Lewis Award Paper: Some Perspectives on Chemical Engineering Analysis

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DOI 10.1002/aic.12796
Published online November 3, 2011 in Wiley Online Library (wileyonlinelibrary.com).

Personal teaching experiences are discussed using an analysis logic diagram which stresses experimental efforts and the need to make students aware of uncertainties in any significant problems they will face. The critical issues are illustrated using a reactor analysis which has been made into an interactive design game for the Web. The analysis logic is also briefly illustrated for mass contactor and heat exchanger analysis. © 2011 American Institute of Chemical Engineers *AIChE J,* 58: 2634–2638, 2012
Keywords: analysis logic, reactor analysis, mass contactor analysis, heat exchanger analysis

Introduction

Stanley I. Sandler, the then *AIChE Journal* Editor, invited me at the time to write an article on my work ''so that the readership can understand the reason you have received the Warren K Lewis Award, which recognizes distinguished and continuing contributions to chemical engineering education, what the Institute values, and how our profession continues to evolve.''

I shall attempt to meet Stan's request based on my experience of several decades of teaching chemical engineers in the university and outside the academic environment in various continuing education programs. My experience has greatly benefited from collaborations with others, and I will acknowledge their contributions in the article that follows.

Chemical Engineering Analysis

The chemical engineering profession has been successful because it is able to combine experiment and modeling to quantitatively understand complex technical issues. Our educational programs build upon the basic sciences of chemistry, physics, mathematics, and more recently biology to educate students capable of identifying and solving problems essential to society's wellbeing. The logical steps to do this are presented in Figure 1.[1,2]

Ours is a profession greatly dependent on experiment, some of which we do ourselves and some of which are carried out by others. Most situations requiring analysis by chemical engineers are complex and to understand them effectively requires that we use a shorthand description to describe them. We make use of mathematical models to do this. If we are careful as educators, we can teach students how to obtain the model of any physical situation by applying the laws of conservation of mass, energy, and momentum. In addition to using these laws of physics, we need a secondary source of relationships, such as kC_A, $Ua(T_1 - T_2)$, and $K_m(C_A^I - MC_A^{II})$. These are commonly known as constitutive relationships. Careful and clever experimentation is required to develop them. They must be verified by experiment. To do this, the model behavior must be determined. There are many ways to do this depending on the complexity of the model equations. Simple models can be solved analytically using algebra, or differential and integral calculus. More complex models may require numerical methods, fast computers, and the use of the extensive software now available. This essential step, however, is not the most critical part of the analysis process although it can be the most tedious.

Most mathematical descriptions are a compromise between the complexity required by including in every detail and the simplicity needed so comparison with experiment can be carried out effectively. This is not trivial and the problem objectives, time constraints, and uncertainty must be considered in reaching this balance. What constitutes agreement with the model depends upon these three issues, and they cannot be easily quantified. Nevertheless, a decision must be made as to proceed to use the model to design a set of new experiments or a piece of process equipment, or to return to the physical situation and modify the model. The ability to do this effectively defines an engineer. It is not easy to teach this and as a result, many professors prefer to concentrate on model behavior as there are definite rules and few ambiguities.

A properly verified model can then be used for the analysis of existing systems, the design of new processes, or the design of a set of experiments. This is important not only for traditional chemical engineering but is essential if we are to quantitatively understand how the chemical plant inside the cell functions. In a traditional chemical processing unit chemical reactions to make product direct how the rest of any process should be designed, operated, and controlled. In the cell we are faced with a difficult measurement and analysis problem. We must quantitatively identify what is possible and feasible to measure and then determine how the organelle ''reactors'' in the cell affect its performance. Since we have played no role in designing the cell this analysis problem is extremely

