An Exploratory Study of the Role of Modeling and Simulation in Supporting or Hindering Engineering Students' Problem Solving Skills

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Background and Motivation

In the context of problem-solving in science and engineering, the use and creation of computing artifacts are being used to understand and design systems [1]. Specifically, the role of modeling and simulation has become the new form of literacy in engineering domains. In educational contexts, simulations have been primarily used for inquiry learning and conceptual change [2]. Modeling and simulation are promising learning tools for understanding concepts in science, technology, engineering and mathematics (STEM) education [21, 24].

Kim and Pak[28] investigated the relation between traditional physics textbook problem solving and conceptual understanding. The findings of the study indicated that there was little correlation between the number of problems solved and conceptual understanding, suggesting that traditional problem solving has a limited effect on conceptual understanding [28]. Sometimes, instruction focusing on problem-solving overlooks intellectual goals and could encourage students to focus on algorithms instead of on concepts, which may eventually lead to fundamental conceptual difficulties [35, 36]. The integration of computer modeling and simulation within learning environments fosters a deeper understanding of complex engineering problems through visualization. With the growing use of software and the ease in availability, computerized science simulations are becoming increasing popular among engineering students. Complex calculations can be offloaded to the computer so that the problem solver can work more efficiently and focus on the core aspects of problem solving.

Many researchers have acknowledged that simulations facilitate the visual representation of otherwise unobservable microscopic phenomena (molecules, coarsening etc.) and abstract concepts (electric and magnetic field lines) [26, 27]. Additionally, several authors have attempted to investigate the value of using concrete material and virtual apparatus and material (computer-based simulations) in science education [25, 27, 32, 33]. Previous research suggests that a combination of simulation and real experiments is more beneficial for learning than using only virtual experiments [33]. On the contrary, the results of a research for the study of electron flow suggests that students using simulations perform better than students using the real circuits [26]. The results from some bodies of research suggest that conceptual change can occur among learners with the use of simulation and modeling tools [11, 12]. Similarly, research in Model Eliciting Activities (MEA) suggests that model developers are able to progressively develop productive ways of solving a problem [31].

An important factor which guides the learners' ability to solve a problem is their prior knowledge. Learners' prior knowledge may provide them with the ability to understand the crucial problem features more clearly. Research done in a variety of problem domains shows that learners with better prior knowledge interpret key problem features more accurately than learners with less prior knowledge [13]. A problem solver is able to categorize a problem better if there exists an understanding of the deep structure of a problem, and this supports the problem solver in the quest of finding the correct solution approaches [17].

Therefore, to effectively integrate these tools in engineering contexts, students can also develop problem solving and design skills in addition to inquiry skills, the adoption of a "practice perspective" is needed [3]. In a practice perspective the focus of learning is on participation in authentic contexts where the learning experiences: (a) are personally meaningful to the learner, (b) relate to the real-world, and (c) provide an opportunity to think in the modes of a particular discipline [4]. Since practice consists of a process of action and reflection in context [5], we argue that learning through practice requires involving learners in original "field" experiences where they participate in (i) the process of collecting, transforming, and summarizing data and (ii) the representation of the relationship between the observed event and its re-representation [3]. To explore the role of computing in engineering problem solving, the guiding research questions for this study are:

(1) How modeling and simulation practices support or hinder problem solving processes?
(2) How do students perceive process scaffolding in the form of engineering problem solving phases?

Theoretical Framework

The current research design is inspired by the "integrated model of problem solving (IPMS)" [9]. The model, which builds upon the Text Diagram Symbol (TDS) model, involves three phases: problem representation, problem framing, and problem synthesis [10]. In the representation phase, the learner reads the problem and creates a mental representation of the problem. This phase involves setting the goals and identifying the deep structure of the problem scenario. During the framing phase, the problem solver focuses on creating a physical diagram to represent the problem. The final phase of problem synthesis involves formulating a mathematical representation of the problem and the solution implementation. In the current research design, we adapt from IPMS and break down the problem synthesis phase into two more specific phases – *problem synthesis* and *problem implementation*. The *problem synthesis* phase involves building the solution approach and the *problem implementation* phase involves the actual implementation of the solution. Simulations and computational models are implemented in the *problem synthesis phase* and using these simulations and models, the problem solution is implemented in the *problem implementation phase.*

