A Course in

MODELING

What differs from tradition is the strong emphasis on modeling blended with mathematics. The required text is "Your Last Calculus Book" . . .

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For a number of years our Department taught a rather traditional course along the lines of Mickley, Sherwood and Reed's *Advanced Mathematics in Chemical Engineering*. The content varied a bit with the inclinations of the instructors but was, mathematically, "soup to nuts." Such a course is literally applied mathematics: take a large measure of calculus from ordinary to partial and another measure of examples and problems from Chemical Engineering. Blend well and serve.

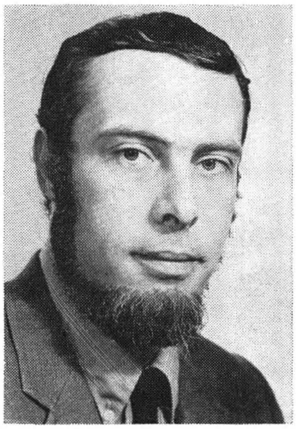
Over the years it was found that the students had little difficulty with the mathematical content. Once the bag of mathematical tricks had been presented and practiced, few had difficulty in finding the right tool for the given *mathematical* situation but this was not the case with the *physical* situation. If the student could formulate the problem, he could solve the solvable mathematics; inevitably, the problem was in the formulation. There seems to be a lesson in the organization of all engineering math texts: a dozen chapters on mathematical tools and one on formulation or modeling. Perhaps we should try to teach *modeling*, and pass along the mathematical stuff as we go, almost as entertainment!

The first thing that had to go was a one-term marathon. After the mathematics is crammed in, there is no time for contemplation of what one is actually doing when obtaining a model, or one of several possible models, for a situation, nor for carrying out with any deliberativeness an analysis of what one has done in the process of going from a problem statement to the mathematical statement. The second thing that had to go was the title! Start with "Advanced mathematics..." and the students' minds are already made up that they are there to learn mathematics, the preliminaries being just trying to cast this week's problem into this week's mathematics. So we called it, naturally, Mathematical Modeling in Chemical Engineering, with a I and a II.

Splitting the conventional content of an advanced calculus course into two terms is not a hard thing to do. We proceeded by straddling the undergraduate transition, the first course being offered at the Senior level (ChE 407), and encompassing mostly problems in one dimension, and the second offered at the graduate level (ChE 507), but available to qualified undergraduates, and extending into multidimensional problems. But if a structure of mathematical dimensionality can be called a vertical ordering of mathematical content, the philosophy and practice of modeling is orthogonal — horizontal — and cannot be divided in the same fashion. In fact, the *same* concepts of modeling apply unaltered to both categories of mathematics. The pedagogical problem, then, is to provide for the students taking both courses an interesting second course using the same philosophy of modeling superim-

TABLE 1. Interaction of Mathematics and Modeling

MATHEMATICS	MODELING
ChE 407	1. Problem Definition
Algebraic Systems	2. System(s)
Ordinary Differential Eqns.: Linear; Nonlinear	Coordinate systems
Series Solutions: Method of Frobenius; Well-known Functions	Assumptions and Presumptions
The Laplace Transform: Formalisms; The Spectral Domain	Notation, symbols
Partial Differential Eqns.: Reduction to o.d.e.	Differential balances
	Laws, correlations
	3. Preliminary Combination
	4. Initial Conditions
	Boundary conditions
	Constraints
ChE 507	5. Simplification
Partial Differential Eqns.: Solvable; Linear	Dimensional considerations
Matrix Methods	6. Selection of Solution Procedure
Separation of Variables	Mathematics (← ChE 407, ChE 507)
Orthogonal Functions: More well-known functions; Sturm-Liouville	Interpretation
Fourier Integral and Transform	7. Calculation
Laplace Transform and p.d.e.	8. Reporting



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His teaching interests include rate processes, mathematics and statistics. His research is in areas of liquid-liquid dispersion interaction, mass transfer with and without chemical reaction and karst geomorphology.

posed upon the higher dimensional mathematics. The key to doing this is to introduce more advanced *formulational* methods along with the more advanced "equations."

This interaction is shown in Table 1. The list of mathematical topics is typical, but not inclusive of all topics that have been treated. There is little new here. The complementary list of modeling topics is also unoriginal; they are necessary no matter how "advanced mathematics" is to be taught. What differs from tradition is the strong emphasis on modeling blended with mathematics. The required text is "your last calculus book"; we can use no other as we seek to avoid giving modeling a mathematical framework.

