A PHENOMENA-ORIENTED ENVIRONMENT FOR TEACHING PROCESS MODELING

Novel Modeling Software and Its Use in Problem Solving

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New avenues to teaching process modeling are sorely needed in our discipline. The methods we have been practicing seem to have been ineffective; they have not been active and concerted. We have instead depended too much on students individually inventing some sort of approach as they struggle to find their way through the modeling maze in homework assignment after homework assignment. Missing has been an articulation of a natural and intuitive hierarchy and its use in declaring the character of a process representation, a hierarchy comprising such matters as conservation principles, thermodynamic constraints, phase conditions, phase equilibria, reaction phenomena, and transport phenomena. Missing also is an awareness of many in academia that process models are presently at the heart of industrial control systems and optimization methods for process operations, and that our graduates ought to be prepared to contribute to that technology.

In an attempt to address this shortcoming, we propose a new avenue for teaching modeling and have brought into being new software embodying a model-building hierarchy that can guide students in using their engineering science background in crafting models for problem solving. Our approach is unconventional, and the opportunity extraordinary for breaking through this instructional omission and breaking through hurdles that students see in their path.

Our motivation further derives from having observed that many students are at a loss in identifying the physics and phenomena operative in a process and how to use their background in engineering science to make an integrated representation of the process. Moreover, many sense their weakness or lack of confidence in writing the equations to represent the physics. A disciplined focus on stating the physics and a release from incessant equation writing is the major contribution that this software brings to student learning. Through a selection of examples, we illustrate how the teaching of modeling can be enhanced with features of the software.

"ModelLA" is the name we have given to this program. Be prepared for something different.

The program offers students a phenomena-oriented environment expressed in the fundamental concepts and language of chemical engineering, such as mass and energy

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balancing, phase equilibria, reaction stoichiometry and rate, modes of heat and species transport. Through a freely accessed hierarchy of declarations of such elements of engineering science, the user is assisted in recognizing, for example, that energy balances must be declared, that chemical equilibrium constrains species behavior, and that a zero entropy increase must be imposed to attain minimum compression work. All levels of the hierarchy are accessible at any time by user request. Unlike the rigid lists of earlier modeling software, elements of the hierarchy are not "pre-wired."

It is just the physics that has to be declared—no equations; the software writes the equations. That is what is unconventional. And, by simply requesting a solution, the equations are solved numerically in a few seconds without user intervention in the numerical method. The results are displayed graphically for rapid assessment of the characteristics of the model. The feedback about misinformed declarations of the physics is instantaneous—certainly a major improvement over the one-week turn-around time of homework sets.

Such modeling capability can complement instruction in modeling throughout the curriculum. Modeling, in our opinion, should be a part of all instruction in engineering, and it should be done in the context of resolving an engineering problem. By teaching modeling in a problem-solving context, one can better demonstrate how the nature of models is influenced by the context, how models serve problem solving, and how the structure of efficient problem solving is shaped by the use of models. The program can be especially helpful in the process-design course as a complement to the use of process simulators such as Aspen and Chemcad, providing students, through model building, a means for understanding the nature of the relations hidden in the simulator modules. ModelLA is different, having modeling rather than simulation objectives; its modeling capability is what complements.

HELPING STUDENTS IDENTIFY THE PHYSICS AND THE PHENOMENA

Knowing where to start is not easy for beginning and inexperienced students. Take, for example, the double-effect evaporator process in Figure 1. There is a lot going on here. In the first place, the instructor will have introduced this project as one of trading off energy and equipment costs in synthesizing an economical process for the desalination of sea water. To build a model for decision making about a process design, students will need to recognize the presence of the phenomena identified in the ellipsoidal bubbles. We emphasize that the evaporators have to be modeled. Unlike the process units displayed on the screens of process-simulation programs, the pictorial icons here are empty shells; there is no model associated with them. The model has to be built. Through interactive Q-and-A with the instructor and concurrent use of ModelLA to declare the physics in the bubbles, students can build a model suitable for investigating, for example, the influence of the temperature drop across the train, the degree of concentration of the brine, and other decisions.