In this study, we investigate the impact of coupling the integrated model of problem solving with the use of modeling and simulation for learning the concepts of kinetics of materials in graduate engineering students. The theoretical framework guided our learning and research design as follows. Students first conducted a preliminary literature review on a given topic, then they were asked to implement a computational solution for the corresponding design challenge. Students completed their designs following the four steps of the problem solving process as follows: *Problem recognition phase:* students investigated the conceptual aspects of the problem to be solved, that is, students identified concepts associated with the kinetics of materials. *Problem* *framing phase:* in this stage students elaborated possible conceptual models of their solutions and identified a possible mathematical model that can represent the physical phenomenon associated with the design challenge. *Problem synthesis phase:* in this stage students work in implementing their models by means of domain-specific software (e.g., Virtual Kinetics of Materials Laboratory (VKML), Gibbs, MATLAB); they also validated their own implemented models by comparing and contrasting them upon existing simulations, empirical data from journal articles, test cases provided by the instructor, or theoretical models described on textbooks. *Problem implementation phase:* in this stage students use their validated implementation to solve the problem or design challenge. The four stages of problem solving used are shown in Fig 1.

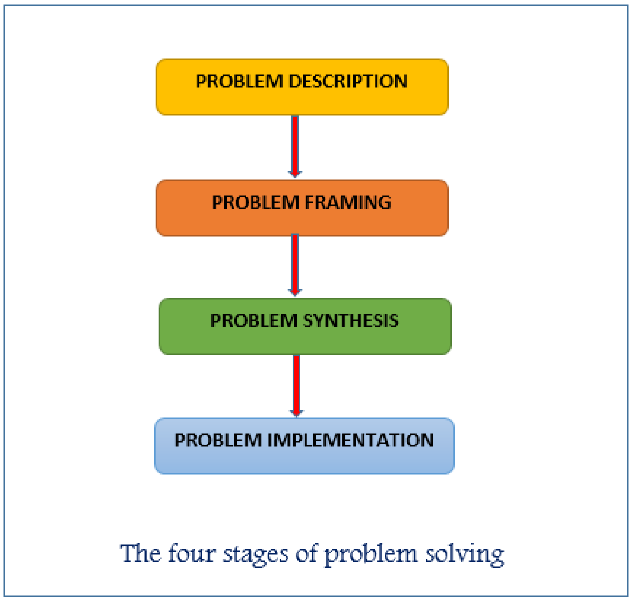


Figure 1. The four stages of problem solving, adapted from the "integrated model of problem solving" (Van Meter et al., 2006)

Methods

Instructional Context

The course entitled "Kinetics of Materials" is an elective course offered to upper level undergraduate students and graduate students interested in developing a fundamental understanding on the underlying atomic and microstructural mechanisms controlling the time-evolution of materials. This is a newly added course to the engineering curriculum and was taught at the university for the first time. The concepts taught in the course included the principles and controlling aspects of diffusion, irreversible thermodynamics, motion of dislocations and interfaces, morphological evolution due to capillary and applied mechanical forces (including evaporation/condensation, coarsening, sintering, grain growth, diffusional creep), phase transformation kinetics, including general features of order-disorder transformations, spinodal decomposition, fundamentals of nucleation, growth, precipitation, and martensitic transformations. This course was designed with an intent to build students' conceptual understanding by using both visual representations and simulations, and promoting an environment where students use computational and mathematical models to complete their assigned term projects.

Participants

The participants consisted of 2 upper level undergraduate students and 12 graduate students who registered for the “Kinetics of Materials” course from a top ranking Midwestern engineering program. To protect the identity of the fourteen participants, demographic information was not disclosed to the researchers. The participants worked in teams of up to three members and were informed by the instructor to form their own teams. The instructor also gave the students the option of working solo for the project. All of the teams worked on a course project which constituted solving a complex computational problem using modeling and simulations. Each team had to come up with a team name. The team and their member pseudonyms are listed in Table 1. Table 1 also describes the problem solving tasks undertaken by the team. Three teams (Kinetics, Star Wars 8 and Super Battery) contained three members each. One team (Ramvik) consisted of two members. Three students (Lone Ranger, Forest and Squash) decided to work by themselves for the project.