WHY MODEL

There is a single statement which sums up the reasons for modeling: It allows the logical restructuring of descriptions, providing insight and the capability to produce quantitative results in response to questions. It is no accident that the fields of study in chemical engineering have organized themselves according to the type of question to be answered and the corresponding modeling and restructuring procedures. These areas, together with the general question asked are as follows:

- **Research.** What are the basic laws, which when used in the structure representing the system, will produce the observed effects?
- **Parameter and Property Evaluation.** What are the numerical values of the symbols which characterize the system (parameter) or the material (property) being described?
- **Design.** Among the parameter and property values which we may choose, what set of values will produce the desired result?
- **Optimization.** Among the sets of values which may be chosen for a given process, what set will yield the best value of the desired result?
- **Simulation.** Given all the parameters and values and functions necessary to determine the operation of the process, what result may one expect?
- **Control.** Given a process and a specified mode of operation, how can one ensure that it will continue to operate in this fashion?

Only the first three of these were generally thought to be important in the quantitative modeling sense until approximate a decade ago. The remainder of the questions were asked, but answering them remained an art until machine computation appeared on the scene.

One particularly important aspect of communication is the ability to read the current literature in an area of interest. The vast majority of contemporary technical writing depends heavily upon and is oriented toward a mathematical approach. To be conversant in these terms requires abilities in both model building and in mathematics.

There is in this connection a common statement that needs a mild rebuttal. It is: "I am (or plan to be) a manager, so I do not care about this mathematical stuff. I need to learn how to deal with people." This is incorrect by virtue of being overstated. It is necessary to use manpower to the limit of its ability in a competitive environment, and to do so requires an understanding of these abilities. Therefore it is imperative to understand mathematical modeling from the viewpoint of "know what it can do", so that one can properly direct the efforts of those who "know how to do."

THROUGH THE LOOKING GLASS

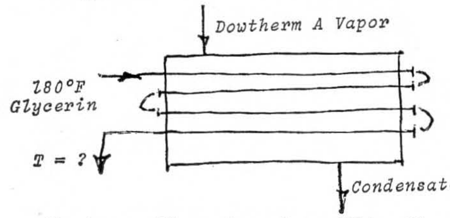
The solution of a modeling problem is a tortuous path, traversed with a cloudy mirror before the engineer. Only experience can give clues as to where the path is leading—while all the work behind is visible, including errors. A prescription on how to proceed is very necessary.

Logically, the first question is: Where am I going? A clear problem statement must be had. To illustrate:

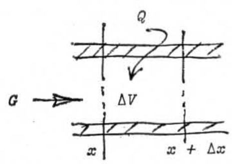
> *1.* **Problem Statement:** *Glycerin is to be heated with condensing Dowtherm A at atmospheric pressure. The glycerin enters a 360 ft. multipass exchanger at 180°F. The tubes are 1¼ inch BWG 12 copper. The glycerin mass flow is 2.7 x 10^6 lb_m/ft^2hr per tube. Calculate the exit glycerin temperature.*

Next, all pertinent information is assembled. It helps to draw a picture of the physical process to be described. Labeling such a sketch provides instant organization of some nomenclature; the whole can be listed eventually. Now select the portion of the system which can be described by the basic laws available. This may be an entire process, a process unit such as a reactor, or a differential portion of a process unit if spatial variations are anticipated.

> *2.* **Assembly of Information.**
> *Diagram:*



System: V = *glycerin within the exchanger*
Nomenclature: x = *length, ft*
L = *total tube length, ft*
T = *temperature*
G = *mass velocity,* lb_m/ft^2hr
Subscripts: i = *inside tube*
o = *outside tube*
e = *entrance to exchanger tube*
L = *exit from exchanger tube*
Subsystem: ΔV = *glycerin within a differential length of tnbe*



The selection of the basic laws — both kind and number—is deeply affected by the assumptions and presumptions made concerning process behavior. There is an often-neglected difference between these which should be pointed out. An assumption refers to something taken for granted, and hence is usually not checked. A presumption is a belief unsupported by evidence—or in other words an assumption about which we feel uneasy. There is no safe course in making as-

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sumptions and presumptions. Assume too much and you get a wrong answer; assume too little and complications prevent getting any answer. Presume too much and you are called ignorant; presume too little and you are called a coward. The proper approach is to occupy the most defensible position while obtaining results in the desired length of time.

Presumptions:
1. *Constant properties*
2. *Turbulent flow on tube side*

Assumptions:
1. *No Multiple-tube effects (horizontal arrangement, one tube thick)*
2. *Constant (saturation) temperature for Dowtherm*
3. *Arithmetic average inlet film temperature difference, can be used in the correlation for condensing coefficient*
4. *Steady state*

The selection of the basic laws to be used is influenced somewhat by the choice exercised above, and in turn influences that choice. Should a statistical or deterministic approach be taken? Are we worried about time behavior? Is it necessary to know distribution of variables within a process unit? We must discard some of the very small, the very large, the very fast, the very slow aspects of the process, depending upon the desired result. A partial explanation is all we can ever expect.