A perennial difficulty in assigning such a project is the lack of physical feel of many students for the qualitative cause-effect relations of the process variables to one another. With the availability of the software, those students can explore an instructor-built model and acquire insight into the effect of changes in operating conditions before attempting to craft his or her own model. Figure 2 shows one such set of explorations: the effect of condenser coolant flow rate on pressures and vapor flow rates in the various units.

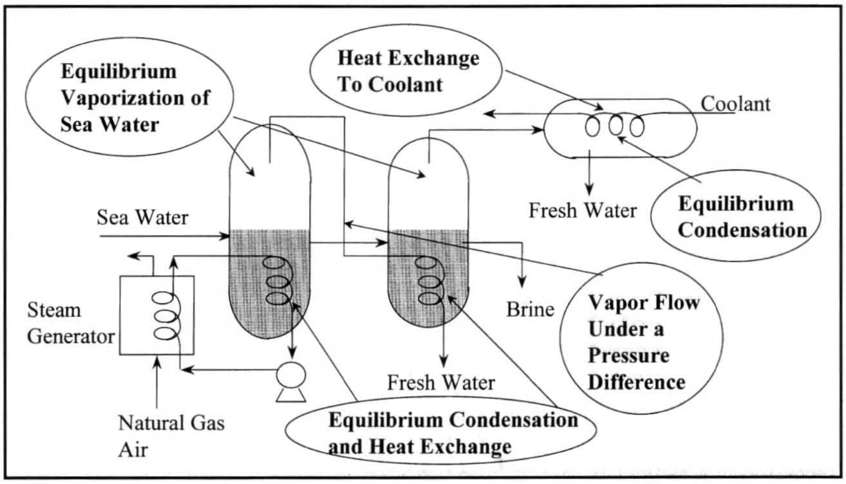

Figure 1. *Double-effect evaporator modeling project illustrating the spectrum of phenomena for incorporation in a model.*

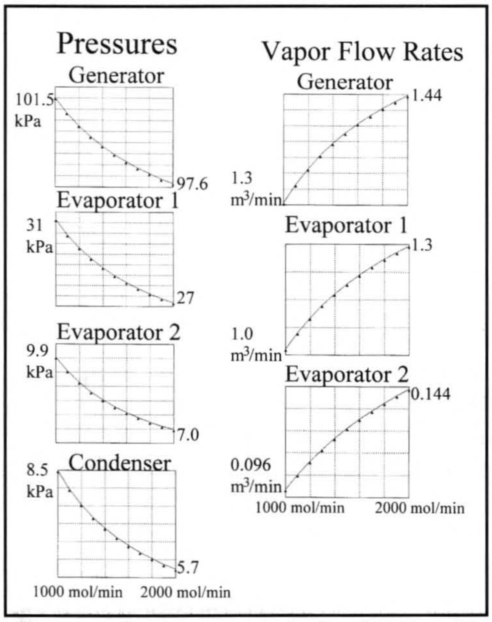

Figure 2. *Students can gain familiarity with the evaporation process by interrogating an instructor-built model for the effect of coolant rate on pressures and vapor rates.*

All this is calculated in a few seconds with a single request for such an analysis. The results reveal, perhaps for the first time for some students, that pressure in the condenser decreases with increasing coolant flow, that the pressure decrease propagates upstream to the steam generator, that there is a pressure gradient from one unit to the next, and that vapor rates in the units differ. Then the question for the students is, "Why does all this happen?" With such knowledge, students should be able to make intelligent declarations of the physics far better than had they not explored the behavior.

PUTTING THOSE INSIGHTS TO WORK IN MODELING THE EVAPORATOR

Exploration of the instructor-built model alerts students that there are two component parts of the evaporator, that they are linked by heat exchange, and that they are different—one a boiling liquid mixture and the other a condensing pure vapor. Such recognition suggests that declarations about the internal structure and the character of the evaporator parts need to be made in crafting a model. This is accomplished in ModelLA by disaggregation of a process unit into its internal parts. Figure 3 shows how a modeler would use the disaggregation window (Level 2) to state his or her view of the evaporator internals through placement of a mixture unit, a tubes unit, and linkages of convective flows to those of the parent (Level 1) located on the edges of the disaggregation window. A heat flux between the tubes and mixture is declared as an essential linkage for effecting evaporation. One can see that all of this is done in a visual, graphical manner, a feature quickly grasped by the user.

