Process Simulators in the ChE Curriculum

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ABSTRACT

Process Simulators has become an indispensable tool for design and retrofit of refineries and petrochemical plants. Originally created for the commodity industry, the advantages provided by these tools have made them also an attractive option for other industrial application such as pharmaceutical and specialty chemicals. Software companies are constantly increasing the capability of simulators to include novel technology and expand their applications market.

In the last twenty years simulators have also become much more user friendly and have been expanded to incorporate equipment design and costing tools. As a result, Chemical Engineering programs throughout the nation started using them for a variety of reasons. Some professors see process simulators as a must-do-must-teach so students are familiarized with their use by the time they graduate. In this case process simulators are generally introduced during the senior design sequence or simply in plant design courses. Others have found in process simulators a valuable teaching aid as well.

At Rowan we introduce process simulators starting at freshmen year and use them as a teaching aid in several courses throughout the curriculum. This process has allowed us to develop valuable lab writeups to use process simulators in all different courses in the curriculum and case studies to show students of the importance of reality checks and the immediate consequences of "blindly" trusting the process simulators results. This paper describes some of the process simulators exercises used throughout the curriculum at Rowan.

FRESHMAN YEAR

Rowan's two-semester Freshman Clinic sequence introduces all freshmen engineering students to engineering in a hands-on, active learning environment. Engineering measurements and reverse engineering methods are common threads that tie together the different engineering disciplines. Previous reverse engineering projects have involved common household products such as automatic coffee makers [1,2,3] hair dryers and electric toothbrushes [4]. Recently, the human body was added to the repertoire of familiar machines to be reverse engineered. In a semester-long project, freshmen engineering students explore the interacting systems of the human body in a hands-on, active learning environment. They discover the function, interaction, and response to changing demands of various systems in the human body: the respiratory, metabolic, cardiovascular, electrical, and musculoskeletal systems. During this project, the students performed several laboratory experiments in which they are introduced to engineering measurements and calculations, mass balances, and process simulation through their application to the respiratory system.

In an in-class workshop, students perform a HYSYS simulation of the respiration process [5]. Students input their own experimental data from a previous experiment in which the compositions and flow rates of inhaled and exhaled air were measured. Students then use HYSYS to perform material and energy balances on the respiration process, and compare the results of the simulation to hand calculations. Several simulations are run to explore the effect of ambient conditions on the relative contributions of sensible and latent heat during respiration. Students explore a range of temperatures and relative humidities that correspond to a range of weather conditions (for instance, a dry winter day, a rainy winter day, a hot desert, and a hot steamy swamp).
The respiration process is represented by two unit operations: a heater which heats the inhaled air to body temperature, and a humidifier that saturates the inhaled air with water. The HYSYS respiration process flow diagram is shown in Figure 1.

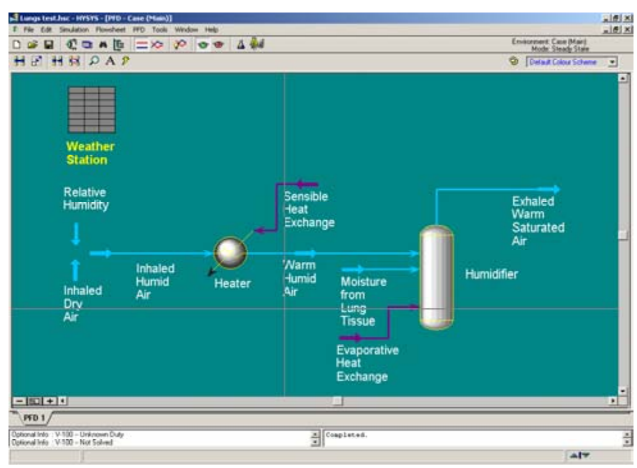

Figure 1: Process flow sheet diagram to simulate the lungs' physiology

The HYSYS flow sheet has been set up to simulate the respiration process by providing the experimentally measured values of flow rates, composition, temperature, pressure and relative humidity. Students enter the

