ENHANCED UNDERGRADUATE LEARNING THROUGH INTEGRATION OF THEORY AND COMPUTATIONAL TOOLS

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BACKGROUND

In the engineering discipline, it is of utmost importance to value applied learning because as engineers we are expected to innovate, and innovations happen when theoretical ideas are implemented successfully. Utilizing programming and simulation tools is one way of demonstrating the virtual implementation of ideas at low cost and minimum risk. Designing computational modules that can support such learning initiatives are very well known and have shown evidence of better student understanding and preparation for future careers. Moreover, prior research in chemical engineering education has indicated the need for revisions in the traditional curriculum and teaching methods to meet the needs of a modern chemical engineer.[1–4]

The Chemical Engineering department at Rowan University was founded in 1995 as a part of the Henry M. Rowan College of Engineering located in Glassboro, New Jersey. It has been a consistently high-ranking department in the US News rankings since 2002 (when it was first ranked) with its unique Engineering Clinic program integrated throughout the four-year curriculum.[5] The undergraduate curriculum is presented in Figure 1. The Engineering Clinic courses are shown with black borders. Freshman and Sophomore clinics are common activities for all students irrespective of their engineering discipline. Junior/Senior clinics are discipline-specific where students get an opportunity to choose their projects. These projects are offered by the engineering faculty based on their research expertise. The core chemical engineering courses and electives in the department are highlighted with grey borders. Enhanced learning through the integration of theory with computational tools is proposed for the Process Dynamics & Control course and two new approved electives: Process Optimization and Experimental Methods in Chemical Engineering (shown with star markers in Figure 1).

Among these, the Process Dynamics & Control and Process Optimization courses have benefitted from this integrated approach. For each course topic, a supporting computer lab session was designed to substantiate student learning and simultaneously enhance mathematical modeling and computational skills. Additionally, team projects promoting the novel approach were assigned in the Process Optimization course. Guidelines for topic selection, project development, and evaluation rubrics were also provided. The training in computer labs to solve state-of-the-art problems via multiple programming and solution platforms provided the students with an opportunity to select computational tools best-suited for their team projects. Furthermore, allowing students to work on the in-class assignment problems and discussing their computing issues provided insights into learning barriers as compared to traditional lecture-based teaching. We were able to discuss problem formulation errors, incorrect module selection, programming syntax errors, illogical initial guesses, incorrect solvers, lack of an output function, and illogical results generated from ill-conditioned problems.

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Process Dynamics & Control (Required Senior Level)

This course introduces the concepts of process dynamics, modeling, and control of process systems when subjected to input disturbances or pre-determined changes. Principles of mathematics, science, and engineering are integral aspects of this course. The students apply concepts from mathematics, such as linear algebra, differential equations, and Laplace transformations. Scientific concepts from chemistry and physics are applied while solving specific problems in class, homework, and computer labs. Engineering principles are employed for process identification, model development, and controllability studies.

Process Optimization (Senior-level and Graduate Elective)

The course focuses on methods and algorithms for solving optimization problems and also introduces the applications in areas of chemical engineering process design, supply chain management, reaction kinetics, etc. The topics included in this course are linear optimization, nonlinear optimization (convex and nonconvex), discrete (integer) and mixed-integer optimization, network flow problems, heuristic optimization methods, uncertainty characterization, stochastic optimization, optimal control, and multi-objective optimization. Some case studies involving process modeling and optimization are also included in the computer labs.