At this level, declarations can also be made about the phases present in each subunit, the species in them, equations of state, the equilibrium relations between the phases, and the "mechanisms" for heat transport and vapor flow. Such declarations are made through a hierarchy of dialogs. As these declarations of species and phase equilibrium are made, a linkage is established to a physical-properties data base for the estimation of quantities such as vapor pressures, activity coefficients, densities, and enthalpy of phase change that are eventually needed in the numerical solution of the model equations. We have operated with a relational database containing data for over 2000 chemical compounds. The user may also supply any special data particular to the process being modeled.

It is at this level where the engineering science concepts and facts are introduced into the model. To accomplish this in an organized manner, students need disciplined guidance in an environment familiar to chemical engineers. They get it through the hierarchy of declarations of structure and phenomena shown in the right side of Figure 3. That set of hierarchical elements applies to just the declarations needed for this part of the model. The full set available in ModelLA is much more extensive. The Modeling Assistant shown at the bottom in Figure 3 guides the user in branching to the major elements of the hierarchy.

Learning about the physics of the process takes place very rapidly here because the guidance given by the program at each juncture is centered on the logical consistency of the declarations made and because the feedback about inconsistency is essentially instantaneous. One of our student evaluators remarked that ModelLA guards the user from accumulating mistakes. A good amount of self-learning takes place about the modeling process without instructor prompting.

PROCESS SYNTHESIS—EXECUTING A TOP-DOWN APPROACH

The top-down synthesis of a process system can be shown to students as an orderly and rational way to evolve the structure of a process[1] and provides a good example of the use of the hierarchical structure of the software. Unlike the bottom-up approach usually employed with process-simulation programs, the top-down approach affords the user a view of the direction of subsequent development and the type of model needed to support that development. Some

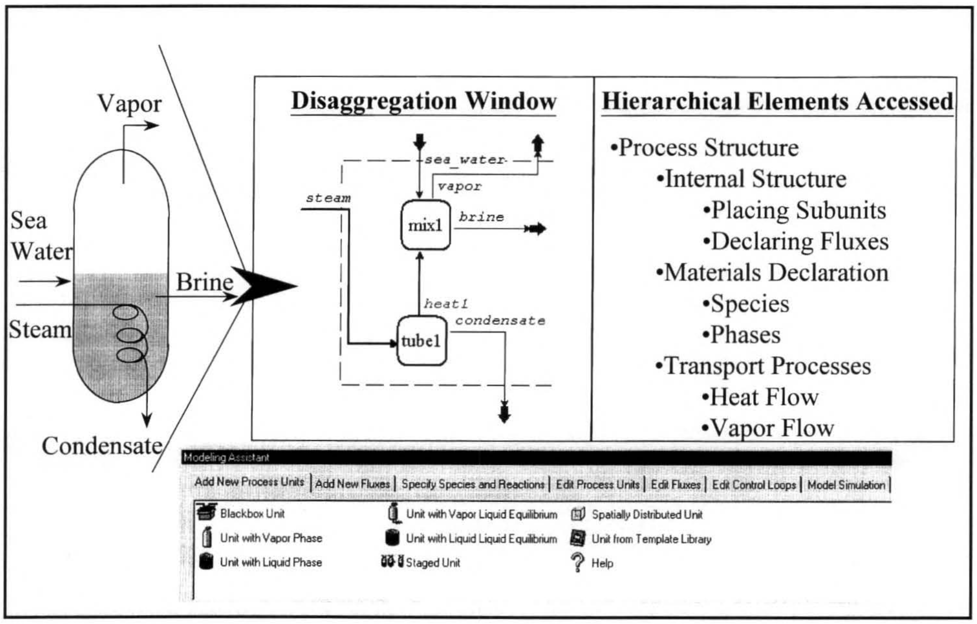

Figure 3. *The subunits of the evaporator are identified in a disaggregation window, fluxes stated, and material properties declared.*