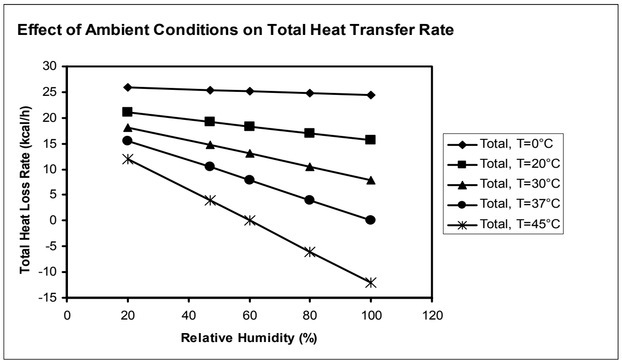

Figure 2: The effect of ambient temperature and relative humidity on the total heat transfer rate during respiration**.**

ambient conditions of temperature, pressure and relative humidity into a spreadsheet operator named the *weather station*. A hidden spreadsheet takes these data and calculates the mole fraction of water in the inhaled air, using the Antoinne equation to determine the vapor pressure of water at the ambient temperature. These steps were necessary because HYSYS requires a water vapor mole fraction rather than relative humidity, to calculate water content of a given stream. The "inhaled humid air" stream represents inspired air at ambient temperature, pressure and relative humidity. The stream called "exhaled warm saturated air" represents the exhaled air at body temperature and pressure, saturated with water vapor; students supply temperature, pressure, flow rate and composition of this stream using their experimental data.

Temperature and pressure values for the intermediate streams called "warm humid air" and "moisture from lung tissue" are also supplied by students. HYSYS completes the material balances and students compare their process simulation results with their hand-calculated results.

Using the HYSYS process simulator to simulate the sensible heat and latent heat changes during respiration, the role of respiration in thermal regulation of the body is investigated. Figure 3, Figure 2, Figure 4 show the total, sensible, and latent heat transfer rates (respectively) under varying ambient temperature and relative humidity. Using the resting data from the experiment, the overall rate of heat transfer through respiration at rest (and at ambient conditions of the experiment) is about 19 kcal/h, or 23% of the total resting energy expenditure.

By performing HYSYS simulations at different combinations of ambient temperature and relative humidity, students can make the following important observations about heat transfer during respiration:

1. The total rate of heat loss via respiration decreases with increasing RH and with increasing temperature. Heat loss is

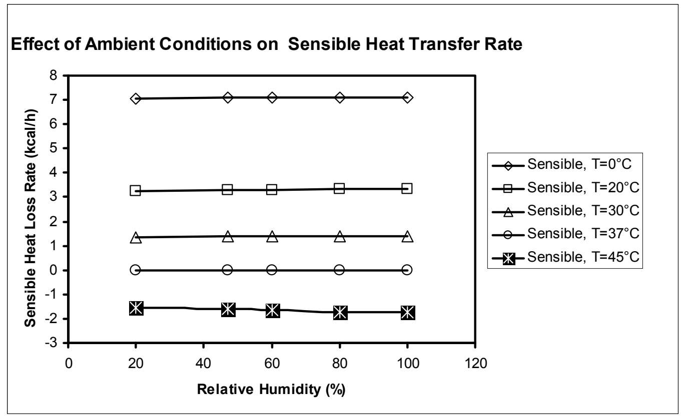

Figure 3: The effect of ambient temperature and relative humidity on the sensible heat transfer rate during respiration

positive except under the most extreme conditions of high T and RH when the heat loss is negative and heat is transferred to the body via respiration. This extreme combination of high temperature and humidity is an uncommon weather condition; however, the transfer of heat to the body under these conditions explains why it is necessary to limit steam saunas to short periods of time. Heat loss occurs via evaporative cooling in dry conditions, and this causes a net cooling effect even when the ambient temperature is higher than body temperature.

