INCORPORATING COMPUTER-AIDED SOFTWARE
in the Undergraduate Chemical Engineering Core Courses

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The chemical engineering curriculum at the American University of Sharjah (AUS) incorporates computer-aided software packages at an early stage to promptly familiarize the students with plant operations and professional practice, and enhance their overall experiences and successes. As will be discussed in this paper, ideas for the integration of computer software into the ChE curriculum are outlined within journal papers.[1,2]

The Chemical Engineering Department at AUS was established in 1997. Currently, the department has 11 Ph.D. faculty members and three laboratory instructors. Each course has approximately 30 students and convenes for one hour, three days a week. The program is ABET accredited, first in 2006 and again in 2012. Teaching methods include a combination of PowerPoint presentations and standard whiteboard use. At present, the number of chemical engineering students enrolled in our program is 408, with 55 percent being female. The new M.S. graduate program has an enrollment of 20 graduate students. A Bachelor of Science in ChE degree requires a total of 140 credits hours. The general educational requirements consist of 12 credits in English language, three credits in Arabic heritage, six credits in mathematics, eight credits in science, and 15 credits in humanities and social sciences. Figure 1 (page 18) displays a flowchart of the course sequence. Approximately 40 students graduate each year, and the graduates are hired by various chemical industries. Additionally, 10% of the graduating students proceed to complete a graduate degree, either at AUS or abroad in Europe or North America. Within the two engineering buildings at AUS, there are five computer labs, each equipped with 25-30 desktops. Software including HYSYS, MATLAB, MATHCAD, PRODESIGN, Control station, and SIMULINK are installed on all computers.

The incorporation of computer-aided software instruction in the undergraduate ChE courses begins in sophomore-level courses, namely Chemical Engineering Principles II (ChE 206) and Computer Methods in Chemical Engineering (ChE 240). ChE 206 is a sophomore course designed to familiarize students with material and energy balances. AUS educators apply process simulation as an educational tool at such an early stage to enhance the learning process. Early exposure to such valuable tools enables students to understand and better relate to existing chemical engineering problems and also allows them to experiment with different operating conditions

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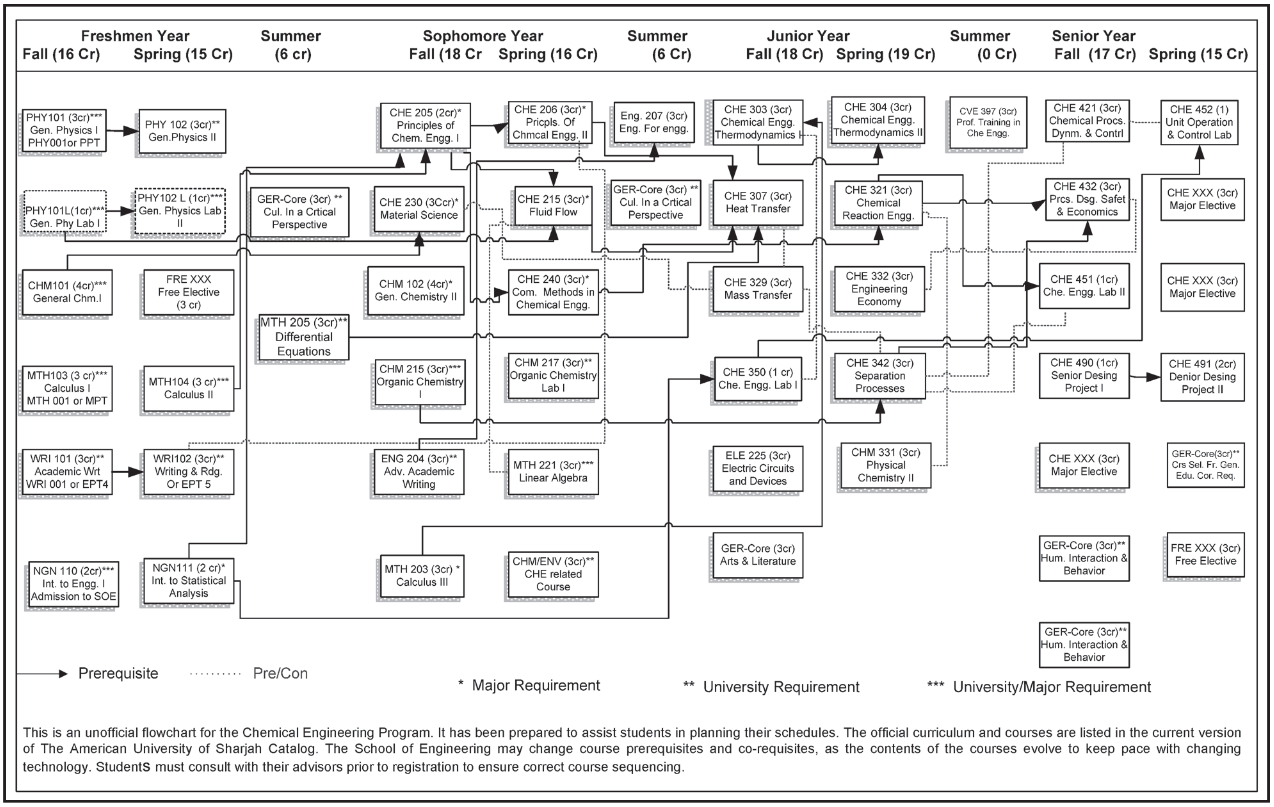