FIRST YEAR			
FALL	CR	SPRING	CR
Rowan Core Elective	3	Composition I ENGL01.111	3
Calculus I MATH01.130	4	Calculus II MATH01.131	4
College Chemistry I CHEM06.100	4	College Chemistry II CHEM06.101	4
Fresh. Engineering Clinic I ENGR01.101	2	Fresh. Engineering Clinic II ENG01.102	2
Intro to Sci Prog CS01.104 (3 CR) *OR Intro Prgm CS01.102 (3 CR) OR Comp Sci & Prgm.*	3	Introductory Mechanics PHYS02.200	4
Total	16	TOTAL	17
SECOND YEAR			
FALL	CR	SPRING	CR
Principles Chemical Processes I CHE06.201	2	Principles Chemical Processes II CHE06.202	2
Calculus III MATH01.230	4	Math for Engrg Analysis MATH01.235	4
Approved Biological Science Elective	3	ChE Fluid Mechanics CHE06.241	2
Organic Chemistry I CHEM07.200	4	Approved Advanced Chemistry Elective	3
Soph. Engineering Clinic I ENGR01.201	4	Soph. Engineering Clinic II ENGR01.202	4
TOTAL	17	TOTAL	15
THIRD YEAR			
FALL	CR	SPRING	CR
ChE Thermodynamics I CHE06.310	3	ChE Thermodynamics II CHE06.315	3
Separation Processes I CHE06.312	2	Separation Processes II CHE06.314	4
Process Fluid Transport CHE06.309	2	Chem Reaction Engineering CHE06.316	4
Jr Engineering Clinic I ENGR01.301	2	Jr Engineering Clinic II ENGR01.302	2
Heat Transfer Processes CHE06.311	2	*Rowan Core Elective* or ChE Materials CHE06.381	3
ChE Materials CHE06.381	2		
Rowan Core Elective	3		
TOTAL	16	TOTAL	16
FOURTH YEAR			
FALL	CR	SPRING	CR
Chem Process Component Design CHE06.401	4	Chemical Plant Design CHE06.406	3
Unit Opns Expt Design & Analysis CHE06.403	2	Unit Operations Lab CHE06.404	2
Process Dynamics & Control CHE06.405 ✱	3	Approved ChE Elective III CHE06.___	3
Approved ChE Elective I CHE06.___	3	Approved ChE Elective IV CHE06.___ ✱	3
Approved ChE Elective II CHE06.✱	2	Sr Engineering Clinic II ENGR01.402	2
Sr Engineering Clinic I ENGR01.401	3	*Free Elective*	3
TOTAL	17	TOTAL	16
TOTAL CREDITS 130			

Figure 1. *Undergraduate chemical engineering curriculum of Rowan University.*

Experimental Methods in Chemical Engineering (Senior-level and Graduate Elective)

This is a newly proposed elective course that provides hands-on experience with experimental techniques and computer-aided methods for materials characterization and solutions to contemporary research problems in Chemical Engineering as well as in a variety of other engineering disciplines. This is a modular course that includes experimentations and computer-aided software packages such as ASPEN®, GAMS®, COMSOL®, MATLAB®, Python®, and ImageJ®. Each topic listed in the module involves an independent computer laboratory session where pre-defined tasks are provided to the students.

APPROACH

Design thinking is one approach[6,7] that can enhance the understanding of theoretical concepts and their applications to different types of problems in more meaningful ways. The five stages of design thinking (Figure 2) include: (1) Empathize, (2) Define, (3) Ideate, (4) Prototype, and (5) Test.[8] The traditional engineering curriculum focuses on the last four stages and thus leads to a skewed perspective among students with regards to problem definition, formulation, and solution. Thus, the development of the 5-stage design-thinking inspired computational labs and group assignments as part of the Process Dynamics & Control core-course and the two elective courses, Process Optimization and Experimental Methods in Chemical Engineering, are presented in this paper. Team projects from the Process Dynamics & Control and Process Optimization courses, along with the detailed guidelines and evaluation rubric that mapped onto each of the design thinking stages, are also discussed.

The Process Dynamics & Control course has been offered every fall semester, the Process Optimization course has been offered twice, and the new elective course, Experimental Methods in Chemical Engineering, has been offered once to the graduate students in the chemical engineering department. Thus, this paper focuses on the computational labs that were accomplished in the two courses offered more than once to the undergraduate students as well as their team projects. The computational labs were a short introduction to the design