describe it as a target-directed approach. In a top-down approach, the progression of one's thoughts about creating process structure is intuitively organized as a hierarchy, proceeding from overall (top level) objectives and successively broken down into levels of finer detail. That hierarchy matches exactly ModelLA's hierarchy of declarations of process structure and content. As an example of how a top-down synthesis can evolve with the use of ModelLA, we show three levels of the synthesis of a process for the hydrodealkylation of toluene to benzene, the HDA process.[1]

The synthesis starts at Level 1 in Figure 4 with simple declarations of the products to be produced from candidate raw materials, the chemical species present in the process, the expected chemical reactions, the expected byproducts and waste products, and energy fluxes between the process and environment. ModelLA's hierarchical elements accessed for such declarations are shown to the right of the Level 1 depiction in Figure 4. Next, with an appreciation that a reaction section and a separation section would be needed, a modeler would place such elements in Level 2, a disaggregation of Level 1, as shown in Figure 4. Such a step is a top-down step in the synthesis, the educational benefit being an opportunity for the student to express his or her perception of the big picture. Such declarations are made by accessing the hierarchical elements shown to the right of Level 2 in Figure 4.

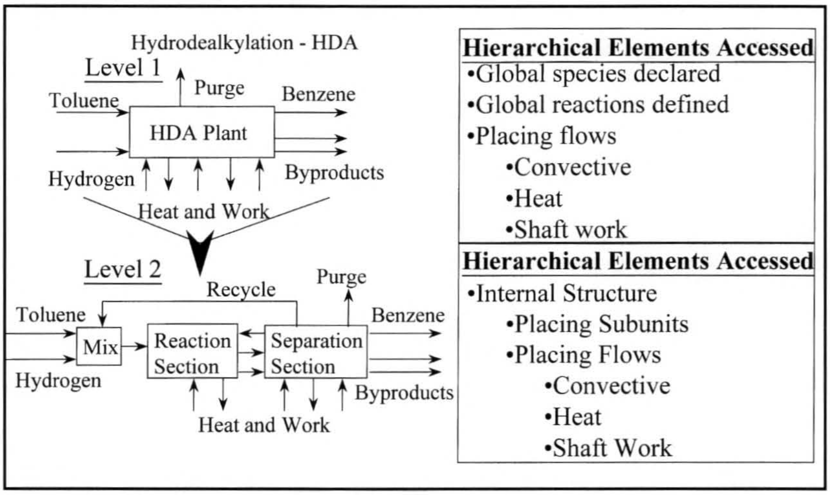

Figure 4. *Process synthesis pursued through successive sublevels corresponding to the multilevel hierarchy of ModelLA.*

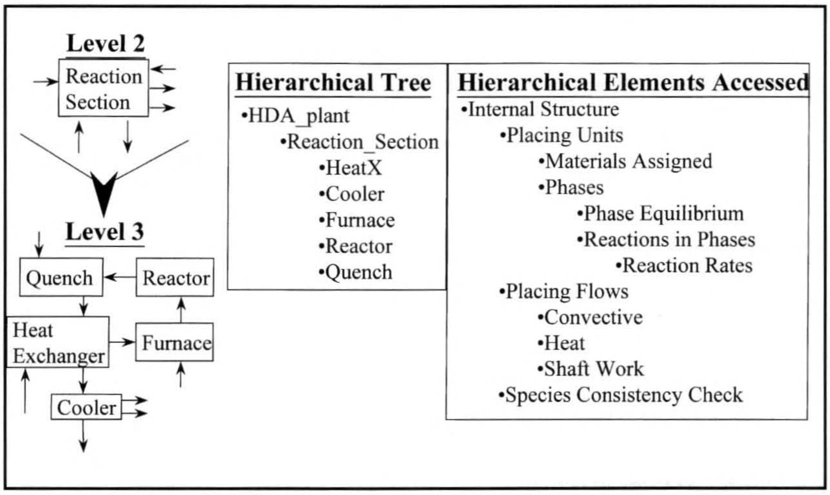

Figure 5. *Successive disaggregations bring one to the point at which process subunits can be fully defined and modeled.*