Figure 1. *Curriculum flow chart of the Chemical Engineering Program at AUS, Catalog 2012-2013.*

without the need for a laboratory. The course ChE 240 uses MATLAB[3] to solve numerical computational problems in chemical engineering.[4] Moreover, Aspen HYSYS[5] is used to assist students in solving a number of process flowsheet problems, fitting equilibrium data to different thermodynamic models, defining reaction kinetics, and optimizing process performance under different operating conditions by performing sensitivity analysis. As students' knowledge and abilities in the simulators increase, more complicated scenarios and processes of vapor-liquid separations using HYSYS challenge the students along every step of the way.

At the senior level, the process simulator HYSYS is not only employed in the capstone course Process Design, Safety, and Economics (ChE 432), but also in several undergraduate technical electives, such as Oil and Gas Chemical Processes. The use of HYSYS and other simulation tools appears to increase student interest regarding the subjects and improve their process of learning. Plant design case studies taken from Reference 6 are assigned as group term projects, typically constituting 20-30% of the total grade for the entire course.

Likewise at the senior level, educators integrate MATLAB, Simulink, and Control Station Loop-Pro software[7] in the Process Dynamics and Control course (ChE 421). The students immediately become more comfortable with control theory applications as these tools alleviate the burden of the mathematical complexity associated with tackling more realistic process cases, such as distillation columns, heat exchangers, and reactors. In Loop-Pro, real processes are interfaced with a virtual operator console view in which the students can monitor various control instruments within the process and attempt different controller settings to visualize closed-loop responses.

IMPLEMENTATION MECHANISMS

This section approaches the process of incorporating computer-aided software in three undergraduate chemical engineering core courses. For the core courses and their accompanying workshops, faculty overcame one of the major obstacles encountered when teaching design in the capstone courses by exposing the students to existing industrial experiences. In this regard, we strongly agree that our experiences may be helpful in improving the design and implementation of capstone courses in chemical engineering.

1) Chemical Engineering Principles II (ChE 206)

ChE 206 is a sophomore course designed to familiarize students with material and energy balances. Equipment simulation used as an educational tool enhances the course textbook material covered in Reference 8. Students are initially introduced to HYSYS after 4 weeks of instruction, after which they have studied and solved problems relating to the First Law of Thermodynamics including calculating the work shaft of compressors, turbines, and pumps, and the heat required for heat exchangers, condensers, evaporators. The