2. The sensible heat transfer contribution becomes more significant when ambient temperatures are farther from body

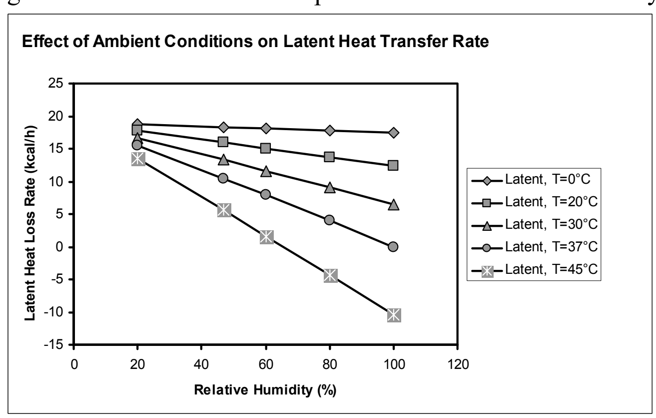

Figure 4: The effect of ambient temperature and relative humidity on the latent heat transfer rate during respiration.

temperature (at cold and hot extremes). Sensible heat losses are greater at cool temperatures and show little dependence on relative humidity. When the ambient temperature exceeds body temperature (37 °C), sensible heat losses are negative.

3. The latent heat loss rate decreases with increasing RH and with increasing temperature. When the ambient air is at 37°C and 100% RH, the total sensible and latent heat losses are exactly zero. In very hot and dry conditions, an overall cooling effect is achieved by a high rate of evaporative cooling (note that at 45 °C and dry conditions the total heat loss and the latent heat loss are both positive, while the sensible heat loss is negative). In extreme hot, humid conditions, the latent heat loss becomes negative because water can theoretically condense in the respiratory system (causing further distress to the person who stays in the steam sauna for an extended time!). (In order to obtain the data for hot humid conditions in which water condenses in the respiratory tract, the order of the heater and humidifier were reversed on the HYSYS flowsheet).

A HYSYS handout can be found at
http://engineering.rowan.edu/~farrell/hohb/HYSYS.htm

SOPHOMORE YEAR

All Rowan Chemical Engineering students have a two-semester sequence of courses in material and energy balances. During the sophomore spring semester, in Principles of Chemical Processes II, the students are presented with a chemical process which it has been dissected into a sequence of homeworks and labs assignments. The objective of the course and the assignments is to teach them how to carry out more complex material and energy balances such as those dealing with phases changes, recycles, and chemical reactions. Students performed mass and energy balances in all units by hand and when necessary, they calculate and/or estimate physical properties, enthalpies, transport properties, etc. They are also taught how to calculate the utility needed in a chemical plant.

Once the student cohort has a good understanding of the principles and the techniques used in solving such problems by hand, they are given a set of computer lab exercises to perform similar calculations using a process simulator. In the past five years we have designed several HYSYS and ASPEN Plus exercises to use in this calls. We currently use three modules that have proven to be very useful as teaching aid. These are:

1. Introduction to Bubble Point, Dew Point and Flash Calculations.
2. Introduction to Piping Calculations.
3. Introduction to Heat Exchangers

The first of the three modules is designed to aid in teaching degrees of freedom of a given system, bubble point and dew point concepts for multicomponent systems, and finally the concepts of isothermal and adiabatic flashes. The module is usually the first in the sequence and therefore it allows the instructor to discuss the importance of picking the appropriate thermodynamic package. This cohort has not yet had a thermodynamic course but they do know about cubic equations of states such as Peng Robinson and SRK. The instructor can also address the issue of property estimation vs. experimental data by using the available ASME Steam thermodynamic package and showing how water and steam properties come out different when using an equation of state that estimate them instead of using the experimental data that the steam package provides. This is also the first time the students are asked to set up the complete simulation since in the case of their freshman experience, they are provided with a template created by the instructor and they just enter data in it. Once they have selected the chemical species, the units system and the thermodynamic package, the students create the first stream and they vary the vapor fraction from zero to one to calculate the bubble point and the dew point respectively. The data provided in this exercise was taken from Example 2-1 of Wankat [6]. After this part of the exercise has been completed, the students are instructed to solve and extension to the prior problem is which they enter a temperature between

