PROCESS SIMULATION AND McCABE-THIELE MODELING

Specific Roles in the Learning Process

KEVIN D. DAHM
Rowan University • Glassboro, NJ 08028-1701

Standard texts on equilibrium staged separations[1,2] present the McCabe-Thiele, graphical approach as a primary tool for modeling and designing staged separation processes such as distillation, absorption, extraction, and stripping. The development of process simulation software, however, has impacted the way this material is taught. In a recent survey[3] of U.S. chemical engineering departments, 57% of the respondents indicated that they now use process simulators in teaching equilibrium-staged operations, and this number is presumably still growing. Recently, authors have discussed methods of integrating process simulators into lecture courses[4] and of using simulators to facilitate major project work.[5]

Simulators certainly have not, and should not, entirely replace "hand" solution techniques. The primary pedagogical concern regarding process simulators is that they function as black boxes. In many cases students can use them to solve specific problems without necessarily understanding the physical process they are modeling.[3] They are likely to accept the results of the simulation blindly, with no thought of the potential limitations of the modeling approach used.

One merit of traditional graphical approaches is that they provide some insight into what the simulator is actually doing. A further consideration is that graphical approaches provide a convenient framework for visualizing the process. Wankat[6] points out that even experienced engineers "commonly use McCabe-Thiele diagrams to understand or help debug simulation results." But the merit of extending the hand calculations significantly beyond simple graphical models, such as using the Ponchon-Savarit method to include the energy balance, is less clear in the era of process simulation.[7]

It is such considerations that led Wankat to recommend "an eclectic approach that includes classical graphical and analytical methods, computer simulations, and laboratory experience."[6] This paper examines how an effective balance between these various components can be attained, using research into cognition and the learning process as a guide.

> ***The course organization is consistent with what is known about cognition and the progression of student understanding, and it appeals to students with varied learning styles.***

Over the past three years, the author has taught a 2-credit-hour, 14-week course (two 75-minute periods per week) on equilibrium staged separations (see Table 1 for a summary of its content). Enrollment varied between 14 and 22 first-semester juniors. In the fall of 1999, the course was taught using a lecture format almost exclusively. Material was presented in a purely deductive manner, closely following Wankat's textbook[1] and making little use of process simulation.

In the fall 2000 and 2001 semesters, the course was organized as described in this paper (still using the Wankat text-

Kevin Dahm is Assistant Professor of Chemical Engineering at Rowan University. He received his PhD in 1998 from Massachusetts Institute of Technology. Prior to joining the faculty at Rowan University, he served as Adjunct Professor of Chemical Engineering at North Carolina A&T State University. His primary technical expertise is in chemical kinetics and mechanisms, and his recent educational scholarship focuses on incorporating computing and simulation into the curriculum.

book). Active learning exercises were employed throughout, with lab demonstrations, McCabe-Thiele modeling, and process simulation playing specific, complementary roles that are discussed in detail in this paper. Significantly, restructuring the course did not affect the class time requirements summarized in Table 1 and required no increase in preparation time on the part of the instructor aside from the one-time investment of learning to use HYSYS.

COURSE ORGANIZATION

In a series of articles in *Chemical Engineering Education,* Haile[8-12] discussed the operation of the human brain and the learning process. This paper discusses how these insights on cognition were used to guide the course's organization and the specific role McCabe-Thiele modeling and process simulation should play. This paper uses column distillation as an example, but the approach is readily applied to other physical processes and was integrated throughout the course.

TABLE 1
Topics in Equilibrium Staged Operations and Approximate Number of Class Periods Spent on Each

Topic *(Number of 75-minute periods devoted to it)*

- Introduction to Separations *(1)*
- Vapor-Liquid Equilibrium, Bubble/Dew Points *(3)*
- Flash Distillation, VLE Models *(3)*
- Binary Column Distillation *(6)*
- Multi-Component Distillation, Shortcut Methods *(4)*
- Absorption and Stripping *(3)*
- Liquid-Liquid Extraction *(4)*

Haile described[9] a "special hierarchy"—a progression of seven levels at which a student can understand concepts. These levels are summarized in Table 2 along with examples of capabilities of students who understand distillation at a particular level. The table assumes McCabe-Thiele is the primary modeling tool used.