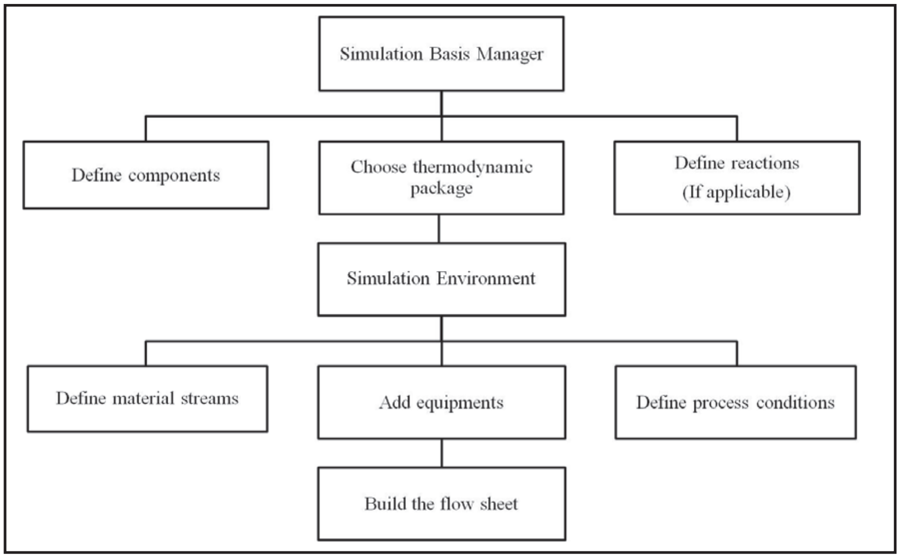


Figure 2. *Flow chart for explaining steps in HYSYS simulations.*

first HYSYS recitation introduces general concepts associated with the software, *e.g.*, compound listing and formulas, the database of physical properties, and add-on required chemicals: organics, electrolytes. The available thermodynamic packages are also discussed, including the equations of state, kinetic equations and models, and solver toolboxes. The second recitation explains how HYSYS works. First, students are taught how to select components and their thermodynamic packages. Streams are selected together with their flow rates and energies. Next, the equipment is selected and connected to the specified streams, and during the same recitation, the flow chart in Figure 2 is discussed. Thereafter, students are instructed on how to define units. The third and fourth recitations discuss the following three simulation examples:

a) *Mixing Water Streams*

b) *Modeling a heat exchanger*

c) *Lowest energy requirement of a Reboiler.*

The fifth recitation concerns the reactors. Students are requested to simulate a simple continuously stirred tank reactor (CSTR), during which they are instructed how to specify reaction kinetics.

These examples are selected to help students in future thermodynamics, heat transfer, and reactor design courses. The three courses expand on the HYSYS usage and provide more detailed and involved simulations problems.

To ensure that students have acquired the basic HYSYS understanding needed for their future chemical engineering courses, two homework assignments are given that involve the simulation of a simple refrigeration cycle. The students must calculate the work shaft of the compressor, the heat absorbed by the evaporator, and the heat released by the condenser. Additionally, students must answer multiple-choice questions on the final exam relating to their basic HYSYS skills, which typically constitute 10% of the final exam grade. Two examples of such questions are displayed in the supplementary material section.

2) Separation Processes course (ChE 342)

Chemical engineering students enroll in the Separation Processes course (ChE 342) during the second semester of their junior year. ChE 342 entails the design of chemical separation systems, and topics include the design of equilibrium-based single and multistage separations (distillation, absorption/stripping, and extraction).[9] Mass balances, thermodynamics, and engineering equipment design are used to simulate separation processes. Students must submit a term project that requires them to perform both hand calculations and HYSYS simulation to design a separation process. To enhance students' understanding of separation processes, visual demonstrations involving laboratory and industrial processes are presented in class during the first week of the semester. The use of visual aids, such as CDs, appears to improve students' understanding of the current topics as evidenced by the course outcomes and the senior exit surveys. Afterwards, both analytical and graphical methods are employed to design single and multiple stages in distillation, absorption, stripping, and solvent extraction.

The HYSYS package was successful in designing the above separation processes as evidenced by the students' response to whether "the approach of teaching appears to be effective and is able to balance between the different components (analytical and graphical) to enhance students' understanding." See Table 1.