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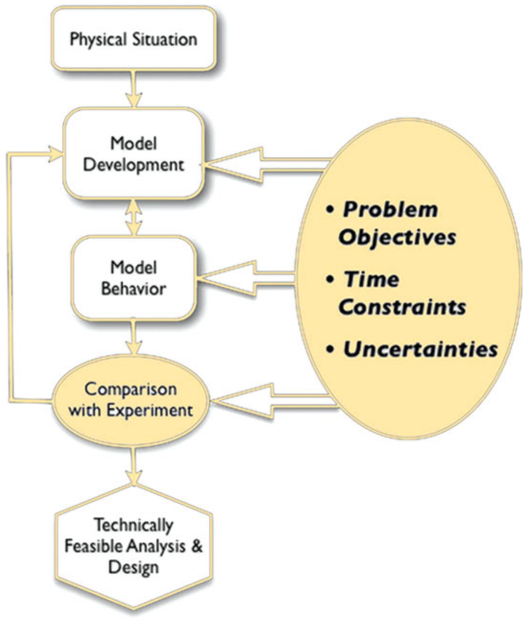

Figure 1. Chemical Engineering Analysis.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

complex compared with the analysis of a traditional chemical processing unit. We need to modify our curriculum to prepare students to meet these new challenges. Some of my thoughts on how we can do this are as follows.

Chemical Reaction and Reactor Analysis

The reaction and reactor analysis course which now is taught in most curriculum best illustrates the steps from experiment to process design and operation and provides a tested methodology that can be applied effectively to the different types of problems beyond our traditional ones in which chemical engineers are successfully making significant contributions. The chemical engineering analysis illustrated in Figure 1 can be applied to any situation.

If one considers single phase reactors and simple kinetics, a reactor analysis can be used to illustrate the critical elements of analysis in the first course that students take. We have done this for several decades in our program at the University of Delaware, several continuing education courses with practicing engineers and courses taught to nonmajors (chemists, other engineers, and even some secondary education math majors). I know these works because I am careful to observe the student response when I am in front of the class; this is a far better way to judge teaching effectiveness than asking students to fill out survey forms on the web usually long after they have been taught the material. We keep our maximum class size between 30 and 40 students so the in-class feedback can be effective. Our aim is to convince students that a model is essential if one is to thoroughly understand any physical situation. Morton Denn and I spent several years teaching the first course that Delaware students take. We each taught a section of the class at the same time. The material was coordinated on a lecture-to-lecture basis, and its impact on the students was evaluated after each lecture and again after each major topic had been covered. This resulted in our text "Introduction to Chemical Engineering Analysis"[1] and a paper "Introduction to CHE Analysis" published in Chemical Engineering Education.[3]

If one ignores time constraints and uncertainties, it is relatively easy to teach analysis using the simple reaction example. One can, of course, solve much more complicated problems but this example serves to illustrate concept without mathematical complexity. The critical educational challenge is to get students to deal with uncertainty at an early stage in their education. My concern with this has been influenced by my process design experience at Union Carbide Canada and many years consulting with a number of firms. I am particularly grateful for my 30-year consultation with the Engineering Department of the DuPont Company. All practicing engineers must cope with uncertainty, which can arise from many sources: time constraints that limit the amount of experimentation which can be carried out, errors in the market predictions, poor knowledge of the competition's production capacity, inadequate product specifications, to name just a few.

Students come into the university believing that there is a firm unambiguous answer to all problems. Unfortunately, some of them leave with the same impression because we educators tend to stress model behavior over the more critical parts of analysis.

To solve this problem, we designed a computer game and played it with over 2000 participants in the early 1970s. This was described in a paper in Chemical Engineering Education.[4] We have recently updated this effort and developed it into an online review and game, which can be played by one, two, three, or four players. The game requires the participant to develop the algebraic model equations for a simple CFSTR reactor and then operate it for five periods in competition with three firms. Predicted sales and selling price for the firms producing the product, which we have designated as D are supplied (demand curve). Laboratory data is supplied and must be modeled and a numerical value for the reaction rate constant obtained from concentration, time data. The program contains time limits for completion of each task. A penalty is imposed if the time limits are exceeded. After each operating period, a report is issued for each firm stating their market share, profit or loss, and unsold product. The winner is the person or team with the highest profit at the end of the fifth period. The website can be accessed at http://www.mht.che.udel.edu/static/activities.html and should be accessed for a complete understanding. There are two sets of activities in the site heading: one is marked "Graded Activities" and is for student use when grades need to be assigned, the one in the URL provided does not require one to proceed step by step and allows for more experiment with no grade penalty.

It is much more effective to go to the website than to have me continue with a prose description. The game has turned out to a very effective way to introduce students to uncertainty as they do not know what reactor size and flow rate the competing firms are using. This game, although simplified, is based on a real process and was developed with assistance from industrial business people.