Haile[11] also described a general hierarchy of modes of understanding that includes

> *Somatic Understanding* • Tactile learning. Observing and handling something lays the groundwork for understanding it at higher, more abstract levels.[13]
>
> *Mythic Understanding* • Oral traditions. Levels 1 and 2 of the special hierarchy fall within this realm.
>
> *Romantic Understanding* • Characterized by abstractions such as writing and graphs. Level 3 of the special hierarchy is an example.
>
> *Philosophic Understanding* • Logical reasoning. Levels 4 through 7 of the special hierarchy require a philosophic understanding.

The progression from Somatic to Philosophic understanding, in this case, suggests a course structure in which students are first exposed to a real distillation column, then they are exposed to an abstract model of a column (such as a HYSYS model) that is already complete, and finally they learn to derive their own abstract model, namely the McCabe-Thiele model. The special hierarchy is also a useful guide. In Chapter 5 of Wankat's book, for example, the McCabe-Thiele model is derived and then used as a framework for illustrating such patterns as the trade-off between reflux ratio and the number of stages. The special hierarchy, however, suggests an alternative organization in which students are exposed to such concepts and patterns first (levels 1 through 3). This was accomplished by using HYSYS to generate simulated experimental data supporting an inductive presentation of the patterns. Derivation of a model came later in the context of solving problems (levels 4 and 5).

TABLE 2
Levels of Understanding in the Special Hierarchy as Described by Haile[9] and How They Might Manifest in Students Learning about Distillation

Level of Understanding	*Examples of Student Capability*
1. *Making Conversation*	• Describe in general how distillation works • Recognize a distillation column when seen
2. *Identifying Elements*	• Compare/contrast column distillation to flash distillation • Identify individual components of a column and explain their function
3. *Recognizing Patterns*	• Correctly predict relationships between column parameters, *e.g.,* what happens to the heat duty in the reboiler when you raise the reflux ratio?
4. *Solving Problems*	• Use McCabe-Thiele model to determine the number of equilibrium stages required, given reflux ratio, top and bottom product compositions, and feed rate and composition
5. *Posing Problems*	• Use McCabe-Thiele model to solve a variety of distillation problems in which different sets of variables are used as "givens"
6. *Making Connections*	• Apply the McCabe-Thiele model to a column configuration (open steam heating, multiple feed, side stream product) that the student has never seen before
7. *Creating Extensions*	• Recognize that the McCabe-Thiele model is not valid for a given application and articulate how to modify the modeling technique to solve the problem at hand

The following sections give a step-by-step discussion of strategy for advancing the students through the levels of understanding and the tools used to facilitate each transition.

■ *Introduction to Column Distillation*

Haile[8] stated that because "learning creates new structures in the brain by modifying existing structures, learning can only begin from things the student already knows." Flash, or single-stage, distillation is the logical lead-in for column distillation. The limitations of flash distillation were demonstrated by an example problem in which it took five flash stages to produce a desired product of >98% pure A from a feed of 50% A and 50% B. (This is similar to the presentation in Chapter 4 of Wankat's text.) Students began to calculate flow rates and compositions for all streams, given equilibrium data, but they quickly recognized that, practically speaking, the process makes no sense. The "saleable" product stream had a tiny flow rate and there was a clear need to somehow recycle the intermediate fractions.

The class then moved to the Unit Operations Laboratory, where the ten-stage distillation column had been prepared and was operating at steady state. The instructor explained the counter-current functioning of the column and discussed the purposes of the various components of the column (condenser, reboiler, etc.). Next, the instructor posed the question, "How is this like flash distillation and how is it different?" This exercise followed the active learning strategy advocated by Felder, *et al.*[14] The class broke into groups of two to three students each, where they brainstormed lists of similarities and differences, and then the instructor led the full class in a discussion.

These activities were viewed as a vehicle to bring the students to Level 2 of the special hierarchy (Table 2). The next step, as outlined above, was to expose the students to an abstract model of the process and to help them recognize patterns.