The project topics were discussed midway through the semester. The students had six weeks to work on the project and design a solution for the chosen computational problem.

Table 1. Team pseudonyms, team member pseudonyms and the chosen project topics

Team Name Pseudonyms	Team Member Pseudonym	Project Topic
Kinetics	Whiskers	Modeling of Two Phase Coarsening Effects at High Volume Fractions
	Mittens	
	Buttons	
Super Battery	Tom	Optimal Grain Microstructures & Film Thickness for Thin Film LiCoO2 Batteries
	Harry	
	Sam	
Lone Ranger	Ranger	Determination of the crystallization time of liquid-liquid phase separated model hydrophobic drug in buffer
Ramvik	Ram	Ostwald Ripening in a system with high volume fraction of Coarsening Phase
	Vik	
Star Wars 8	Solo	Stress Modification of Oxide growth rates in Alumina Layer for Thermal Barrier Coating Systems
	Skywalker	
	Kenobi	
Forest	Rogue Elephant	Hydrogen Storage: Size Effects in Magnesium Hydride
Squash	Squash	Size and Temperature Effects in Magnesium Hydride

The instructor introduced the following topics for the term projects in class:

- Hydrogen Storage: Size Effects in MgH_2

• Thermally Grown Oxide Kinetics (Aging of Thermal Battery Coatings)
• Grain Boundary Design in Thin Film $LiCoO_2$ Batteries
• Non-Ideal Coarsening Kinetics

In addition to the topics mentioned above, the students were given the option to come up with their own topic, provided they would use the concepts learnt in class to propose a solution to the problem they intend to solve. For each of the topics listed above, the instructor introduced the problem and proposed the challenge that the students needed to solve as a part of their term project (see project topics Appendix B). Data and simulations from relevant research papers were used to present the scenarios of the computational problem.

Software Tools Taught in the Course

The instructor covered three software tools and packages that could be used by the students to build simulations and computational models for their projects. The instructor conducted laboratory training sessions to introduce these tools to the students. The use of these tools or software packages was optional and the students were given the option to choose any other tool for the purposes of the project. The three tools introduced by the instructor are described in the Table 2.

Table 2. Software packages to help students build simulations that were introduced by the instructor

Software Package/Tool Name	Description
VKML	The Virtual Kinetics of Materials Laboratory (VKML) is a web environment to develop microstructural evolution models by using FiPy, a powerful set of python-based libraries to write Partial Differential Equations [14, 15]. A basic set of examples is provided to simulate: a) the electrochemical transport kinetics of rechargeable lithium-ion batteries; b) simple diffusion and spinodal decomposition problems; c) Symbolic Thermodynamics using the Gibbs infrastructure; and d) basic examples to learn how to write a program with a simple GUI. Each example can be readily edited, debugged, and run online. VKML is a computational simulation tool developed initially for experts and is now integrated into courses in engineering and sciences at the university level [16].
OOF2 - Object oriented finite element analysis tool	OOF2 is public domain finite element analysis software created at the National Institute of Standards and Technology (NIST) to investigate the properties of microstructures. At the simplest level, OOF2 is designed to understand the effects of far fields (boundary conditions) on the local microstructural fields, or to assess the mechanical, electrical, and thermal reliability of a material with a complex topology[19].
Gibbs	Gibbs is a general-purpose python-based Object Oriented set of libraries designed to simulate the multiphysical equilibrium of materials. The developed framework enables the rapid prototyping, validation, and comparison of thermodynamic models to describe the equilibrium between multiple phases for binary systems[20].

Data Collection and Data Analysis Methods

Once the professor introduced the topics for the term projects, the students were given a week's time to choose one of the topics or come up with their own topic for the term project. The following week, each team was required to submit a one page write up about the topic they chose. This submission was considered as a homework assignment. The homework assignment submitted by the students was qualitatively analyzed to understand how the students framed the computational problem at a very high level.