This teaching tool for undergraduates led to a senior student thesis, a master's level research, and a PhD thesis. The papers resulting from this activity[5–7] show that the theory developed closely tracks the actual development of a product produced by Union Carbide and Dow Chemical.[7] Another one of these papers[5] has been used by a firm to help develop new businesses. The game experience also helped motivate me to join with J. Wei to coauthor a text: *The Structure of The Chemical Processing Industries*.[8] This text uses the

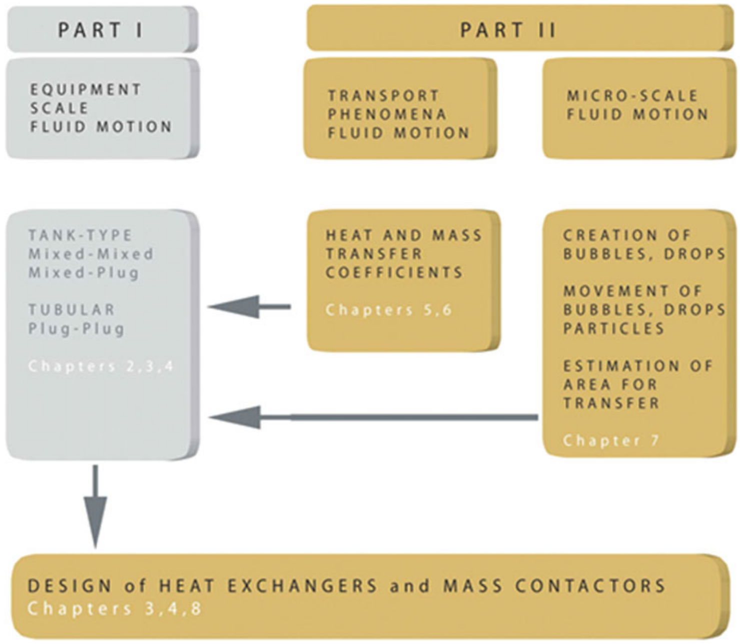

Figure 2. Organization of transport phenomena.

Reproduced from Ref. 2, with permission from Cambridge University Press. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

game concept to illustrate the need for microeconomic analysis in process design.

The chemical engineering analysis illustrated in Figure 1 can form the basis for the teaching of other courses in the curriculum since experiment and its analysis is such a critical part of our profession. Discussing material by stressing experiment also makes any subject more interesting to students and they better learn how to rationally use models. Robinson, Wagner, and I along with several of our teaching fellows have experimented with the approach for several years in teaching our transport phenomena course in heat and mass transfer and are convinced that it is effective and allows for more flexibility in covering the material. This is a critical issue since our educational programs must recognize that both chemical and biomolecular issues are becoming increasingly important. The profession must allow for the inclusion of new material without adding to the total credit hours for a degree.

Mass and Heat Transfer

Our course in heat and mass transfer reorganized as shown in Figure 2, reproduced with permission from "Mass and Heat Transfer—Analysis of Mass Contactors and Heat Exchangers."[2]

Traditional transport phenomena courses start in Part II as shown on Figure 2 under the heading "Transport Phenomena Fluid Motions" and concentrate on derivations of the equations of change with time and three spatial dimensions as the independent variables for the model equations. There is value in this approach since it can introduce the key constitutive equations commonly known as Fouriers Law, Ficks Law, and the relationship defining viscosity (Newtonian Fluid). Cussler[9] does present a particularly clear discussion of Fick's experiment but the experimental efforts, which produced the other relations are almost never discussed. The major issue I have observed in several ABET visits and examining these courses in other situations is that most of the class time is taken up with heat transfer in solids and laminar flowing liquids for which model behavior can be determined analytically, thus little time is left to devote to significant mass transfer problems which along with reactor analysis helps to define chemical engineering.