■ *Use of HYSYS for Inductive Presentation of Concepts*

Induction consists of starting with observation and inferring the governing physical principles, as opposed to deduction, which consists of deriving the specifics of the case at hand from the general principles. Educators have begun to recognize that induction is a more natural learning mode,[15,16] but most traditional textbooks are written deductively. The chemical engineering department at Rowan University has previously implemented experiments to promote inductive learning of heat and mass transfer.[17] Here, the students gained a qualitative understanding of the physical process of distillation inductively, using the simulator as a rapid way to generate simulated "experimental data."

After seeing the real column, students moved to the computer lab and loaded a HYSYS model of a distillation column, which had been prepared and converged ahead of time by the instructor. Students then went through a short (about five minutes) tutorial on the software, learning how to access significant column parameters (Qc, Qr, reflux ratio, product compositions, temperature profile, internal liquid and vapor flow rates) and how to specify them. The class discussed why each of these parameters is of interest to the engineer—for example, the reboiler heat duty is significant because energy is expensive.

Next, the students were asked to collect simulated data in order to quantify certain patterns, such as

- *The effect of reflux ratio on product purity*
- *The effect of feed stage location on product purity*
- *The effect of reflux ratio on condenser and reboiler heat duty*
- *The effect of number of stages on product purity*

In response, the students took the column through a series of configurations and plotted graphs of the relevant data. After collecting the information, students broke into small groups to brainstorm physical explanations for the trends in preparation for full-class discussion.

During this stage of the process, students also observed that liquid and vapor flow rates throughout the column were nearly uniform. The physical reason for this, involving the energy balance on each individual stage, was another topic for discussion. Students were thus exposed to the physical justification for the constant molal overflow approximation before they knew of its significance in simplifying by-hand calculations.

HYSYS was specifically chosen for this process as part of a department-wide effort to introduce students to process simulation before the senior design sequence. Burns and Sung,[18] however, have created McCabe-Thiele models on spreadsheets and used them for comparable classroom demonstrations. The McCabe software package[19,20] developed at the University of Michigan is also ideally suited for inductive exploration of cause/effect relationships within a column.

The activities described in this section are viewed as a vehicle to instill a romantic understanding (Level 3 in the special hierarchy) of distillation in the students. The transition to a philosophic understanding (Level 4) was achieved by challenging students to devise their own model of the process.

■ *Hand Calculations*

After receiving this thorough introduction to the physical process, students were able to derive the model equations with relatively little guidance from the instructor beyond the simple posing of questions. The sequence of questions is given here; for each, the students spent time working in teams before the full class discussed the results.

1. *The instructor drew a control volume around the entire column and asked the students to list the process variables and brainstorm which of them would likely be given and which would likely be unknown.*
2. *The instructor then asked the students to write balance equations relating these variables to each other. The ensuing discussion led to a determination of the number of degrees of freedom in a column and the most likely ways of fulfilling them.*
3. *Next, the class wrote lists of variables and constraints (mass balance, energy balance, and equilibrium) for an individual stage and determined that no "new" degrees of freedom are introduced when one stage is added to the column.*

At this point, the instructor pointed out that HYSYS models a column by solving these equations simultaneously with the constraint that all stages are at equilibrium. Thus, the function of the "black box" is elucidated.

Next, students were given an example problem involving a ten-stage distillation column and were able to demonstrate that the number of variables and constraints were equal—thus it was possible to attain a complete solution of all column parameters of interest. They also recognized the complexity of solving this many simultaneous equations "by hand." The strategy of solving a system of equations that includes mass balances and equilibrium constraints by plotting both on the same y-x diagram was familiar to the students from the module on flash distillation. The instructor reminded the class of their observation that liquid and vapor flow rates throughout the column were essentially uniform and pointed out how the assumption of constant molal overflow led to mass balances in the form of straight operating lines. Students then learned the graphical technique of stepping off stages. This completed a deductive derivation of the McCabe-Thiele method, which was primarily carried out actively rather than in a lecture format.