TABLE 1

Students' response (based on the last 7 semesters) to whether "the approach of teaching appears to be effective and is able to balance between the different components (analytical and graphical) to enhance students' understanding."

Semester	# of students	Weighted Average response
Fall 2010	24	4.17
Spring 2011	23	4.35
Summer 2011	13	4.23
Fall 2011	34	4.28
Spring 2012	27	4.46
Summer 2012	16	4.36
Fall 2012	25	4.32

3) Chemical Process Dynamic & Control (ChE 421)

Students explore the use and benefits of the Control Station Loop-Pro training simulator, MATLAB, and SIMULINK for the Process Control and Dynamics (ChE 421) course. A process-control training simulator provides an interactive learning environment that enhances learning by integrating the theoretical abstraction of textbooks with the tactile nature of the lab or simulated plant. The primary objective of a training simulator is education; it can motivate, help with visualization, and provide hands-on practical experience. These benefits are evident from the high level of student participation and interest in classroom activities. Further, students' demonstrations on the simulator during assignment presentations highlight their greatly improved skills.

The first workshop is devoted to reviewing some basic MATLAB commands learned in earlier courses, yet with additional emphasis on ODE solutions. For example, a 5-stage absorption dynamic model,[10] a CSTR dynamic model,[11] and three heated-tanks in series dynamic model[12] are examined. Students are asked to simulate the dynamics of such processes using the ODE solver in MATLAB (*e.g.*, ode45) by stepping several forcing function inputs. The students are then able to visualize outputs and quantify the effect of different input(s) on the model output(s). The second workshop introduces students to MATLAB commands used for calculating dynamic responses utilizing transfer function models. Dynamic responses of first-order and second-order transfer functions are explored using commands such as "step" and "impulse." Students also learn how to evaluate ramp, sinusoidal, and other forcing dynamics using the "lsim" command. Finally, the Simulink program introduces students to its graphical user interface for the simulation of dynamic systems.

Upon completion of both workshops on MATLAB and Simulink dynamics, students must apply the learned tools to the transfer functions derived from the dynamic models given in their prospective projects. The students compare open-loop dynamic responses from the rigorous dynamic model (with the ODE package) with others evaluated with transfer function models using MATLAB commands and Simulink. Such methods provide the students with insight on how the linearization of the model can affect the accuracy of the model predictions as transfer function models are derived using Laplace transforms.

A follow-up workshop is available after the students learn about PID controllers in class. Closed-loop simulation using Simulink is demonstrated, and the students are given a simple example of how Simulink blocks can be applied to different components of closed loops, including the PID controller, the process transfer function, the sensor, the valve, set-point and disturbances, and the scope.

Furthermore, students explore PID tuning and closed-loop simulation using the Loop-Pro (Control Station) case studies and also apply Internal Model Control (IMC) tuning-based rules for tuning the PID controller based on model parameters fitted previously for the case study.[10] The case studies processes available in the Control Station include level control of a tank, temperature control of a heat exchanger, concentration control of a reactor, and purity control of a distillation column. The controllers available include P-only, PI, PD, and PID, as well as cascade, feed forward, multivariable decoupling, model predictive (Smith predictor), and discrete sampled data controllers.

STUDENT QUESTIONNAIRES

As discussed above, computer-aided modeling and simulation are incorporated early into the chemical engineering program in an effort to familiarize students with plant operations and professional practice. Students' perceptions of this approach are extremely positive and encouraging. Students' testimonies also affirm that utilizing such tools greatly enhanced their learning capabilities and understanding of the theoretical course materials. Responses from former students include:

"I have to say that the Chemical Engineering Program at AUS is very good and so powerful that I did not need further training after graduation."