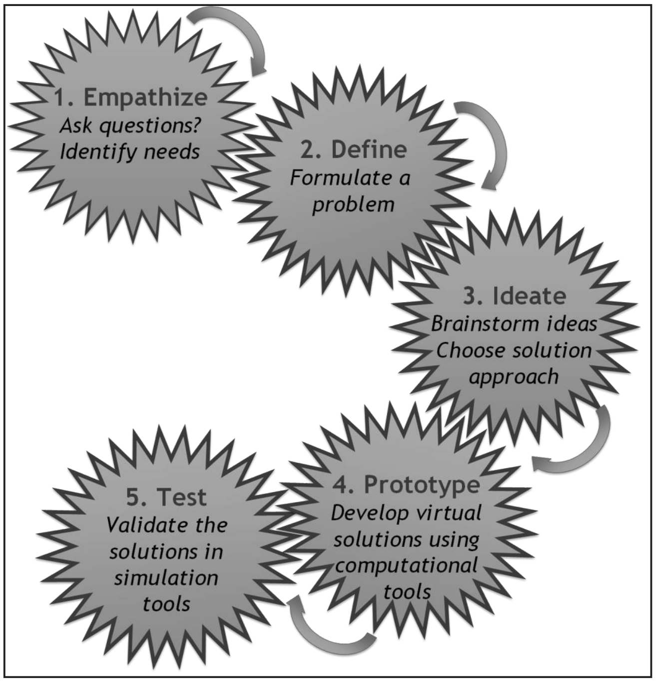


***Figure 2.** Design thinking and its five stages that can enhance chemical engineering education. Graphic designed by the author.*

thinking concepts. Later when students selected team projects and worked on them for about 5-6 weeks, they became more familiar with these concepts.

There are a lot of supporting studies on including systems design in solving engineering problems, especially wicked problems,[9,10] using the design thinking approach. Many real problems do not have a single solution, and sometimes one solution may be applicable under one set of conditions, whereas some other solution is appropriate for the second set of conditions. This is also the case when dealing with multiple criteria [11,12] or uncertainty.[13–15]

Stage 1 in design thinking (Empathize) is implemented by relevant data collection and analysis in computational modules and team projects. For data collection, the students use resources such as peer-reviewed journals, case studies, reports by the US Environmental Protection Agency, National Institute of Health, national labs, public databases,[16] market reports,[17] conferences, and networking events. The collected information is analyzed using data analytics and machine learning methods in tools such as RStudio® and Excel® Data Analytics solver. In Stage 2 (Define), the problem is defined by including the insights from the data collection and analytics aspect. The solution strategies in Stage 3 (Ideate) are implemented in programming tools such as GAMS (General Algebraic Modeling Systems), MATLAB, Simulink®, and P-Graph®.[18–20] The solutions are compared with analytical results (if possible). Virtual implementations of the results are done via simulation tools such as ASPEN and SuperPro Designer®,[21] allowing the students to complete Stage 4 (Prototype) and Stage 5 (Test).

Integrating machine learning,[22] programming, and simulation tools while developing the overall computational modules in courses highlighted using the star markers in Figure 1 is novel because Rowan students are introduced to the capabilities of computer-assisted methods in decision making for real-world problems, and applications. Additionally, they gain the ability to analyze different datasets, solve large-scale problems, and evaluate outcomes and impacts from different perspectives such as economical, commercial, environmental, social, and political. The overall exercise of implementing the design thinking approach is challenging, but at the same time, very motivating to our students. For example, finding an appropriate location for building a plant site among multiple options is a very valid problem for the industry. However, when designing a plant location, we have to evaluate the profitability of the process, its vicinity to the market, transportation accessibility, storage facility, market-demands, political climate, competition, public acceptance, environmental impacts, etc.

EXAMPLES OF COMPUTATIONAL LAB MODELS

1. Computer Lab for Process Dynamics & Control

Students in this Process Dynamics & Control course were able to design a controller configuration (feedback/cascade with P/PI/PID parameters) in MATLAB/Simulink for a temperature-sensitive explosive material to be transported on the interstate with regional limitations and seasonal changes (Figure 3).

In this example the students thought about the seasonal variability in ambient temperature conditions as well as the regional temperature variations in the United States. For example, winter temperatures in Florida will be significantly higher as compared to that in Massachusetts. Additionally, they learned about the controller design and parameter tuning by testing candidate values for K_C (controller gain), τ_I (integral time constant), and τ_D(derivative time constant). This led to the understanding of the controller design under different control configurations with various types of controllers available.