Students then prepared a report where they included all the components shown in Table 3. These reports were qualitatively analyzed and scored with a rubric that would evaluate the outputs from each of the stages of the problem solving process (see Rubric on Appendix A). The rubric was prepared by three researchers and proposed to the course instructor. With feedback from the course instructor, modifications were made to the rubric. Revisions to the rubric were completed after three iterations. Even though the seven teams worked together on the project, they submitted individual final project documents. The evaluation included aspects of how students used their own created models and simulations to solve an engineering design problem and the degree of effectiveness of their solutions. Students were also asked to fill out a survey which was designed to understand: (1) students' thought processes and design decisions, (2) the challenges they encountered in solving the problem and (3) the strategies they used to overcome those challenges. The four questions included in the survey were as follows:-

- Q1. Considering the outline provided for the term project, which step in the project was the most challenging for you? Why?
- Q2. What strategies/resources did you use to overcome those challenges?
- Q3. Considering the outline provided for the term project, which step helped you the most in your learning? Why?
- Q4. How did you apply the concepts you learned in the course in solving the problem?

Students' responses were studied using open-coding analysis to identify the themes and patterns embedded in student responses [18]. In particular, an inductive analysis was conducted to investigate the activities, operations and conceptual process that upper level engineering students employed in modeling the problem solving task at hand. As patterns or themes emerged, each one of them was examined to identify similarities and differences in the set of processes and operations taken by the different individuals. In addition, we looked for insight into understanding the relationships of these processes and operations to the process outcomes and how these outcomes were relevant in understanding students' use of computation tools and conceptual understanding.

Table 3. Project template provided to the students to document the different stages of the problem solving process.

Section	Description
Problem Description	Students need to describe the problem that is being solved and provide a justification using the scientific literature from relevant research papers. The students need to use the research papers provided or other relevant literature to come up with the problem statement
Problem Framing	
a. Conceptual Model	The students need to define a model that will help them define goals, information, assumptions, in terms of relevant models used in class or from the literature, concepts or theories
b. Mathematical Model	The students need to justify the proposed model using concepts developed in class. Also, the students need to work on identifying assumptions and limitations.
Proposed Problem Solution	

a. Define the approach	The students need to predictively compare and contrast alternate solution processes in terms of relevant metrics (e.g., accuracy, precision, efficiency, reliability, feasibility, risk, impact, etc.) The students need to build a program or solution that will help them solve the problem. Describe how this simulation or code implements the model. They also need to provide an explanation of why they chose a particular computational tool.
b. Validate the solution	The students need to thoroughly validate the approach they choose. This can be validated by means of experimental data, a theoretical model, or by means of test cases using a computational tool
Problem Solution Implementation	The students need to use the simulation or program to solve the problem and explain the solution.
Results and Conclusions	The students need to interpret the output and show how the proposed solution addressed the problem/project

Results

The data analysis for the current research are discussed in two separate sections. The first section titles "Problem Recognition" summarizes the inductive analysis from the homework assignments submitted by the teams at the end of the first week after the introduction of the project topics. The homework assignments served like an initial phase of the problem description process. The second section "Problem Solution" summarizes the quantitative analysis of the scores of the final project documents submitted by the students using the template provided in Table 3. Based on the scores of the individual students' documents, they were categorized into high performers and low performers. Categories and themes were identified in the problem solving approach of high performers and low performers. It also separately summarizes the analysis of the students' perceptions for learning from the questionnaire submitted by the high performers and low performers. The inductive analysis of the data in the two sections was aimed at understanding how modeling and simulations support or hinder problem solving processes and the students' perceptions about process scaffolding in the form of engineering problem solving processes.

Problem Recognition

The students submitted a single page report about their project topics. The instructor had not requested for any specific format, but had conveyed to the students that they need to present an initial understanding of the problem. Members of all the teams worked in collaboration to present one report as a team. A common pattern observed in all the homework assignments was a brief problem description with the relevant literature, the problem specifications and principles or models that would be used in implementing the solution. The Star Wars 8 team divided their objectives for the project into primary and secondary objectives. They enlisted their primary objectives and mentioned that they would aim to achieve the secondary objectives if they had more time. Lone Ranger chose a project topic, which was related to the thesis project she had been working on. Some instances of her use of prior knowledge in problem description can be seen in her homework report:

> Lone Ranger: "My lab has shown for drugs such as darunavir and dannazol, LLPS systems provide the highest increase in solubility comparison to other solubility enhancing techniques."