There are certain *axiomatic rules* which are not violated except under extremely unusual circumstances, and may be considered to be universally applicable. In contrast, there are also *descriptive laws,* which apply only in a limited number of circumstances and which are never universally applicable. This latter group originates either from a theory regarding material behavior in a given situation, or from the correlation of a body of physical data.

The remaining laws, which apply to only specific situations, may be divided into two groups. They are either algebraic statements of the observed relations between system variables or statments of the dependence of the rate of an elementary process variables.

There remains a class of mathematically true statements which are in no way related to the real world. Certain definitions bear a remarkable resemblance to either basic laws, rate laws or correlative equations.

Axiomatic Laws: Conservation of Energy

$$[G_i C_i (\Pi D_i^2/4) T_i]_x - [G_i C_i (\Pi D_i^2/4) T_i]_{x+\Delta x} = Q(\Pi D_i \Delta x)$$

Rate Laws: Heat flow

$$Q = U_i (T_o - T_i)$$

Correlations:

$$Nu = 0.023\ Re^{0.8}\ Pr^{0.4}$$

$$h_o = 0.725 \left[\frac{k_f^3 \rho_f^2 g \lambda}{D_o \mu_f \Delta T_f}\right]^{1/4}$$

Added Nomenclature:

G = *mass velocity,* $lb_m/hr\ ft^2$
D = *diameter, ft*
C = *heat capacity,* $BTU/lb_m\ {}^\circ F$
ρ = *density,* lb_m/ft^3
μ = *viscosity,* $lb_m/ft\ hr$
κ = *thermal conductivity, BTU/hr ft°F*
Re = *Reynolds number*
Pr = *Prandtl number*
h = *heat transfer coefficient,* $BTU/hr\ ft^2\ {}^\circ F$
U = *overall heat transfer coefficient,* $BTU/hr\ ft^2\ {}^\circ F$
R = *heat transfer resistance, hr ft°F/BTU*
Q = *heat transfer rate,* $BTU/hr\ ft^2$
g = *acceleration of gravity,* ft/hr^2
λ = *latent heat of condensation,* BTU/lb_m

Subscripts:

f = *film (outside)*
w = *wall*
F = *Fouling*

Following this listing of the mathematical relations, a certain amount of "condensation" is usually possible. Added bits of information, such as boundary conditions, are found to be necessary.

3. **Combination.** *Divide energy balance by*

$$[G_i C_i (\Pi D_i^2/4)]$$

and let $\Delta x \to 0$.

$$\frac{dT_i}{dx} = \frac{4Q}{G_i C_i D_i}$$

Substitute rate law:

$$\frac{dT_i}{dx} = \frac{4U}{G_i C_i D_i}(T_o - T_i)$$

4. **Boundary Conditions.** *at* $x\ v = 0$, $T_i = 180°F = T_{ie}$
5. **Simplification.**

$$A = \frac{4U}{G_i C_i D_i}$$

Then:

$$\frac{dT_i}{dx} = A\ (T_o - T_i);\ T_i\ (o) = T_{ie};\ A = A\ (T_o, T_{ie})$$

Having formulated a mathematical structure, it is quite unlikely that one may immediately proceed to compute the desired answer. It is far more likely that the next step is to restructure the math problem—e.g., solve differential equations.

Modeling allows the logical restructuring of descriptions, providing insight and the capability to produce quantitative results in response to questions.

6. **Mathematics.** *Separate variables and integrate.*

$$\int_{T_{ie}}^{T_{iL}} \frac{dT_i}{T_o - T_i} = \int_0^L A dx \quad \text{or} \quad \ln\frac{T_o - T_{iL}}{T_o - T_{ie}} = -AL$$

$$T_{iL} = T_o - (T_o - T_{ie})e^{-AL}$$

7. **Numerical Results.** *The information given plus data on the two fluids, yield a value of* $A = 4.18 \times 10^{-3}$ *and* $T_O = 495.8°F$, $T_{iL} = 425.3°F$
8. **Discussion of Results.** *With the assumptions given, the glycerin is heated to 425.3°F. However, a check of the constant property assumption shows that it is seriously in error. For example, at 180°F,* $\mu_i = 29cp$; *at 425.3 F,* $\mu_i = 1.2cp$. *Therefore, it appears necessary to "iterate" back to step 2 and change the presumptions. Only part of the next iteration will be shown here. Presumption 1 must be abandoned; flow on the tube side is confirmed to be turbulent.*

Words and numbers are ultimately required from the model. One does not submit a differential equation to management, nor does one frame a computer program and hang it on the distillation tower. It is the responsibility of the modeler to communicate his results either by interpretation, or by providing statements so clear that others can interpret them easily and without possibility of error. This feature of modeling is frequently ignored, fostering battles of misunderstanding between the model builder and the potential model user.