2. Computer Lab for Process Optimization

In the Process Optimization course the students were able to perform kinetic inversion (parameter estimation) for a consecutive reaction system by applying their knowledge of non-linear programming. They were also able to predict the time of reaction to maximize the production of an intermediate product by using the dataset of species concentrations with respect to time (Figure 4).

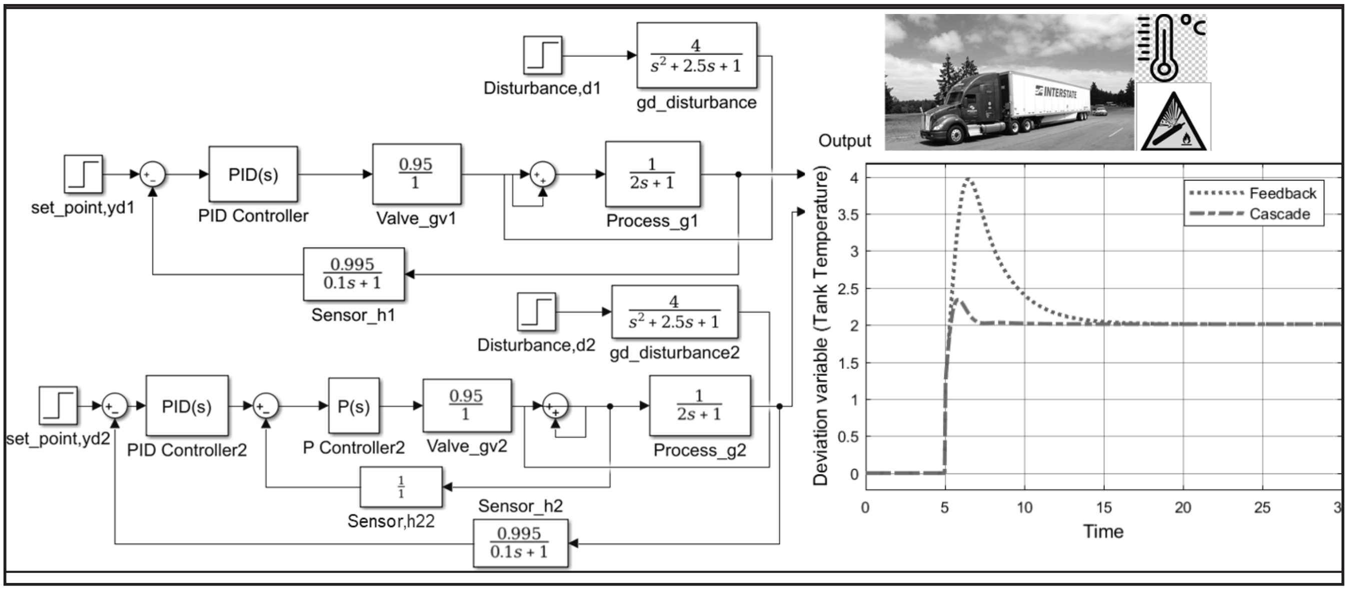


Figure 3. Cascade control loop design implemented in Simulink in a Computer lab session for the Process Dynamics & Control course. The feedback control, shown by the blocks with #1 (e.g. Process_g1, Sensor_h1, Valve_gv1, set_point, yd1, Disturbance, d1), response is denoted by the light grey curve (dot) in the output figure. The cascade control, shown by the blocks with #2 (e.g. Process_g2, Sensor_h2 and h22, Valve_gv2, set_point, yd2, Disturbance, d2), response is denoted by the dark grey curve (line-dot) in the output figure.

