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Work in Progress: Building Conceptual Understanding in the Mass and Energy Balances Course through Qualitative Analysis and Interactive Demonstrations

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Introduction

Many students in chemical engineering are adept at solving systems of equations, but they struggle with understanding the meaning behind the variables and values, which leads to a lack of conceptual understanding and reduced critical thinking. This often hinders the students' abilities to apply the concepts while solving practical problems [1]. To address this issue, we restructured some problem statements in the Mass and Energy Balances course. To isolate conceptual understanding from mathematical ability, we dedicated questions on exams where the students were asked to qualitatively analyze relationships between different variables. We developed active-learning computational demonstrations that students could explore in a self-paced manner by manipulating variables and observing the effects on other variables, working in groups and guided by a teaching assistant (TA) and a problem set during recitation [2, 3].

Assessment of conceptual understanding

In the Mass and Energy Balances course during Fall semesters, we divided the semester into four units: Mass Balances, Reactors, Separators, and Energy Balances. After each of these units there was a written exam. In the Reactors unit, we spent multiple lectures analyzing a reactor process with recycle and assigned multiple homework problems that asked to solve for the values of all system and stream variables in the entire process. This recycle system was a valuable model process for instruction in the course because it used each of the four basic process units: a mixer, a reactor, a separator, and a splitter (Figure 1) [4]. With just two reactions and three species, the number of process variables is large, and yet with this fairly complex model we could facilitate discussion of reactor parameters such as fractional conversion, selectivity, and yield.

To teach students to break down complex systems, we encouraged students to look both at the overall system as well as at each individual unit in the block flow diagram. We introduced the "tear method" [4] to enable students to solve these recycle problems by hand and to demonstrate their ability to track species between different process units.

While asking for students to implement the tear method evaluates their mathematical abilities, we also wished to evaluate their conceptual understanding of the various variables. We dedicated a separate exam question on the Reactors exam to qualitative analysis. The recycle system they analyzed involved reactant cyclobutene isomerizing into a desired product methylcyclopropane and an undesired byproduct 1-butene via parallel reactions. The first part asked students to rank-order the molar flow rate of reactant into the overall process, the molar flow rate of reactant directly into the reactor, and the molar flow rate of product out, assessing whether they could understand the physical meaning of these flow rates.

The remainder of the exam question asked students to predict the effects of changing one stream or system variable on another. Students were asked to fill in the blanks in the following statement: "If the engineer increases recycle ratio, at the new steady-state overall fractional conversion will have ____ because ____,” where the first blank required choosing from “increased”, “decreased”, or “stayed the same”; and the second blank required a brief justification. We chose three manipulated variables (recycle ratio, single-pass fractional conversion, and input molar flow rate) and three dependent variables (overall fractional conversion, molar flow rate of desired product out, and mole fraction of undesired byproduct in the purge stream), and all nine pairings of variables were asked.

In the Separators unit, we discussed vapor-liquid equilibrium, Txy diagrams, and flash drums. Intended learning objectives for qualitative analysis in this section included identifying the relevant regions of a Txy diagram; deriving the “lever rule,” a useful tool in analyzing separator systems [4]; analyzing a Txy diagram to estimate bubble and dew point temperatures and phase compositions for a given inlet feed; and, at the highest level of mastery expected, predicting the effects of changing parameters of a system of two flash drums connected in series. The exam question aligned with these learning objectives.

In the first semester when we taught this course and implemented these conceptual exam questions, students anecdotally reported that they found qualitative reasoning for these questions to be challenging. Initial attempts to rectify this before the onset of this study included dedicating more class time to lead students through the thought processes and providing practice exams with similar conceptual questions. To facilitate more active learning, we developed computational demonstrations for these problems where students could manipulate different variables and observe the effects on other variables.