"Though it was very difficult, I can see the difference now

TABLE 2
The questions asked in the five-point Likert Scale questionnaire:

1	Computer-Aided Software helped me in solving ChE problems
2	The use of Computer-Aided Software enhanced my understanding of ChE problems
3	I would rate my experience of Computer-Aided Software during my sophomore courses as excellent
4	Using the software as part of my modeling and simulation lab work enhanced my education experience
5	Using Computer-Aided Software in my sophomore courses increased my ability to simulate case studies in higher courses
6	Introducing simulation in Principles of ChE course improved my understanding of materials and energy balances
7	Use of simulators in the separation processes course enhanced my understanding of process separation units and their operations
8	Flowsheet simulators provided a useful tool for equipment design and operation performance rating
9	Use of simulators has improved my understanding of process control theory
10	Use of control software trainer helped me to understand and communicate complex control theory in a practical and meaningful manner
11	Use of computer-aided software in many ChE courses provided me with superiority over my peers in my profession or other colleges

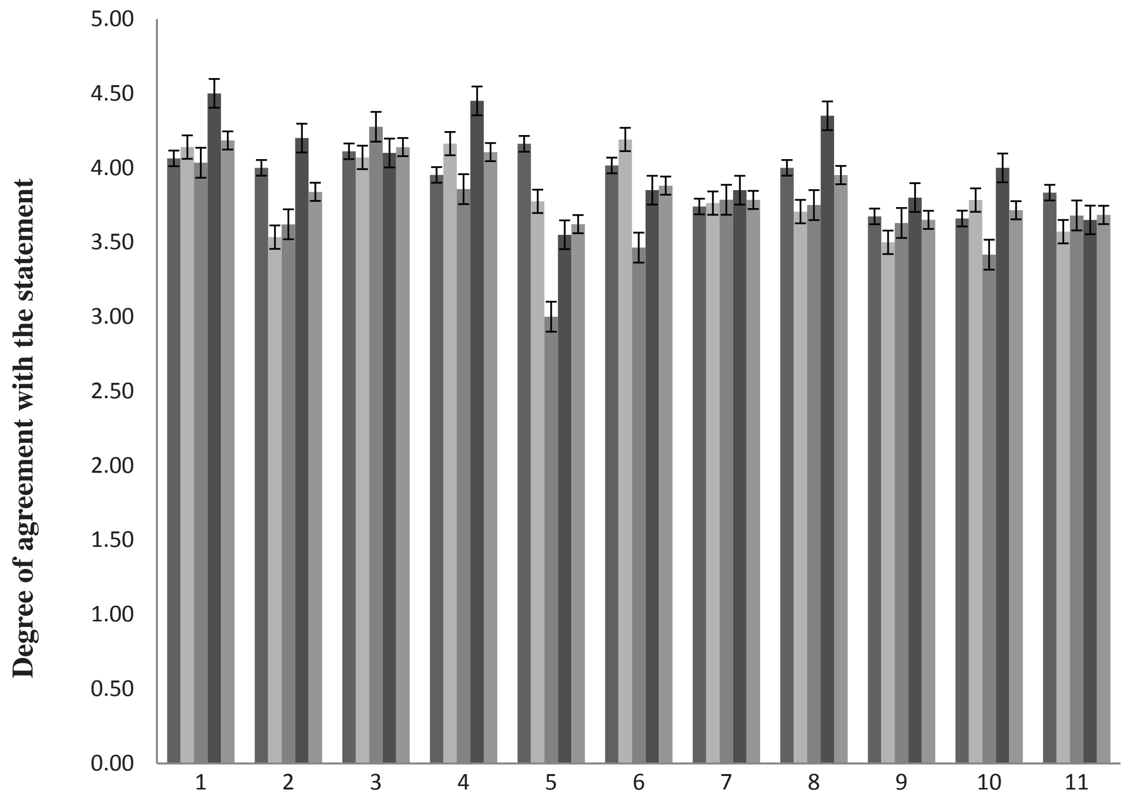
between myself and other fresh-graduate engineers from other universities."

"At AUS, we start using the simulation software during the second year while other universities do not even have it in their program."

"Working as a process engineer is very easy and enjoyable, but it's only because I had a very good base from AUS."

"We are well prepared for working in the industry."