The big picture now has to be fleshed out with some definite proposals for accomplishing the reactions and the separations. A fleshing out of the reaction section is illustrated by the disaggregation of Level 2 in Figure 5. In Level 3 of this example, the modeler must function in a bottom-up mode, placing and connecting process units whose functionality the modeler must eventually describe, stating substructure, species, phases, reactions, and fluxes. This is the level where process inventions are made.

The educational value here is the direction of attention on a well-defined segment of the entire process so that decisions about process structure and the modeling of the set of units in that segment can be made and tested without interference from other segments. For example, the type of reactor model, ways to prevent catalyst coking, and conditions to enhance reaction selectivity can be scouted. There is plenty of opportunity here for the instructor to point out the place and need for a model in problem solving and synthesis. The opportunity is also there to point out the structure of problem solving. The top-down strategy comes to meet the bottom-up inventions of the sub levels as the process is further and further disaggregated into elementary operations and basic phenomena.

One can also see here an opportunity for collaboration among team members in a networked environment, say, in the design course, where one member would develop the reactor section and another the separation section.

As the user's invention of model structure proceeds, the software assembles information about the hierarchy of model units and their connections and displays it as the hierarchical tree of model units shown in Figure 5 for the purpose of keeping the user up-to-date on the model so far constructed. Such a display is especially useful when moving back and forth between several levels of the model.

Completion of the models of the units placed in Level 3 of Figure 5 is accomplished through the hierarchical modeling elements shown at the right. A particularly essential element is the *species consistency check.* It scans the model units of each level to determine whether the distribution of species declared by the user makes physical sense. If it does not, guidance is then given to assist the modeler in rectifying the omissions.

SATISFYING THE DEGREES OF FREEDOM

A very considerable amount of insight and knowledge about the qualitative cause-effect relationships in a process system is needed to identify quantities that fully specify the operating conditions of the process. It is in this aspect of modeling that the students' engineering ability is thoroughly taxed, and in the taxing, further developed. This is also where the instructor can help develop that insight through questions and answers in interactive sessions with the students. Complex processes often bring to the fore perplexing conflicts in satisfying the degrees of freedom, particularly when energy and mass fluxes interact. This is certainly the case in a process as complex as the HDA process.

Even models of modest size can have a dozen or more degrees of freedom. Without some assistance, satisfying these with statements of operating conditions and physical parameters would be a daunting and likely an unavailing task. It is neither of these with the ModelLA program. Candidate quantities are identified for user consideration, unit by unit, flux by flux, phase by phase, variable by variable, species by species. A running count of the degrees of freedom yet to be satisfied is displayed as the user makes selections. This DOF analytical engine also identifies conflicts in the user's selections and offers a list of alternative quantities that can be swapped with the current selection.

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In the case of dynamic models, the DOF analytical engine simultaneously also makes an analysis of the index of the set of differential algebraic equations and informs the modeler when the index exceeds 1. Such an analysis is necessary because selection of a certain combination of quantities to satisfy the degrees of freedom can sometimes result in a large index. Current numerical integration algorithms cannot integrate a differential algebraic equation set with an index greater than 1. Information regarding the source of the high index is reported so that the modeler may reconsider the set of design variables.

CALCULATIONS AND THEIR USE

When it is confirmed that the index is 1 or less and all degrees of freedom have been satisfied, the user may launch a calculation of the model equations. Calculations are made without user intervention by a state-of-the-art numerical engine, gPROMS,[2,3] and for the double-effect evaporator, are completed in 4 or 5 seconds.