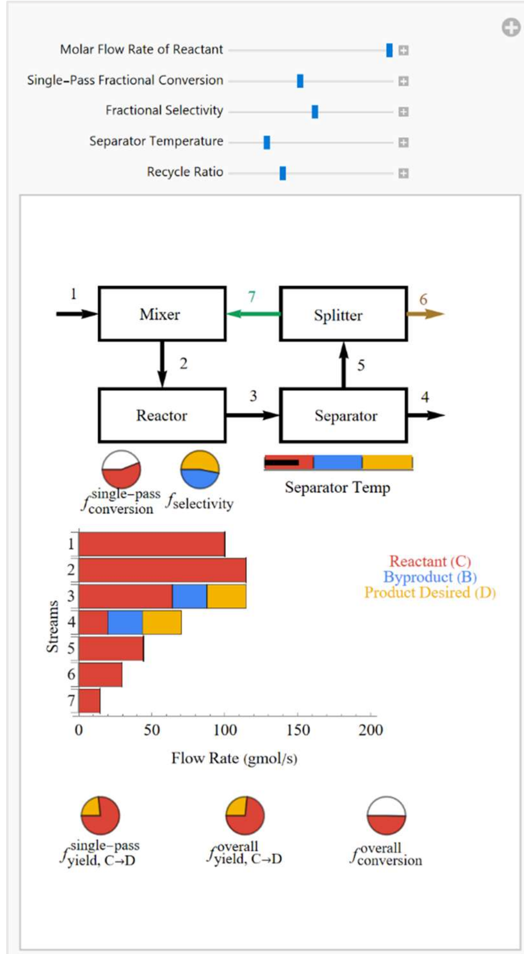

Figure 1. Demonstration for Reactor Process with Recycle. From top to bottom, this demonstration comprises sliders to manipulate variables; a block flow diagram that labels streams and units and visualizes the recycle ratio; accompanying visualizations of single-pass fractional conversion, fractional selectivity, and separator temperature; a bar graph that visualizes partial and overall molar flow rates of each of the three species; and pie charts that visualize single-pass fractional yield, overall fractional yield, and overall fractional conversion.

Design of computational demonstrations and activities

We developed demonstrations for conceptual questions related to recycling and vapor-liquid equilibrium using Wolfram Demonstrations [5]. We chose Wolfram Demonstrations for their built-in slider functionalities, which enabled exploration of variables in a qualitative manner by making increasing or decreasing parameters straight-forward. Each demonstration updates dynamically, adjusting values automatically with each choice of slider position. Manipulating one variable at a time allows the user to observe its effects on the dependent variables.

For the recycle system demonstration, we modeled a steady-state process with two abstracted reactions in parallel, one where reactant C (represented in red throughout the demonstration) produced desired product D (yellow), and the other where C formed undesired byproduct B (blue) (Figure 1). The demonstration allows users to manipulate up to five variables: the molar flow rate of reactant C, the single-pass fractional conversion of C, the fractional selectivity, the separator temperature, and the recycle ratio.

The block flow diagram labels streams and units. The purge Stream 6 (brown) and the recycle Stream 7 (green) arrows grow and shrink in size to visualize the recycle ratio, e.g. with a low recycle ratio, Stream 6's arrow would be large and Stream 7's arrow would be small. Below the block flow diagram are visual representations of the system variables that can be manipulated. Single-pass fractional conversion of C is represented with a pie chart with the fraction of red versus white symbolizing the fraction of C consumed in the reactor in a single pass. Fractional selectivity is represented with a pie chart with the fraction of yellow versus blue symbolizing the fraction of C consumed that becomes D versus B.

The separator model is simplified. The "separator temperature" is not a true temperature, but it is visualized like a thermometer below the block flow diagram to create the analogy. Rather, it determines the fraction of each species that leaves the separator out of Stream 5 versus Stream 4. Like with a separator using vapor-liquid equilibrium, the higher the "temperature", the more "volatile" components leave out the "top" Stream 5. The "thermometer" has three regions, each corresponding to a different species. C was set to be the most volatile, and D was set to be the least volatile. The fraction of each bar that is to the left of the thermometer's temperature level (the right edge of the black bar) represents the fraction that leaves out of Stream 5. Increasing separator temperature elongates the bar to the right and sends more flow up through Stream 5.