We believe that student feedback is crucial in gauging student perceptions related to modeling and simulations in the Chemical Engineering Curriculum at AUS. Hence, to assess student experiences with computer-aided software in ChE courses, we conducted a five-point Likert Scale questionnaire: Strongly Agree (5), Agree (4), Undecided (3), Disagree (2), Strongly Disagree (1), and No Experience (0); see Table 2. Participation was voluntarily and anonymous, and only summary statistics were reported. No penalty was levied for non-participation. Figure 3 summarizes the responses of 155 participants, including sophomore, junior, senior, and graduate students, and alumnus, of a survey conducted in the spring of 2013. The survey results suggest student confidence in process design was strong. The responses to all questions had an average of three or higher, out of five. More than 80% of the respondents "strongly agreed" or "agreed" that computer-aided software helped them in solving chemical engineering-related problems (question 1), and that the use of computer-aided software enhanced their understanding of chemical engineering problems (question 2). Students attested that their knowledge and understanding of process controllers had increased because of the modeling and simulation exercises discussed in class (question 9). Other areas, including the use of flowsheet simulators, provide beneficial tools for equipment design and operation performance rating. Moreover, introducing simulators in the Principles of Chemical Engineering courses improved student understanding of materials and energy balances (question 7), shown also by strong responses. Question 3 is associated with the students' apprehension toward learning and using computer-aided software. More than 70 % of the responses indicate that the use of computer-aided software featured in many ChE courses provided them with superiority over their peers outside of AUS (question 11).



	1	2	3	4	5	6	7	8	9	10	11
sophomore	4.06	4.00	4.11	3.95	4.16	4.02	3.74	4.00	3.67	3.66	3.83
Junior	4.14	3.53	4.07	4.16	3.78	4.19	3.76	3.71	3.50	3.78	3.57
Senior	4.03	3.62	4.28	3.86	3.00	3.46	3.79	3.75	3.63	3.42	3.68
Graduate & Alumni	4.50	4.20	4.10	4.45	3.55	3.85	3.85	4.35	3.80	4.00	3.65
Avg all classes	4.18	3.84	4.14	4.11	3.62	3.88	3.78	3.95	3.65	3.72	3.68

Figure 3. *Results of the five-point Likert scale questionnaire.*

CONCLUSIONS

Incorporation of computer-aided software into the chemical engineering curriculum at AUS enhances students' learning in subsequent courses. The examples presented in this paper illustrate how the standard chemical engineering curriculum is considerably enhanced with a series of hands-on computer exercises and projects. Students' exit surveys and testimonials reveal that a software integration strategy is an effective method for teaching ChE courses. In conclusion, the use of simulation tools significantly increases the students' interest and attraction toward the courses, and the major in general, while simultaneously improving their learning processes and better preparing them for their future positions as chemical engineers.

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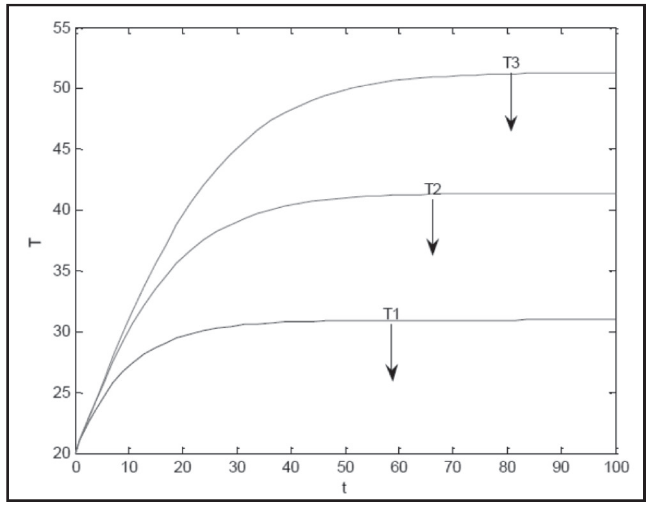


Figure A-1. *The output profiles for the three heated tanks' dynamic simulation.*