Students and instructors like to see trends of process variables over ranges of operating and design conditions like those shown in Figure 2 because insight about the process is more easily grasped. Trends can be calculated and displayed for all variables very quickly. The numerical data of such calculations can be used in deciding on operating conditions or examining the trade-offs among design decisions. The engineering problem can be addressed in this way.

BUT THE EQUATIONS! WHAT ABOUT THE EQUATIONS?

By all means, have the students write the equations—but only after they have gained an understanding of the physics and an appreciation of the qualitative cause-effect relationships among the variables.

One might think that an assignment in writing the model equations after having crafted a model with ModelLA and after having resolved an engineering problem would be unnecessary and anticlimactic. It is neither. First, it is necessary because there has to be a closure to the project that is satisfying to the students. We found that students in our trial group wanted to write equations and to confirm that their model and calculations matched those of ModelLA. Second, one will find that even after having articulated the physics, not everyone is sure-footed in identifying a model envelope and subunit envelopes. That is, some run off in wrong directions. Further, one will find a significant fraction confused about representing such things as the rate of accumulation of internal energy in a mass of material in terms of the process variables and the flux of energy in and out of the process. Instruction is assuredly needed to straighten out those basic matters.

That instruction is one of the activities that sustains an interest in writing equations and saves it from being anticlimactic. We recommend that the instructor work through the equation writing with the students in an interactive workshop environment because many will still need help with matters such as those just mentioned and because there is not much incentive to have students struggle alone through the equation maze at this stage. Focused and concentrated instruction in formulating model equations reinforces an instructor's continuing admonition for physical thinking at all stages of modeling and that the equations are just a symbolic statement of the physics. That will be a revelation to students who have the impression that equation writing is all mathematics.

An alternative approach, which we think ineffective, is to have the software display the equations to the student piece by piece as he or she makes declarations of the process attributes, that is, the materials, phases, fluxes, and reactions. Such displays are unguided and physically uninterpreted and are not an effective pedagogical method.

In the workshops there is the further opportunity for the instructor to point out the character of the set of equations, how a choice of variables can transform a nonlinear model into a linear model, how natural divisions in the process structure result in separate blocks of equations, and how one can order the terms of the equations to form an easily computable structure, as for example, the structure of a linear set. Students left alone in a sea of equations seldom are aware of the equation structure. They can benefit from the instructor's insight here.

A full set of notes for the instructor about writing the equations for every model is given in a set of course modules described in a later section. The equations are laid out following the logic and cause-effect relations articulated in an earlier section of the module and thus should appeal to the physical understanding developed there. Two methods of solving the equations are developed in the course modules for every model. A paper-and-pencil method follows directly, step-by-step, the articulation of the physics, the identification of the unknowns, and the nature of the relations needed to complete the model. Solution by use of general-purpose numerical solvers such as Matlab, Mathcad, and Polymath is also presented. In the case of linear dynamic models of a single state variable, a closed-form analytic solution is derived. Numerical calculations of the derived equations are presented for all models and compared with the ModelLA calculations. Thus, the instructor has material to close the loop for the students.

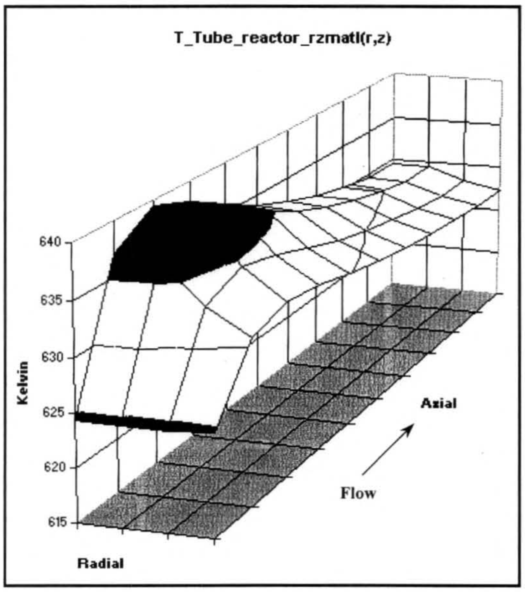

Figure 6. *Two-dimensional temperature profile in a phthalic anhydride reactor calculated by a ModelLA model.*