An approach to teaching this material which builds upon the success our profession has achieved with reaction and reactor analysis has proven to be a better and more flexible way to teach the transport phenomena. This is shown as in Figure 2 as Part I, Equipment Scale Fluid Motion. This is where we begin our teaching. The key elements of this can be illustrated with the model equations for a batch liquid phase chemical reactor, a batch liquid phase heat exchanger, and a batch liquid-liquid mass contactor. The fluids in all the pieces of equipment are assumed to be well mixed, a condition that can almost always be achieved with careful design of the mixing devices. The nature of the information one can obtain experimentally requires equipment in which we have simple fluid motions. This allows us to illustrate important basic concepts, which do not require two or three spatial dimensions in complex model equations. An analysis of the terms and what experiments are required is an effective way to introduce students to the critical role of experiment and the difficulties one faces in carrying out meaningful experiments.

A batch experiment for the reaction A→D requires that we know the chemical equations and that we can measure concentrations. C_A and or C_D as a function of time, verify that the rate expression, kC_A fits the data and k can be determined. The model equations shown below illustrate the process with the simplest possible mathematics:

$$\frac{dC_A}{dt} = -kC_A$$

$$\frac{dC_D}{dt} = kC_A$$

Once this analysis has been completed, one can design a pilot or commercial scale reactor by developing the model equations for a well stirred vessel or a tubular reactor, assuming a well mixed fluid or plug flow. This process has been successful in many commercial applications in the chemical and biochemical process industries. We have illustrated the steps in our website, which can be accessed at http://www.mht.che.udel.edu/static/intro.html.

The batch heat exchanger experiment requires an analysis using two control volumes one for the material being heated or cooled and one for the jacket (or coil) which contains the utility fluid. This can be demonstrated in the classroom with simple laboratory scale equipment using a temperature controlled bath to heat a container of water. The model equations for this are:

$$V_1\rho_1 C_{p1}\frac{dT_1}{dt} = -Ua(T_1 - T_2)$$

$$V_2\rho_2 C_{p2}\frac{dT_2}{dt} = Ua(T_1 - T_2)$$

Using an in-class demonstration allows for a detailed discussion of the intimate relationship between the model equations and the physical situation. This analysis is more complicated than the single phase reactor analysis in that two control volumes must be considered. One must then obtain the temperatures as a function of time to verify that the constitutive relationship, $U\mathrm{a}(T_1 - T_2)$ is valid and that U, the overall heat transfer coefficient can be calculated. "a" the exchange area is calculated from the vessel geometry. The other parameters in the model equation can almost always be found in physical property tables. The design of a commercial scale exchanger is not so easily carried out as with a simple reacting system. We know that U, which depends on the microscale fluid mechanics, is different for a tubular exchanger than it is for a tank type device. Any experiment to obtain U gives a value, which is equipment specific. We need to have additional analysis to provide correlations for U. A combination of experiment and modeling as shown in Figure 2 as Transport Phenomena Fluid Motions produces correlations expressing the Nusselt number as a function of the Reynolds and Prandtl numbers with three constants to be determined experimentally.

Several decades of experiment and analysis on different exchangers have enabled us to determine the constants in such correlations, and we are now able to design a heat exchangers with many different geometries. Process design engineers can by specifying the heat load and the utilities available get quotes on various exchangers (going out on performance) and purchase an exchanger. The heat transfer research (HTRI) will supply the necessary information to its member firms who manufacture exchangers. We then need to ask how much class time we should devote to process heat exchanger design. There are very few if any chemical engineering faculty who carry on extensive research in this area today.

In contrast, mass transfer remains a complex problem. The mass transfer model requires four equations because we are dealing with two phases, in this illustration, two liquids, one continuous phase and one dispersed phase. Other mass transfer situations may require a solid–fluid analysis, or a gas–liquid analysis. We are, as in the case of the reactor and the heat exchanger required to verify the constitutive equation, $K_\mathrm{m}a(\mathrm{C}_\mathrm{A}^\mathrm{I} - \mathrm{MC}_\mathrm{A}^\mathrm{II})$ and determine K_m, the overall mass transfer coefficient and "a." Furthermore we must have information on M, the distribution coefficient, a quantity which must be measured in a thermodynamic equilibrium experiment. The model equations for small amounts of A transferred between the two liquid phases are:

$$\frac{dV_1C_\mathrm{A}^I}{dt} = -K_\mathrm{m}a(C_{\mathrm{A}_1}^I - MC_\mathrm{A}^{II})$$

$$\frac{dV_1C_\mathrm{A}^I}{dt} = K_\mathrm{m}a(C_\mathrm{A}^I - MC_\mathrm{A}^{II})$$