Reaction mechanism

$$A \overset{k_1}{\rightarrow} R \overset{k_2}{\rightarrow} S$$

Kinetic model equations

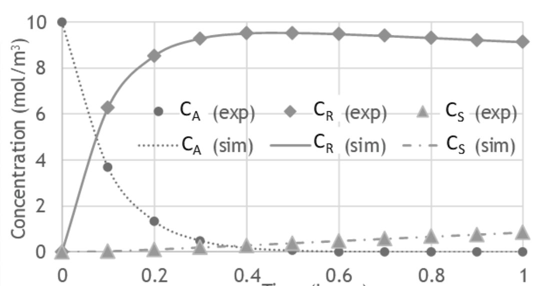
$$C_A(t) = C_{A0}e^{-k_1 t}$$

$$C_R(t) = k_1 C_{A0}\left[\frac{e^{-k_1 t}}{(k_2-k_1)} - \frac{e^{-k_2 t}}{(k_2-k_1)}\right]$$

$$C_S(t) = C_{A0}\left[1 + \frac{k_1 e^{-k_2 t}}{(k_2-k_1)} - \frac{k_2 e^{-k_1 t}}{(k_2-k_1)}\right]$$

Experimental data

Time (hr)	C_A (mol/m³)	C_R (mol/m³)	C_S (mol/m³)
0	10.00	0.00	0.00
0.1	3.68	6.28	0.04
0.2	1.35	8.53	0.11
0.3	0.50	9.30	0.20
0.4	0.18	9.52	0.30
0.5	0.07	9.54	0.39
0.6	0.02	9.49	0.49
0.7	0.01	9.41	0.58
0.8	0.00	9.32	0.68
0.9	0.00	9.23	0.77
1	0.00	9.14	0.86



Results: $k_1 = 9.9941$; $k_2 = 0.100$

Time for Maximum R = 0.42 hour

Figure 4*. The consecutive reaction mechanism of reactant A converted to intermediate product R and R converted to final product S. These reactions are occurring at different rates. The data for the concentration change of A, R, and S are used to determine the values of* k_1 *and* k_2 *(rate constants) and subsequently the concentration for species R is maximized to obtain the time value for the highest availability of R within the reaction mixture.*

GROUP PROJECTS

Along with computer labs, the students also participated in semester-long group projects as a team of four students. The project topics were selected by the teams following an initial literature review, discussion with the instructor, and selection of appropriate programming tools and solution platforms. The concept of design thinking was well integrated in the proposed solutions as a part of these group projects. The topics covered within these group projects varied from traditional chemical engineering design problems such as the optimal design of a shell and tube heat exchanger to practical day-to-day life examples of diet and nutrition optimization. Innovative and interesting examples such as recipe and ingredient cost optimization, ski trail distance, and bar-crawl path optimization were also presented by student teams. They used programming and software tools, which they learned in the computer labs, and they sometimes presented a comparison of results and computing times in different optimization platforms to discuss computing issues, efficiencies, and realistic results.

Project Guidelines

The students were provided with the team formation, topic selection, and stage-wise implementation guidelines within the first month of the semester. The implementation was expected in three phases: (1) project topic selection and team formation, (2) literature review and list of objectives, and (3) final presentation and technical report. Students were made aware of the basic literature review tools like Google Scholar™, SciFinder®Scholar and citation managers like Zotero® and Mendeley®. Some guidelines on categorizing journal articles into reviews as well as original research articles containing experimental data, model information, or optimization and control methodology were also provided to the students. In phase 2 students were expected to find and report on at least one paper from each category. The review articles helped them understand the problem relevance, and the original research articles assisted in data collection and problem formulation. The solution approaches were based on the course concepts as well as the computational labs conducted for each course.

Evaluation Rubric

The evaluation rubric (Table 1) that maps to the 5-stages of design thinking was provided to the students. This rubric was developed through resources provided by the Experiential Engineering Education (ExEEd) department at Rowan University and the Kern Entrepreneurship Education Network (KEEN).

TEAM PROJECT EXAMPLES

Process Dynamics & Control: Wind Turbines for Harnessing Energy

A team of four students worked on the problem of controlling the operation of a wind turbine for harnessing energy. As per the design thinking approach, the students were able to empathize with the fact that to meet the needs of the growing population, renewable energy is the solution. They investigated the growing energy demands as well as conducted a literature review on renewable energy sources. They understood the variability of wind velocity and the influence of weather conditions and formulated the problem of controlling the rotor speed of a wind turbine with two specific objectives: (1) creation of transfer functions to model rotor speed with wind speed disturbances, and (2) implementation of feedback control using P/PI/PID controller.