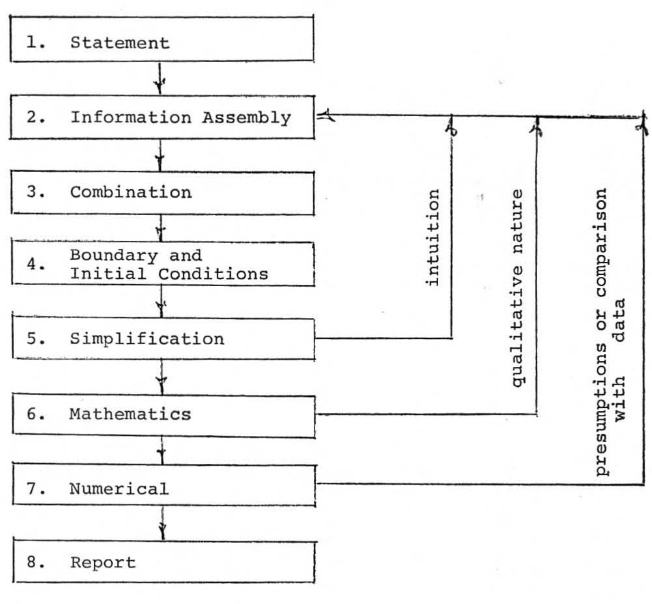

Figure 1. A Model Building Algorithm with Iteration

In the example that we have been carrying along as a guide, we find that we aren't ready to communicate our results as they violated a presumption. An iteration of the *model* is required. However iterations are possible at several different levels, as shown in Figure 1, which rests on the lists of modeling steps in Table 1.

2-II. **Assembly of Information.**

Assumptions:

1. *Temperature dependent fluid properties.*
2. *Turbulent flow on tube side.*
3. *No multiple tube effects.*
4. *Constant Dowtherm temperature.*
5. *Variable film temperature, and Temperature difference.*
6. *Steady state.*

New correlations are needed, and the solution method becomes a computer technique.

8-II. The value of the exit temperature is 464.7°F.

PEDAGOGY

It is moderately difficult for the instructor, and unsatisfactory for the student, to spend much time talking about the philosophy or even the structure of modeling. It seems so self evident that it is boring—but still the students go astray simply by virtue of overlooking a modeling step. Therefore, to make all this work, and to make it interesting at the same time, a variety of pedagogical tricks have been developed and used. These have included:

1. **Omit problem statement.** The "problem" is presented as a demonstration: a vessel is allowed to drain through a square hole and the level measured vs time; a hot sphere is immersed in a vessel of water and its temperature measured; a beaker of molten paraffin is allowed to solidify. Model this situation is the instruction. This focuses thought upon securing a precise problem definition. The students must pry it out of both the instructor and reality.
2. **Give problem solution.** A problem from a preceding course (where it is presumed that the principles of modeling had *not* been taught!) is chosen and the instruction is to recast it into the algorithmic solution format given in Figure 1. This focuses the student's attention upon *procedure*: the work of "solution" has been completed in advance within some other procedure, be it derivation or formula-plugging.
3. **Trial by fire.** A student is asked to solve a problem before the class, with no prior preparation. The whole reasoning process is thus brutally exposed. A kinder approach is to successively question class members to develop the model step-by-step, following the modeling algorithm of Figure 1.
4. **Tweak by paradox.** A "completely logical" example is presented, which leads to a clearly ridiculous result. The location of the flaw in reasoning is a superb educational device.
5. **Math made illegal.** A fairly detailed report, containing no math but explaining the model and results, is requested on a problem. □

BELL **(Continued from page 157)**

The lecturer has a small monitoring screen on the desk in front of him that shows exactly what is going on to the viewers. (The monitor is an insidious and ruthless device: lecturers have been known to start yawning in boredom while watching it.) The studio audience mostly watches the two TV screens, because that's where the action is when the lecturer is working on the note pad; this is somewhat distracting to an experienced lecturer, who relies upon eye contact to see if the audience is with him. I don't use the board because it is hard to remember to work in properly scaled modules so that the whole image fits the TV screen and yet is legible. This is readily controlled by using a 6 in. by 8 in. buff-colored note pad. The material to be presented in class is written or drawn upon the pad in yellow ink, which is readily visible to the lecturer and nearly invisible to the camera; during the lecture, the notes, etc. are made visible to the audience by writing over them with a black felt-tip pen. (By forcing the lecturer to do the writing, the speed of the presentation is held closer to the speed at which the students can make notes.)

Acclimatization to the TV system took only two or three lectures. The most important single change that I noticed was that I was better prepared to lecture when I came to the studio. Having to prepare the notes in yellow ahead of time not only forced me to review, but also to organize the material so that the contents of each sheet made sense. □