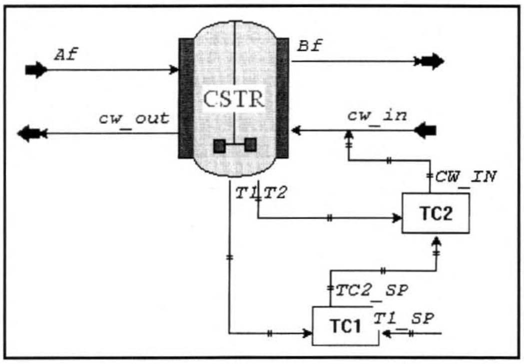

Figure 7. *Cascade control system for a CSTR is constructed after identifying variables that can be measured and manipulated.*

CURRICULUM-WIDE MODELING CAPABILITIES

Modeling of spatially distributed and dynamic processes is a frequently encountered challenge for students throughout the curriculum. ModelLA has the capability for both. Further, students can investigate control of processes by placing control systems around dynamic process models.

Spatially Distributed Processes • Tubular reactors, absorption columns, cooling towers, adsorption beds, and tubular heat exchangers all need at least a one-dimensional spatial representation of species behavior and energy flows. ModelLA has 3-D spatial modeling capability, offering rectangular, cylindrical, and spherical coordinates. As an example of that capability, the temperature distribution in a 2-D model of a phthalic anhydride reactor produced by ModelLA is shown in Figure 6.

Dynamic Processes • Instruction in modeling the dynamic behavior of processes can be introduced profitably in the first course in material and energy balancing. We simply remark that early experience in dynamic system modeling gives students an early understanding of interactions in process systems and potentially an appreciation for the evolution of the steady-state condition. Declaration of the attributes of a dynamic process model proceeds in the same way as that of a steady-state model with additional attention needed to specify the initial conditions. Spatially distributed dynamic processes can be modeled.

Multiloop Control Systems • Control loops can be placed on the process flow diagram as shown in Figure 7, for example, by the cascade system on a CSTR. The user can select a PID controller algorithm or craft a custom controller action involving, for example, logic elements and actions triggered by a time sequence. The salient educational merit of ModelLA's use in configuring control systems is the challenge to identify which variables should be measured, which should be manipulated, and how to link them. Other types of process models in other types of software by necessity reveal the measurement transducers and control valves, thus surrendering the educational benefit of this intellectual challenge.

COURSE MODULES FOR ASSISTANCE IN MODELING INSTRUCTION

To assist instructors in using the software for instruction in modeling, we have developed several course modules that can be used in concert with two of the most popular texts on material and energy balancing, namely those written by Felder and Rousseau[4] and Himmelblau.[5] Several modules on more advanced topics have also been developed. The modules treat the modeling of process systems presented in those texts, some being simple "warm-up" exercises of the single-answer variety, and others involving analyses of trade-off in operating costs with product value in a search for optimum operating conditions.

One of the important components of each module is an articulation of the physics and the qualitative cause-effect relationships of the process, thus giving the instructor background about the project. Because students can benefit from such an analysis as well, students are asked in a preliminary homework assignment to identify the process variables, what affects them, how they might be determined, and to name the relations that fully define a model. Students can benefit from a Q-and-A session with the instructor following such an assignment and before embarking on building a model.

The modules also lay out a completed ModelLA model, showing all subunits, fluxes between them, phases, reactions, and transport relations. The full set of design variables and initial conditions is given and the full set of ModelLA declarations is provided on a disk file so that a numerical simulation is ready for execution. For each ModelLA model, tips and reminders are given to the instructor concerning certain declarations that may not be obvious or that might be overlooked. These can be passed on to the students as they develop the model. Some models may be crafted in more than one way. In those instances, we have included a discussion of the philosophy of the approaches and have given the rationale for the approach selected.

Results of the numerical simulation of all models are given in graphical or tabular form and are discussed in relation to the physics and cause-effect characteristics treated in the preliminary homework assignment and also in relation to questions asked in other assignments. Projects involving design or operating trade-offs show the behavior of an objective function as a function of split fractions and fraction conversions, for example.