They identified the four control block components and their transfer functions by analyzing information from different sources.[23–26] The process block consisted of the wind turbine where the control variable was identified as the rotor speed. The wind speed was considered to be the disturbance. The set-point control problem for the rotor speed and the disturbance control problem for the variable wind speeds were formulated. The sensor was assumed to be 100% accurate and hence had negligible dynamics. The drive train actuator was also assumed to be very fast. Using the process block transfer function, they first determined the controller gain stability limits using the direct-substitution method[27]. The four control blocks were modeled in Simulink and using the critical controller gain (K_C) and the critical frequency (ω_C) values, the P/PI and PID controllers were implemented using the Ziegler-Nichols controller tuning rules. The best controller that was able to maintain the rotor speed with minimal deviations was identified as the PID controller. Thus, through a group endeavor, the students were able to formulate a realistic problem of harnessing wind energy, and the computer lab and theoretical concepts of feedback controller design and tuning assisted them in solving the problem in Simulink. A technical report and relevant computation files submitted by the students were evaluated, and it reflected their holistic design thinking approach for problem formulation and solution.

Process Optimization: Dieting Plan

A team of three students worked on the development of a dieting plan to minimize the difference between the individual's current weight and their ideal weight as well as the food cost. Their rationale behind the problem selection was the rising obesity across the United States and its direct link to several chronic diseases such as type-2 diabetes. Along with the primary objective of weight loss over a period, the secondary objective was to determine the decision variables that primarily impact weight loss and ensure that the model adheres to healthy eating practices.

The problem was formulated as a multi-objective mixed-integer linear programming model. The first objective function was the absolute difference between the goal weight and the final weight. This was calculated based on the number of calories, fats, carbohydrates, and proteins the subject consumes, which were constrained based on the amount needed to maintain a healthy diet. The second objective function reflecting food cost was calculated based on how many servings of each type of food were consumed. The number of servings of each food was determined based on macronutrient composition and cost per serving. A general rule of thumb followed by dieticians is that losing one pound per week is the equivalent of burning 3,500 calories per week more than the amount consumed.[28] The number of calories burned each week was calculated using the Harris-Benedict equation.[29]

TABLE 1 **Evaluation rubric for group projects that map to the 5-stages of design thinking**		
Criteria	**Points**	**Explanation of Grade Points**
Project Topic Map to Empathize (1) and Define (2)	5	The report presents a substantial topic and gives a concise and compelling motivation for why the project is significant. This includes a discussion of relevant economic, social, global and economic considerations related to the topic.
	3	The report presents a workable topic that required students to use the principles learned in the course, but the discussion of the motivation and significance of the topic isn't very compelling. There is a cursory mention of relevant economic, social, global or economic considerations.
	1	The topic chosen is badly suited to the project.
Literature Review Map to Empathize (1) and Define (2)	5	The report presents a strong literature review that identifies a variety of relevant and credible sources and gives a thorough and insightful analysis of what was learned from each source and how it relates to the project.
	3	The report presents an acceptable literature review that includes the minimum number of required credible sources. The report gives some insight regarding information learned from the literature, but with noticeable shortcomings (e.g., demonstrates only a surface understanding of the source material, doesn't thoroughly connect the source material to the project)
	1	The literature review has fundamental problems: Doesn't meet the minimum number of sources required, sources are not credible, information from the source material is badly misrepresented or misunderstood, etc.
Application of Relevant Principles Map to Ideate (3)	5	The report demonstrates mastery of principles relevant to the project, including a thorough understanding of techniques learned in this class and general chemical engineering principles as needed. The authors present a sound approach to the problem and execute it accurately and efficiently.
	3	The report demonstrates knowledge of principles relevant to the project, showing the use of techniques learned in this class and general chemical engineering principles. The authors have a strategy for approaching the problem but make some minor errors in executing it.
	1	The report is fundamentally flawed in its discussion of relevant engineering principles. The authors give no evidence of a strategy for solving the problem or describe a strategy that is unsound and won't produce useful results.
Conclusion/Solution Map to Prototype (4) and Test (5)	5	The report presents a thoroughly optimized solution to the stated problem and presents a clear, valid and compelling explanation for how the solution was reached.
	3	The report presents a plausible solution to the stated problem and presents a rationale for how the solution was reached, but some shortcomings are evident (e.g., some missed opportunities for improvement, lack of clarity regarding how some decisions were made, questionable interpretations of some facts or evidence)
	1	The report presents no clear conclusion or solution, or the conclusion or solution presented is fundamentally wrong.