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While the McCabe-Thiele method was presented as a "pencil and paper" technique, the spreadsheet models[18] or McCabe[19.20] software package mentioned above could also be introduced at this stage. The crucial point is that the students have received a thorough exposure to the physical process, intended to provide the philosophic understanding required for true model building. They are therefore more likely to appreciate the capabilities and limitations of the McCabe-Thiele model (in whatever form) and less likely to regard it as an arbitrary ritual.

HIGHER LEVELS OF UNDERSTANDING

The activities outlined in the previous sections required, in total, approximately two weeks of class time. Progression through the higher levels (Levels 5 through 7) of the special hierarchy requires practice in problem solving through repetition and examination of variations.[10] In the fall of 2000 this was done exclusively using the McCabe-Thiele model for both in-class examples and homework problems, but in 2001 some homework problems were also completed on HYSYS so that students would have the experience of constructing models from scratch on the simulator. The final assignment in the 2001 module on distillation was one in which students designed the same two-column system both by hand and with HYSYS, comparing the results. This was intended to reinforce the students' understanding of the assumptions and methodology behind both modeling approaches and the limitations of each, consistent with the highest levels of Haile's special hierarchy of student understanding.

LEARNING STYLES

The course structure presented here used both process simulation and McCabe-Thiele modeling in a sequence that is logical according to the learning progression described by Haile. It was also consistent with the variety of learning styles[21] represented in any class

Visual vs. Verbal Learning • The students spent most of their class time discussing the system, either in small groups or with the full class. Throughout the process, however, visual learners were also stimulated. Introduction to distillation was carried out in the lab with a real, working column. Students transcribed the simulated data from HYSYS into graphical form and used the graphs as the basis for the discussion.

Active vs. Reflective Learning[22] • Small-group, active learning exercises were a feature of the entire course. The full-class discussions allowed the instructor to insure that the work from these activities was accurate and that no salient points were missed. But they were also intended to benefit the reflective learners in the class.

Sensory vs. Intuitive Learning[23] • Students were quickly immersed in studying and explaining physical phenomena, a

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Process Simulation

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process that should appeal to an intuitive learner. They did this, however, in a practical context that would also appeal to a sensory learner; they first saw a real column and did an example validating its importance, and then they used HYSYS, which is recognizable as a tool used by "real engineers."

Sequential vs. Global Learning[16,24] • The structure was methodical and well-suited for sequential learners, but was also interspersed with "big picture" insights that were meant to benefit all students, particularly global learners. The first thing the class learned about column distillation was why it was useful. The class discussed the significance of each process parameter before attempting to calculate it or to even relate it to anything else.

TABLE 3
Summary of Course and Teacher Evaluations
Responses were on a scale from 1-5, with 5 being best.

Question	*Fall 2000*	*Fall 2001*
Were the additional activities (HYSYS) helpful for understanding the subject matter?	4.63	4.88
Considering everything, how would you rate this teacher	5.00	4.71
Considering everything, how would you rate this course	5.00	4.65

STUDENT RESPONSE

The course structure described in this paper was used in the fall 2000 and fall 2001 semesters at Rowan University. Table 3 summarizes the results of the course and teacher evaluations of it. Feedback was very positive, both toward the use of HYSYS for inductive teaching on concepts and toward the overall course. Specific student comments included, "Learning HYSYS and seeing what actually happens in a distillation column, etc., was very helpful," and "The in-class HYSYS days were helpful for seeing how the whole process works."

SUMMARY

In assessing how modern process simulators should affect teaching of separations, chemical engineering educators have suggested a blend of simulation with traditional graphical modeling approaches. This paper describes an effective strategy for using these two modeling approaches that was successfully implemented in the fall 2000 and fall 2001 semesters at Rowan University. Students' first introduction to distillation was exposure to a real column and discussion of the practical significance of distillation. Process simulation was used as a tool for inductive presentation of concepts to promote a thorough understanding of the physical process. This was followed by a deductive derivation of the McCabe-Thiele model. The course organization is consistent with what is known about cognition and the progression of student understanding, and it appeals to students with varied learning styles. It was an effective presentation, as evidenced by student feedback. This paper focused on column distillation as an example, but the approach is readily extended to other physical processes.

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