The Ramvik team introduced the problem with the relevant mathematical models and described their objectives in a mathematical context:

> Ram: “The concepts we want to focus are: (1) Different diffusion paths (2) Gibbs-Thomson equation for non-spherical particles (3) Irreversible Thermodynamics”

The Super Battery team did not submit the homework assignment.

Problem Solution

Student individual solutions to their problems were scored by the course instructor using the rubric shown in Appendix A. The individual scores of all the students for the final project documents are tabulated in Table 4. For each of the four phases of problem solving, the students were graded on a scale of 1 to 4 (1= Unsatisfactory, 2=Needs Improvement, 3=Meets Expectation, 4=Exceeds Expectation). Based on the individual scores of the final project document, the students have been classified into the high scoring and low scoring groups (See Table 4).

Table 4. The scoring chart for final project documents submitted by students for the rubrics shown in Appendix A.

	Student Pseudonym	**Team Pseudonym**	**Problem Description Score**	**Problem Framing Score**	**Problem Synthesis Score**	**Problem Implementation Score**	**Organization of Report**
High Scoring Students	Squash	Squash	4	4	4	4	4
	Rogue Elephant	Forest	4	4	3	3	4
	Buttons	Kinetics	4	4	4	4	4
	Mittens	Kinetics	4	4	4	4	4
	Whiskers	Kinetics	4	4	4	4	4
	Lone Ranger	Lone Ranger	4	4	4	4	4
	Skywalker	Star Wars 8	4	4	4	4	4
	Kenobi	Star Wars 8	4	4	3	4	4
	Solo	Star Wars 8	4	4	4	3	4
	Ram	Ramvik	4	4	4	4	3
	Vik	Ramvik	4	4	3	4	3
Low Scoring Students	Tom	Super Battery	1	2	1	2	2
	Harry	Super Battery	2	2	2	1	3
	Sam	Super Battery	2	2	1	2	3

Problem Solutions from High Performing Students

A general pattern observed in the high scoring documents was the strong connections students were able to make between the conceptual and mathematical models. The transformation of these mathematical representations into visual representations in the form of simulation models proved to be a catalyst for their learning. As an example of the created representations, Figure 2 depicts the microstructural evolution of Ostwald ripening designed by Ram, member of the Ramvik team, using FiPy, which is a Python-based object oriented set of libraries to numerically solve partial differential equations. Figure 3 shows the progression for the phase field for different particle sizes at 700K developed by Squash. Squash observed that the results of the phase field simulation proved that the use of smaller particle sizes lead to faster hydriding kinetics. This result was consistent with the concepts and previous research.

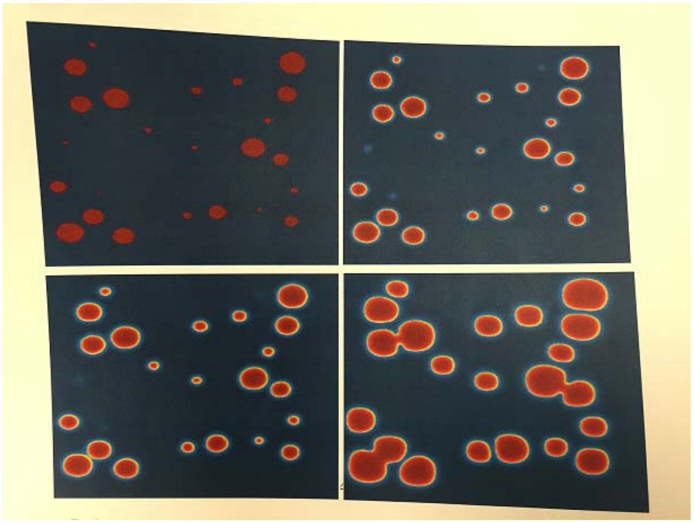


Figure 2. Simulation showing the microstructural evolution of Ostwald ripening in the final project document submitted by Ram