The formula for a male to maintain his weight:

$$BMR = 66.5 + (13.75 \times \text{kg Wt}) + (5.003 \times \text{cm Ht}) - (6.755 \times \text{age in years}) \quad (1)$$

The formula for a female to maintain her weight:

$$BMR = 655.1 + (9.563 \times \text{kg Wt}) + (1.850 \times \text{cm Ht}) - (4.676 \times \text{age in years}) \quad (2)$$

Activity factor to estimate the total daily energy expenditure (TDEE):

$$TDEE = BMR \times 1.35 \quad (3)$$

TDEE is a function of height, weight, age, and gender. Since the weight is not constant, TDEE kept changing over time. An iterative update loop was incorporated to update the individual's weight and corresponding TDEE each week; the difference between energy intake and expenditure was used to determine the change in weight, which was used to calculate the TDEE for the following week. The calories necessary for consumption were broken down into three macronutrients: (1) protein (1 g equivalent to 4 calories), (2) fat (1 g equivalent to 9 calories), and (3) carbohydrates (1 g equivalent to 4 calories) [30] The range of each component in total calorie intake was expected to be 10-35% protein, 45-65% carbohydrates, and 20-35% fat. All this information was implemented into the optimization program as constraints to determine the weekly consumption for each macronutrient. Additionally, the total amount of calories were required to meet a minimum of 1,200 for women and 1,500 for men as per the minimum recommended daily intake.[31] A hypothetical 30-year-old male weighing 100 kg striving to reach a goal weight of 80 kg was used to test the effectiveness of the problem formulation and code. The results showed that if the male were to eat 1,820 calories per day (71.6 g of protein, 292.0 g of carbohydrates, 40.7 g of fat), he would reach his goal weight by week 28 while spending about $16.90 every week.

The students identified that the diet plan still needs to be modified since no individual would like to eat the same food every week. There could be food groups and some flexibility to maintain variety among food choices. Additionally, an exercise regime could be incorporated to increase the overall effectiveness of the predictions. Thus, the group projects enabled the students to think about more realistic issues when designing and solving a problem, and they were also able to comment on future work and revisions needed that were not addressed within the limited timeframe.

SUMMARY

Due to this integrated training, the students were able to solve large-scale case studies and advanced problems with broader contexts. For example, in Process Dynamics & Control, they were able to design a controller configuration (feedback/cascade with P/PI/PID parameters) for a temperature-sensitive explosive material to be transported on the interstate with regional limitations and seasonal changes. In Process Optimization the students were able to perform kinetic inversion (parameter estimation) for a consecutive reaction system by applying the knowledge of non-linear programming. They were also able to predict the time of reaction to maximize the production of an intermediate product. Furthermore, the group projects provided the students with an opportunity to explore their creativity and imagination, which led to solutions to challenging problems by using the tools and resources that they learned during the computational labs. The additional guidelines to implement the group projects in three phases and the evaluation rubric assisted them in systematic thinking, problem formulation, and solution.

ACKNOWLEDGMENTS

I would like to thank the Department of Chemical Engineering at Rowan University for their support and technology resources which helped in the implementation of these ideas. I also thank Dr. Mary Staehle and Dr. Zenaida Gephardt for their assistance in developing the computer lab assignments in the Process Dynamics & Control course.

This work is partly supported by an internal KEEN (Kern Entrepreneurship Education Network) Curricular Reimagination Grant. I thank Dr. Cheryl Bodnar and Dr. Kevin Dahm for their assistance in developing the evaluation rubric for the Process Optimization course.

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