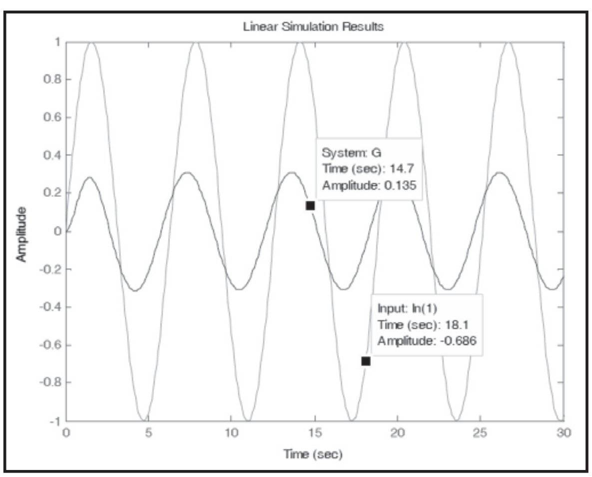


Figure A-2. *Dynamic simulation using Matlab "lsim" command for a sinusoidal forcing function.*

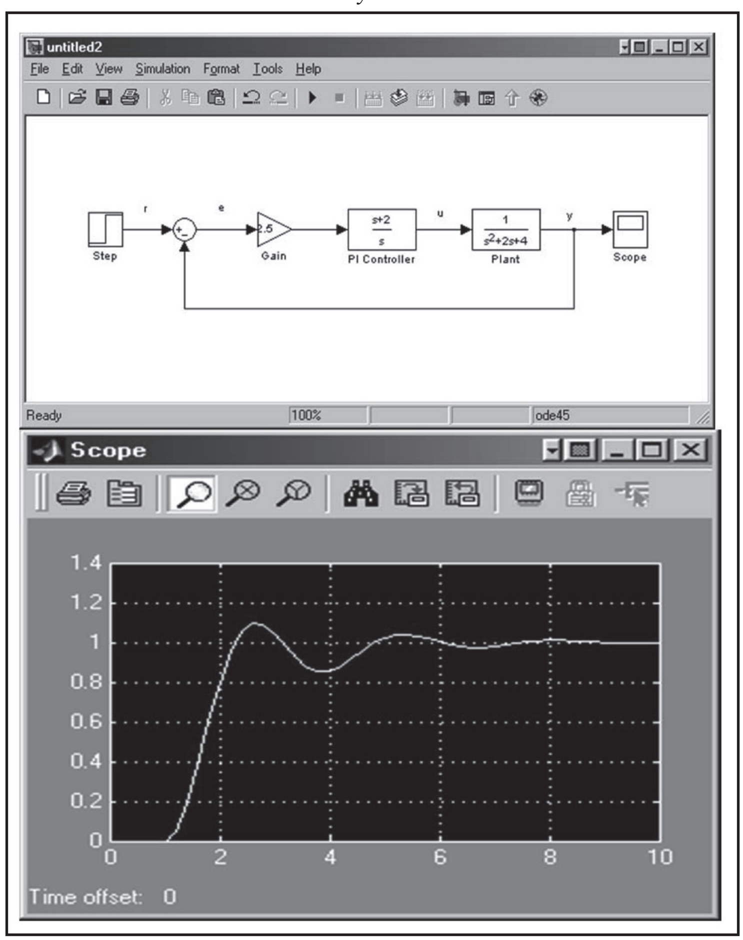


Figure A-3. *Example of Simulink tutorial workshop for closed-loop simulation.*

APPENDIX

Figures A-1 through A-4 are part of the Appendix.