As a means of getting students "up to speed" in use of the program, we have prepared an on-screen tutorial that guides the learner through the several types of declarations in the hierarchy interactively with a "live" ModelLA program running concurrently. Our experience is that students pick up the general structure and features of the program in about a 2-hour session with the tutorial and the finer details with subsequent use in modeling projects.

SUMMARIZING THE EDUCATIONAL INITIATIVES

This phenomena-oriented and hierarchically structured software propels students quickly into model building and problem solving. The model can be built expeditiously because the focus is on the phenomena and because students need not struggle with equation writing. The hierarchical structure of the software embodies the same hierarchy used by engineers in declaration of model characteristics and thus promotes a natural and intuitive flow of model development.

The release from equation writing permits the students to push ahead with model development and problem solving and helps them build a "can-do" confidence in completing an engineering project. Writing equations is deferred to the end of the project. Students at that point are much better informed about process character and more receptive to instruction about formulating model equations. Further, the instructor has the opportunity to describe the structure of the model, a matter rarely treated, but one of value when consistently brought into view across the curriculum. Thus, we favor the inversion of the usual order of equation writing and problem resolution.

The ability to build a model quickly and efficiently with ModelLA is a major contribution to student learning. Students are steadily engaged with the physics and are given instant feedback about inconsistencies or just plain impossible constructions. Waiting for instructor approval is thus unnecessary. Efficiency is very important also in satisfying the degrees of freedom through identification of design and operating variables. There is a good amount of qualitative cause-effect analysis needed on the part of the student in this, and ModelLA helps one to move through selection of design variables rapidly in an orderly sequence.

This new avenue to teaching modeling can speed student grasp of using engineering science concepts in any course environment. Inasmuch as our current method of instruction rests heavily on quantitative models of fundamental phenomena and on models of process systems, there is considerable incentive to improve the efficiency and effectiveness of that instruction. There is a marked commonality of modeling needs across the curriculum that can benefit from this hierarchical modeling environment.

AVAILABILITY OF THE PROGRAM

ModelLA and several course modules will be available in the near future to faculty members interested in helping us evaluate its effectiveness in teaching modeling. Requests should be made on departmental letterhead to Professor George Stephanopoulos at MIT. The program will be available to all interested persons following the evaluation period.

ACKNOWLEDGMENT OF OUR HELPERS

Miklos Gerzson assisted in scouting some early ideas for familiarizing students with process behavior. Michael Lasinski assisted with coding of some of the graphical displays. Berkeley junior-year students Adam Cate, Valerie

Grill, James Comb, and Ryan Overstreet assisted with evaluation of the software and with the development of process models. Professor Terje Hetzberg of the Norwegian Institute of Technology, Trondheim, in a sabbatical year at Berkeley assisted the Berkeley team with modeling techniques and evaluation of the software.

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Universities - Why?

Continued from page 291.

then not only do we hinder student growth, but we also undermine the university and, ultimately, corrupt society.

If this seems farfetched, consider the catastrophic consequences of the Soviet experiment in which a society attempted to provide economic security while suppressing intellectual growth and development. Consider further the grave difficulties now being faced by countries of the former Soviet Union—difficulties engendered because too many of their people fail to understand how modern societies function.

In our society, the difficulties of educating are exacerbated by an astonishing degree of self-satisfaction. It is possible to operate cars, computers, and microwave ovens without knowing anything about how they work; possible to vote and pay taxes without understanding the rudiments of government; possible to work at a job without comprehending the larger workings of the economy; possible to be courteous and well-meaning while ignoring the deeper implications of human psychology. In other words, it is possible for many to live only at the surface of the culture and to be unconcerned about the underpinnings by which the society functions.

The operative question is this: For a society to survive and its culture to continue to evolve, what is the smallest fraction of the population that must comprehend how the society functions? In modern societies, it is the unique responsibility of universities to keep that fraction above the minimum.

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