The dependent variables appear in the bottom half of the demonstration. The bar graph shows molar flow rates for each species within each stream. Each colored segment corresponds to the partial molar flow rate of that species in that stream, and the combined total length of the bar corresponds to the total molar flow rate of that stream. The pie charts show the intensive properties of the recycle system. The single-pass fractional yield and the overall fractional yield of C to D are each represented by the proportion of the pie that is yellow (D) versus remaining red (C). The overall fractional conversion, similar to single-pass fractional conversion, is represented by the proportion of the pie that is red versus white.

For the vapor-liquid equilibrium demonstration, we modeled a hexane-octane binary mixture passing through two flash drums in series at steady-state (Figure 2). The Txy diagram (Figure 2A, top) displays the saturated liquid line and the saturated vapor line. It also displays the temperatures of each of the flash drums, stream compositions, and relevant tie lines, with line colors indicating its corresponding stream. The large black triangle can be dragged to any position on the diagram and sets the temperature of Flash Drum 1 and the composition of inlet Stream 1. The small gray triangle corresponds to the temperature of Flash Drum 2 and the composition of the stream entering it. The temperature of Flash Drum 2 is set by a slider (not shown) to emphasize the single degree of freedom, and the composition depends on the user's selection of how the two flash drums are connected (Figure 2B). The configuration determines whether the small triangle lines up with the composition of Stream 2 (liquid stream connection) or Stream 3 (vapor stream connection).

