knowledge and tools to consider what successful types of reactors are available, what are their characteristics as well as pros and cons, and how to go about doing small scale pilot plant experiments to test feasibility and stability.

## III. Computer-Based Reaction Engineering: Bio, Environmental, etc.

Many of the most skilled masters in reaction engineering relish their ability to provide analytical solutions to important industrial problems, and would look down with scorn on problems that are solved by numerical methods, such as Runge-Kutta for differential equations with highly non-linear terms. There is the intellectual pride of greater knowledge and skill needed to do analysis, in comparison with the more routine application and drudgery of numerical methods. There is also the consideration that with an analytical solution, an impartial referee can easily confirm the accuracy of the results. When the solution is in the form of an equation, an engineer can answer what-if questions such as predicting the effects of changing parameter values, even extrapolations to infinity. However with a numerical solution, a referee can check the accuracy of the results only by repeating the computation, there is little intellectual beauty to boast, and each what-if question requires a new calculation.

Should the chemical reaction engineers stay exclusively with elegant and simple kinetics and reactor problems, or should they boldly tackle the most messy and complex problems important to the industry and to the nation? It is very well that complex first-order kinetic systems under isothermal conditions can be solved analytically by the matrix method, so the heart of the mystery is laid bare. The catalytic reforming reaction in petroleum refining is approximate a system of first order reaction, which works very well under isothermal conditions. The concept of lumping also reduces complexity to the point of being manageable, but at the cost of some lost of detail - similar to data compression in images in digital cameras and sounds in iPods. But an adiabatic reforming tower has a different temperature at each bed elevation, so that a different kinetic matrix would have to be used together with changing eigenvectors and eigenvalues. But the even more important catalytic cracking is carried out as many non-linear reactions, so one can either pretend that it is (any short line is a straight line) and treat it analytically, or admit that it is not and use numerical computational methods. As long as computers were slow and expensive, an investigator has the choice of doing an approximate solution or grudgingly taking on the slow computation task of a more full fledged model. When the path is long and arduous, there is always the possibility that a computation error crept in somewhere, and the results are not accurate.

There is no mistake that using computational methods is regarded as a cop-out for a proud analyst, but I suspect that if you can do computation with Roman numerals, you will look down on people who do computation with Arabic numerals. In 1962 when I was a visiting professor at Princeton, Leon Lapidus was pioneering in using the computer, but I stuck to the high road of analysis for many more years. Half a century later, it is clear that he represented the future, and I joined his team. So a new slate of textbooks of chemical reaction engineering arrived, assuming that the students already know how to do numerical methods on a computer, or can learn it soon, and proceed to deal with much more complex and realistic problems:
1986 H. S. Fogler "Elements of Chemical Reaction Engineering"
The latest edition of this book comes with a CD-ROM in the back, which contains computer software which can be used by the students to compute a number of reactor problems which are too complex to be solved analytically.
1998 L. D. Schmidt "The Engineering of Chemical Reactors"
This book takes an additional tack by considering problems from the bio-reactors, environmental modeling, combustion, and polymerization. While there is a wealth of problems from petroleum refining and petrochemicals to explain, a similar set of meaty problems in these newer industries need to be compiled by a team of writers, each has to acquire deep expertise in an industry, after years of research, practice or consulting. This is too much to expect from a single author. Perhaps a group of experts in different industries should get together to write such a textbook.

Together with the arrival of Computation Chemistry, we have the companion Computation Chemical Engineering. The current crop of reaction engineers have no excuse to deal only with simply reactor problems that can be solved by analytical methods, as they can pile on complex systems and non-linear phenomena and still expect answers. But the price paid is also significant when you want to check the accuracy of their results, to examine the effects of changes in parameter values, and to generalize to other situations.

## Future Challenges

We the chemical reaction engineers should be prepared to solve the problems of the future, instead of refighting the problems of the past. What problems would we encounter in the future? We think about the future either as gradual extrapolations of current trends in society needs and technology capabilities, as well as revolutionary leaps in either. In the 1950, the emphasis was in industrial inorganic chemistry, such as making sulfuric acid and salt. The emphasis has changed to oil refining and petrochemicals, and now to biomedical engineering, electronic processing, novel materials, and environment. In the last few turbulent years, of energy and food shortage, and of global environmental concerns, the future growth appears to be in two scales:
Commodities: petroleum, new energy sources, sustainability

Specialties: bio-processing, biomedical, electronics, advanced material
The scales in tons per year in many of the Specialty industries are much smaller by orders of magnitude than in the Commodity industries, and the products are in much earlier phases of the product cycle. The Specialty industries are more in need of product engineers who can make high speed development to put novel products to the market place, than in need for incremental improvement of mature products. There would be fewer classical products and processes that last many years, and more quick processions of products and processes. This requires an adaption of chemical reaction engineering abilities and skills in ways that remain to be worked out.

This generation of reaction engineers will have more knowledge and tool available in their practice than previous generations. They will have many new challenges, as the needs of society keeps on evolving, and I wish them success and glory.