I. Two examples of final exam questions that deal with HYSYS

1. If a stream has a known temperature, pressure, composition, and flow rate, and it is necessary to pump that stream to a higher pressure, then a HYSYS simulation of such a stream should:

a) Specify the temperature, pressure, composition, and flow rate of the exit stream

b) Specify the temperature and composition of the exit stream only

c) Specify the pressure, temperature, and flow rate of the exit stream

d) Specify the temperature, composition, and flow rate of the exit stream

e) Specify the pressure of the exit stream only

2. In HYSYS, getting a consistency error suggests that:

a) You have over-specified your system and need to review all defined parameters

b) HYSYS is corrupt and you need to contact the company

c) One of the values you defined may be incorrect or unrealistic

LOOP-PRO PID Tuning Report

LOOP-PRO PID Tuning Parameters

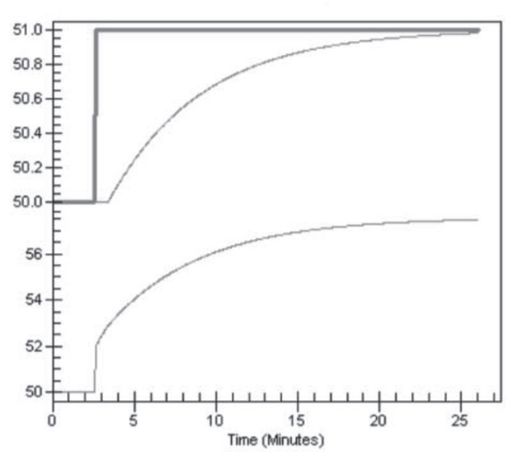
PID Controller Loop-Pro Generic Controller Algorithm

	K_C	τ_I(min)	τ_D(min)	α
P-Only	****			
PI	1.977	1.704		
PID	****	****	****	
PID with Filter	****	****	****	****
Existing	****	****	****	****

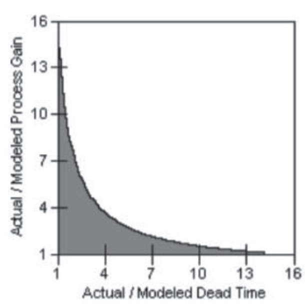
Closed Loop Time Constant, τ_C : 5.8 min

Tuning Style: Moderate Tunings

LOOP-PRO PID Response



Robust Stability Plot



Legend

LOOP-PRO Performance Statistics

	Stability Factor	Settling Time (min)	Percent Overshoot	Decay Ratio	CO Travel (%CO/hr)	IAE	ITAE
P-Only	****	****	****	****	****	****	****
PI	3.753	20.65	N/A	N/A	17.21	6.412	51.44
PID	****	****	****	****	****	****	****
PID w Filter	****	****	****	****	****	****	****
Existing	****	****	****	****	****	****	****

***Figure A-4.** PID Controller tuning output using Loop-Pro Control Station.*

d) (a) and (c)

e) (b) and (c)

f) (a) and (b)

II. Control Workshops Examples

1) Dynamic simulation of three heated tanks in series. See Figure A-1 (page 22).

The model equations are defined in the following m-file:

```
function f=proj_assg1model(t,T)
f=zeros(3,1);
w=100;
m=1000;
UA=10;
Cp=2;
To=20;
Ts=250;
f(1)=[w*Cp*(To-T(1))+UA*(Ts-T(1))]/
(m*Cp);
f(2)=[w*Cp*(T(1)-T(2))+UA*(Ts-T(2))]/
(m*Cp);
f(3)=[w*Cp*(T(2)-T(3))+UA*(Ts-T(3))]/
(m*Cp);
```

2) Exploring dynamics using Matlab commands

Below is a MATLAB example for finding a sinusoidal response for the given transfer function model G(s).

Example:

Simulate the response of

$$G(s) = \frac{s+0.5}{s^2+2s+4} \text{ for } u(t)=\sin(t) \text{ for } t=[0,30].$$

The output is shown in Figure A-2 (page 22).

3) SIMULINK

A simple demonstration was given to show how SIMULINK can be used for closed-loop simulation. Figure A-3 (page 22) shows an example of this tutorial.

4) PID Tuning using Loop-Pro Control Station τ

Based on the identified model done in Workshop III, students tuned a PID controller. Figure A-4 (page 23) shows typical program output for control design tools using Loop-Pro with PI control. Students explored the effect of changing controller tuning parameters (K_c, τ_I, τ_D, and τ_c) on the controller performance. ❒