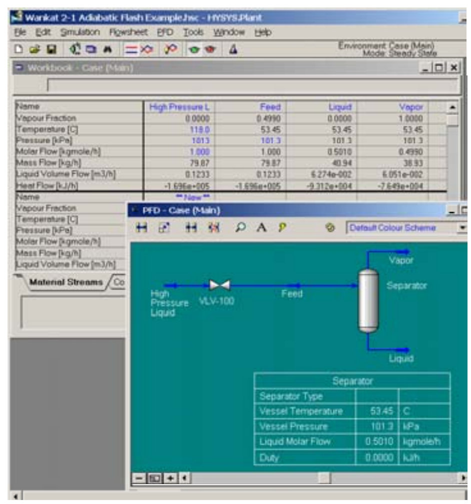

Figure 5: HYSYS adiabatic flash results page

the bubble and the dew point temperatures and they report the vapor fraction so they can realize that it lies between zero and one. Finally, the students add a simple two-phase flash unit, a heater and a valve to simulate either an adiabatic or and isothermal flash process. Figure 5 shows one of the HYSYS screens the lab write-up provides so students can compare their results.

In module two, the students simulate two heat exchangers of the Rowan Cogeneration Plant (Figure 6). First, the students go to the plant and they take readings of temperatures, flowrates, and pressures throughout the entire power generation cycle. Second, the students are provided with a computer lab handout to guide them through the simulation of the two heat exchangers identified at the cogeneration plant. This lab gives the students an opportunity to simulate real plant data and compared the simulator's results against those measurements taken at the plant. Figure 7 shows a typical HYSYS output for the simulation of the two heat exchangers [7]

The final sophomore module presents student with a set of exercises to calculate pressure drops in piping systems.

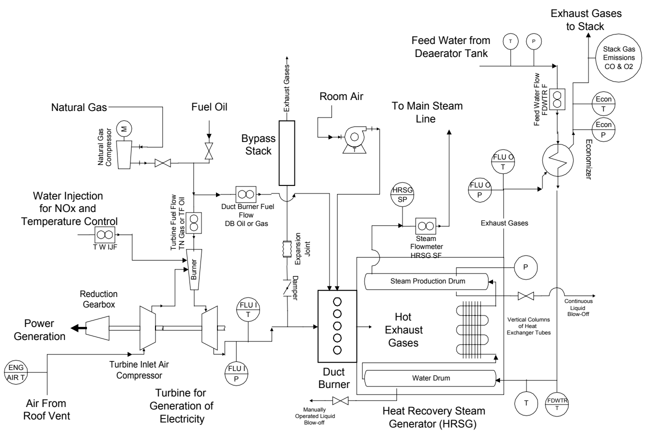

Figure 6: Rowan Cogeneration Plant

The module also introduces the concept of feedback controller in a problem in which students let the simulator find the maximum liquid flowrate that could circulate in a piping network given a total pressure loss constraint. This is obtained by adding and Adjust operator in HYSYS which varies the flowrate of liquid to meet a pipe-outlet-minimum pressure. Figure 8 shows the output from HYSYS.

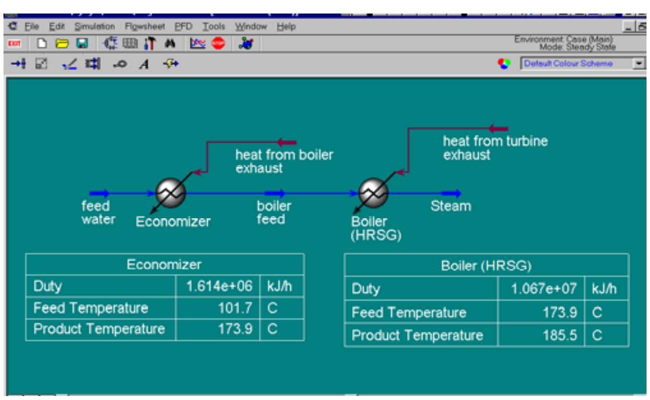

Figure 7: HYSYS screen for the sophomore module on heat exchangers simulation.