In contrast with the heat exchanger analysis where "a" is determined easily from the exchanger geometry "a" in the mass transfer analysis must be determined from a two phase fluid mechanics analysis. This is a much more difficult issue, and most mass transfer experiments and analysis are only able to determine the lumped parameter $K_\mathrm{m}a$, an equipment specific quantity. As a result, scale-up to any other mass transfer contactor becomes extremely difficult. Chemical engineers have avoided this issue for decades by assuming that a mass contactor operates at thermodynamic equilibrium, and all curriculums have a separate course in equilibrium stage operations.

To illustrate how the model equations can give insight into why an equilibrium stage assumption can be valid we solve the mass contactor equations for liquid–liquid systems assuming that the phase volumes are equal and that there is not sufficient transfer of component A to change phase volumes. The tedious algebra I will leave out but it can be shown that the time to reach equilibrium, t_eq (seconds) must lie between the limits of 540d and 54,000d, where d is the diameter of the dispersed phase drop size in meters. The calculations assume a K_m value within an order of magnitude of 3×10^{-5} m/s and an equilibrium distribution coefficient, $M = 2$. It is relatively easy to obtain drops in most low viscosity liquid of 0.001 meters, and if so equilibrium can be reached between about 0.5 and 50 s. Thus, an assumption of phase equilibrium is pragmatically valid for most liquid–liquid systems. The approximate analysis also tells us that if we wish to obtain concentration time data that drop size needs to be greater than 0.005 meters. The corresponding analysis for a gas liquid system such as that encountered in tray or packed columns is much more difficult to do but decades of practical experience indicates that an equilibrium stage analysis is pragmatically valid to determine the number of theoretical stages. It is not possible to design a stage with any degree of confidence but there a number of proprietary tray designs available that have been extensively tested on commercial scale equipment. The Fractionation Research Institute, a research consortium similar to HTRI carries out research on commercial scale distillation equipment.

As shown in Figure 2, Part I, all equipment configurations are considered, and for mass contactors Chapter 4 is organized to deal with solid–fluid, liquid–liquid, and gas–liquid systems reflecting our view of the importance of mass contactor analysis and design in chemical engineering education.

Part II, Chapters 5 and 6 is organized to consider transport phenomena fluid motions and the application of the equations of change to provide insight into the molecular material properties and fluid motions, which provide correlations for K_m and U.

The determination of the interfacial area for mass transfer, a, is dealt with in Chapter 7, which presents the current state-of-the-art for estimating this critical parameter.

Organizing the transport phenomena course using the approach described above produces students with a much clearer understanding of analysis and all its critical elements. Experiment and its essential role in the process equipment design, operation, and control required for the chemical and biochemical industries is stressed. Many of the students we graduate still go into process jobs in this traditional sector of our economy so it is important that we retain some elements of the historical curriculum, which for decades has been successfully serving this society need. It has also produced graduates who can identify and solve technical problems in a wide variety of other situations, and as a result we have students who select Chemical Engineering as it provides an effective understanding of the basic sciences and mathematics through their application.

All the feedback (closing the loop in ABET speak) that we have obtained over the last few decades can be summarized in some form of the following expression "I really learned how to identify and solve problems." No one ever mentions the fascinating lectures on the second virial coefficient, the brilliance of the Sturm–Liouville solution to partial differential equations or the great numerical analysis techniques, which can be applied to design of a finned tube heat exchanger. This should tell us that it is not the content, which is critical to their success but how the material is used to solve problems.

We, however, have not produced successful graduates capable of formulating the critical policy, which our society now desperately needs in a world experiencing a myriad of new threats and opportunities. We have not effectively taught that even technical issues cannot be resolved unless we deal with the critical nontechnical matters.

To be successful, we need to constantly modify our educational programs and our research efforts. To do this effectively as our world rapidly changes we need to go beyond discussions of content and more critically examine how best to have our students learn. We must find effective ways to make our education program more efficient and eliminate material that is no longer quite as relevant. We should consider how to educate technically competent engineers who can be effective in convincing others of a sound course of action.

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Manuscript received Mar. 11, 2011, and revision received Sept. 15, 2011.