Use of Process Simulation and McCabe-Thiele Modeling in Teaching Distillation

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Abstract

The increasing prominence of process simulation has led to new ideas on how to teach separation processes such as column distillation to students. Graphical techniques such as McCabe-Thiele modeling have value in that they provide a compact framework for visualizing the process and illustrating concepts and phenomena, but no longer represent the state-of-the-art in engineering practice. Process simulators are recognizable as practical engineering design aids, but have pedagogical drawbacks. A student can use process simulation to model a distillation column without understanding the physical process of distillation at all. The challenge is to strike a balance that will prepare students for engineering practice, giving them both a thorough understanding of the fundamentals of the physical process and a familiarity with modern computational tools.

This paper will give a detailed description of the method employed in the Equilibrium Staged Operations course at Rowan University during the Fall 2000 and Fall 2001 semesters. The first introduction to column distillation employed a complete HYSYS model prepared by the instructor. This was used for inductive illustration of such cause-effect relationships as the increase in reboiler heat duty that accompanies increases in the reflux ratio. The instructor then led the class through hand calculations that further illustrated physical explanations for the trends uncovered by the HYSYS model. This ultimately led to a deductive derivation of the McCabe-Thiele model. Hand calculations and HYSYS modeling were then combined in the solution of practical design problems. The paper will detail each step in this process, with examples. It will also discuss how this approach engages students with a wide variety of learning styles. The paper uses column distillation as an example but the approach is readily extended to other processes.

Introduction

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 respondents indicated that they now use process simulators in teaching equilibrium-staged separations.

Simulators certainly have not, and should not, entirely replaced "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 into potential limitations of the modeling approach used. One merit of hand calculations 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[4] points out that even experienced engineers "commonly use McCabe-Thiele diagrams to understand or help debug simulation results." However, the merit of extending the hand calculations significantly beyond the simple graphical method, such as using the Ponchon-Savarit method to include the energy balance, is less clear in the era of process simulation.[5] It is these considerations that lead Wankat to recommend "an eclectic approach that includes classical graphical and analytical methods, computer simulations and laboratory experience."[4]

This paper examines how the balance between these various components can be attained and how they can be made to complement each other. It describes in detail how equilibrium staged operations was taught at Rowan University in the fall 2000 and fall 2001 semesters, with primary emphasis on how McCabe-Thiele modeling and process simulation are integrated. The paper focuses on trayed column distillation as an example but the approach is applicable to other physical processes.

Course Organization

In a series of articles in *Chemical Engineering Education*, Haile[6,7,8,9,10] discussed the operation of the human brain and the learning process. These insights are valuable as a guide in organizing a course. Haile described[7] a "special hierarchy," a progression of seven levels at which a student can understand concepts. These levels are summarized in Table 1, 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[9] also describes 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.[11]
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 4-7 of the special hierarchy require a philosophic understanding.

Table 1: Levels of understanding in the special hierarchy as described by Haile,[7] 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 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

These insights are useful in determining exactly how the course can be structured and what specific role simulation and McCabe-Thiele modeling should play. 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. Next, students are exposed to an abstract model of a column- such as a HYSYS model- that is already complete. Finally, students will learn to derive their own abstract model, namely the McCabe-Thiele model. The special hierarchy is also useful. In chapter 5 of Wankat's text[1], for example, the McCabe-Thiele model is derived and then used as a framework for illustrating such patterns as the tradeoff between reflux ratio and number of stages. However, the special hierarchy suggests an alternative organization in which students are exposed to such concepts and patterns first (levels 1-3). HYSYS proved to be an ideal tool for this exposure. Derivation of a model came later in the context of solving problems (levels 4-5).

Introduction to Column Distillation

Haile[6] 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 produced 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.[1]) 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 recycle the intermediate fractions somehow.

The class then moved to the Unit Operations Laboratory, where the ten-stage distillation column was prepared and 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.[12]: The class broke into groups of 2-3, brainstormed lists of similarities and differences, and then the instructor led the full class in a discussion.

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 style[13] but most traditional textbooks are written deductively. The Rowan University Chemical Engineering department has previously implemented experiments to promote inductive learning of heat and mass transfer.[14] 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. The model was prepared and converged ahead of time by the instructor. Students then went through a short (~5 min) tutorial on the software in which they learned 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 are 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.

The activities described in this section are reasonably viewed as a vehicle to instill a romantic understanding of distillation in the students. The transition to a philosophic understanding 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 and then 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 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 number of degrees of freedom in a column and 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, and thus it was possible to attain a complete solution of all column parameters of interest. But they also recognized that solving this many equations without the aid of the computer wasn't reasonable. The instructor then reminded the class of their observation that liquid and vapor flow rates throughout the column was essentially uniform, and pointed out the enormous simplification that occurs in hand solution of the equations when one assumes constant molal overflow. This completed a deductive derivation of the McCabe-Thiele model, which was primarily carried out actively rather than in a lecture format.

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 (4-7) of the special hierarchy requires practice in problem solving- repetition and examination of variations[8]. In the fall of 2000 this was done exclusively using the McCabe-Thiele model for both in-class examples and homework problems.

However, 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 six-week module on distillation was one in which students designed the same two-column system both by hand and with HYSYS and compared 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[15] 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. However, throughout the process, visual learners were also stimulated. The introductory class was carried out in the lab with a real, working column. Students were asked to transcribe the simulated data from HYSYS into graphical form and these graphs were the basis of the discussion.

Active vs. Reflective Learning:[16] Small group, active learning exercises were a feature of the entire course. The full-class discussion led by the instructor 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:[17] Students were quickly immersed in studying and explaining physical phenomena, a process that should appeal to an intuitive learner. However, they did this in a practical context that would appeal to a sensory learner: they had first seen a real column and done an example validating its importance, and they used HYSYS, which is recognizable as a tool used by "real engineers."

Sequential vs. Global Learning:[16,18] 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 needed. The class discussed the significance of each process parameter before attempting to calculate it or even relate it to anything else.

Student Response

The course structure presented here was used in the fall 2000 and fall 2001 semesters at Rowan University. Table 2 summarizes the results of the course and teacher evaluations. Feedback was very positive, both toward the use of HYSYS for inductive teaching on concepts and toward the course overall. 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."

Table 2: Summary of course and teacher evaluations. Student 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 of 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

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, using column distillation as an example, describes an effective strategy for using these two modeling approaches that has been 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 a 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. This course organization is consistent with what is known about cognition and the progression of student understanding, and appeals to students with varied learning styles. It was a very effective presentation as evidenced by student feedback.

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