JUNIOR YEAR

During the junior year, students work with simulations of single unit operations. They receive an initial introduction to physical processes through models prepared by the instructor, and later revisit the processes and construct their own models. [8]

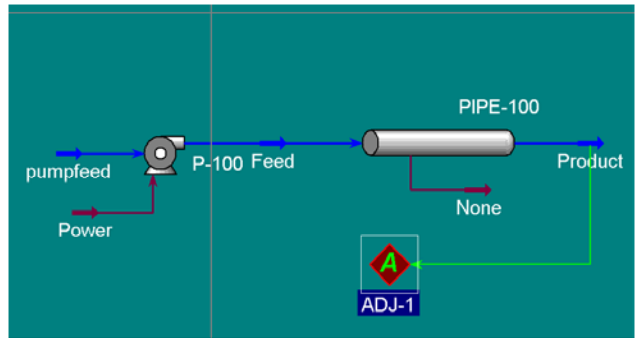

Figure 8: Piping system with feedback controller

Use of Process Simulators for Inductive Learning

Induction consists of starting with observations 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 [9,10] but most traditional textbooks are written deductively.

Here, the simulator is used as a tool for an inductive introduction to a process. Students in Equilibrium Staged Operations, a fall junior course, are first introduced to a new physical process (distillation, absorption, stripping, extraction) through a HYSYS model prepared and converged ahead of time by the instructor. They go through a short (~5 min) tutorial on the software in which they review how to access significant parameters (heat duties, product compositions, temperature profile, product and solvent flow rates, etc.) and how to specify them. The class also discusses 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. Examples for column distillation would include:

- 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

The full class then shares and discusses the results. Students thus have a qualitative understanding of the physical process and the cause-effect relationships between the process parameters before they attempt to derive equations or model the processes quantitatively.

A similar technique is used in Chemical Reaction Engineering, a spring junior course. Students use prepared models of reactors to explore the effects of temperature, initial concentration and pressure on product yields, and explain the results qualitatively, before attempting to solve problems. In subsequent homework problems or laboratories, they are required to produce their own, working models of these processes, "from scratch."

Some of the HYSYS handouts for sophomores and junior courses can be found at:
http://engineering.rowan.edu/~hesketh/0906-316/index.html

SENIOR YEAR

Rowan's design sequence comprises of two courses. In the fall semester, senior students have Chemical Process Component Design. This course is tailored to teach basic engineering. The spring course is the typical capstone Chemical Plant Design course in which students design a complete chemical plant and process simulators are fully employed as design tools.

In Chemical Process Component Design a weekly double class period is used to learn and experience more complex features of process simulators. Students are challenged with complex problems and decision-making strategies starting with thermodynamics property packages selection, followed by an array of simulation problems for short cut distillation, absorption and stripping, multicomponent distillation, rigorous design of shell and tube heat exchangers, optimal diameter of piping system calculations, and chemical processes optimization. In the spring semester, besides using the process simulator for their plant design projects; students are given assignments to explore heat integration, mechanical design of shell and tube heat exchangers, heating utility minimization and process evaluation as well as dynamic simulation techniques.

A strong emphasis is placed on having the students understand the importance of the accuracy of the input data and also the importance of a critical reality check of the results obtained from any process simulator or their peripheral software.

CONCLUSIONS

At Rowan Chemical Engineering process simulators are being used as pedagogical tools to support inductive and deductive teaching as well as to reinforce important principles learned in core courses. A set of exercises is proposed for each year of the entire curriculum.

Students' responses from this type of learning environment are quite positive and encouraging.

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