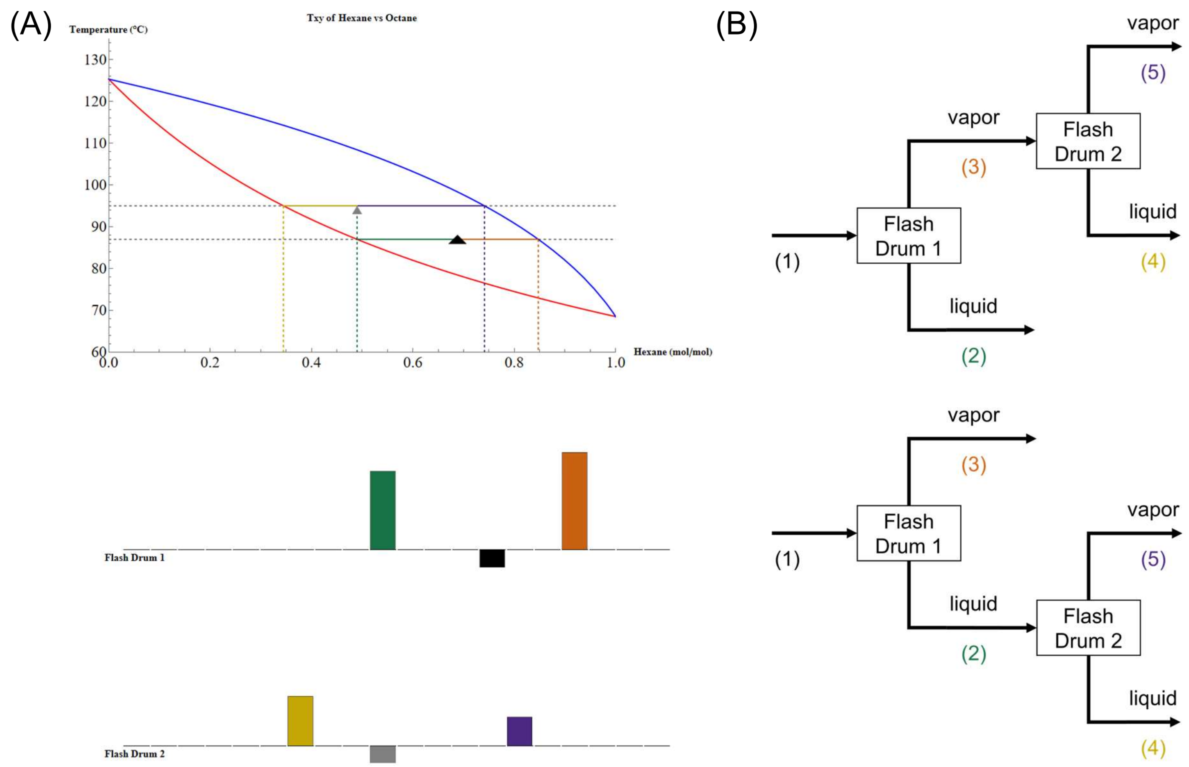

Figure 2. Demonstration for Two Flash Drums in Series. (A) The Txy diagram for a hexane-octane binary system also displays the set temperatures of each of the flash drums, stream compositions, and relevant tie lines. The large black triangle sets the Flash Drum 1 temperature and the inlet Stream 1 composition, and the small gray triangle indicates the temperature of Flash Drum 2 and its inlet composition. Total molar flow rates of Streams 2 (green), 3 (orange), 4 (yellow), and 5 (purple) appear as bar graphs below the Txy diagram, positioned to create a visual representation of the lever rule for each flash drum. **(B)** The user can select whether Flash Drum 2 is connected to the vapor outlet of Flash Drum 1 (top) or to the liquid outlet (bottom). Only one of these configuration diagrams appears within the demonstration at a time to indicate which selection is active. In (A), the bottom configuration is set.

The total molar flow rates of Streams 2–5 appear as bar graphs below the Txy diagram, with their heights showing magnitude and their lateral positions corresponding to their composition (Figure 2A, bottom). With the small fulcrums below each line corresponding to the triangles in the Txy diagram above, this creates a dynamic visual representation of the lever rule for each flash drum, balancing an outlet stream's difference in composition from that of the inlet flow with its relative magnitude of flow rate.

Notably, students are not limited to practical choices of temperature or flash drum configuration. Cases such as working outside of the vapor-liquid envelope are allowed, to demonstrate the effects of all possible design choices on the performance of the separation system.

We chose to introduce these demonstrations during two of the weekly two-hour recitations. These recitations were an existing part of the course, structured to promote peer learning and facilitated by a TA. Thus, they seemed like the appropriate time for students to be encouraged to use the demonstrations. To further guide students, we accompanied each demonstration with a set of questions as part of their normal recitation problem set. The time that students spent on each recitation, with and without these demonstrations, was identical. With no extra time given to these topics, we could make fair comparisons when evaluating the demonstrations' efficacy.

Discussion

In implementing this intervention, we observed some areas we can improve upon in the future. Because few students had Wolfram Player, the software that runs these demonstrations, already installed on their computers, some recitation time was spent on the installation and downloading process. In future semesters, we would ask students to download the software ahead of time. Once the demonstrations are finalized, we can also contribute them to the Wolfram Demonstrations Project library [5] for online access through web browsers.

In addition, these recitations were not directly overseen by the instructor, to give students time with their peers and student TA to explore more freely. Even with a preparatory discussion during the preceding weekly TA meeting, the TAs' familiarity with the software and how hands-on they were in helping students both varied, which may have led to different student experiences. In future intervention semesters, we would provide clearer guidelines for what the TA should and should not do to help the students, to standardize the experience.

Also, because of the complexity of these demonstrations, the software would occasionally lag, which could lead to student frustration as they struggled to manipulate the variables and waited for the dynamic update. We believe this was one of the highest barriers to using these demonstrations, so in future iterations we would look to other programming languages that could provide the same functionalities, including ease of access.

Overall, these demonstrations were promising to promote conceptual understanding. While these demonstrations were illustrative, students could feel even more engaged if the activity were an experience driven by their own curiosity. For the future, we would be interested in gamification of these demonstrations to promote student motivation in addition to active learning [6]. Ultimately, we hope our focus on conceptual understanding will not only build students' intuition and critical thinking skills but also instill more confidence and engagement in the content beyond solving equations.

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