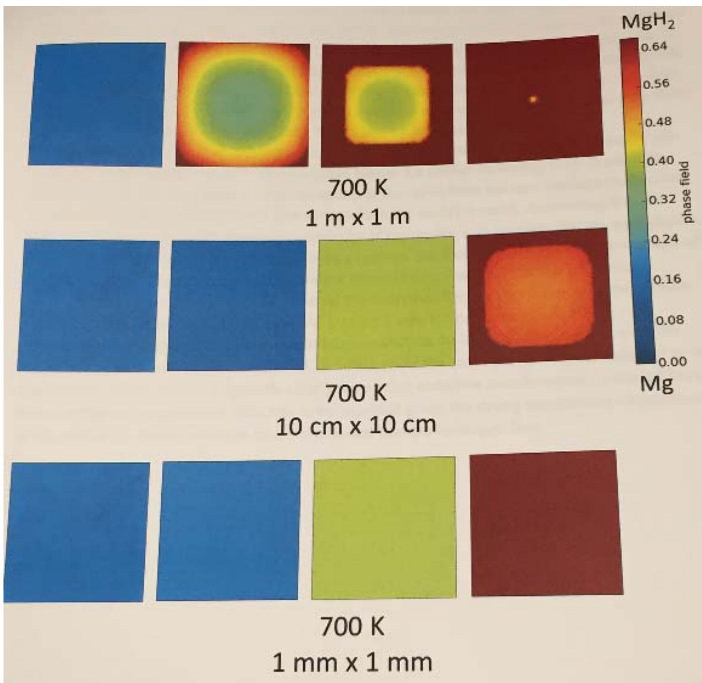


Figure 3. Simulation showing the phase field of the simulation cell at 700K for three particle sizes submitted by Squash

Perceptions of High Performing Students

Most Challenging Component

From the questionnaire responses of the high performers, it can be inferred that problem framing and problem synthesis were the most challenging components of the project. Two categories emerged from student responses:

(1) Students who struggled in the problem framing phase. The student, Lone Ranger, found problem framing as the most challenging step due of the limited availability of data. Rogue elephant and Buttons (Team Kinetics) had a similar response:

Buttons (Kinetics): "Problem Framing I believe was most difficult. We felt that there were several approaches to this coarsening problem, and finding a new way to attack it while still connecting conceptually to class was somewhat difficult."
Lone Ranger (Lone Ranger): "It was challenging to conceptually define the project by reading the short description."

(2) Students who struggled in the problem synthesis phase. Two members of the Star Wars 8 team, Skywalker and Kenobi, faced challenges in the problem synthesis phase, specifically in building the simulation and validating it. Ramvik, Solo and Squash, particularly struggled working with the simulations during the problem synthesis phase. Solo felt that he was ambitious in his plans, while Squash struggled with learning a new language for the simulation.

Solo (Star Wars 8): "It was difficult because we were ambitious in our plans. I tried making my own ID Finite Difference Model in Matlab and it took several iterations to work out the kinks"

Squash (Squash): "I am not familiar with FiPy, so trying to modify the existing code to fit the needs of my simulation proved difficult"

Strategies/Resources to overcome challenges

From the responses to this question, we were able to deduce that the students used online resources, journal articles and the instructor's guidance to overcome the challenges they faced in the problem solving tasks.

Squash (Squash): "I asked the professor about how the program worked and looked through the FiPy examples to figure out how to modify the code."

Kenobi (Star Wars 8): "The resources were mostly the textbook, lectures and relevant papers. FiPy was used for the simulation."

> Mittens (Kinetics): “We tried an extensive literature review and in the end we tried to make assumptions that minimized error in our model.”

Most Beneficial Learning Component

Six out of the twelve high scoring students unanimously agreed problem framing to be the most helpful step. Two students favored the problem description phase. Reading the relevant literature helped them understand the aspects of the problem solving tasks and made them aware of new theories, which depicted the ongoing work related with the topic. Out of the remaining three, two students (Solo and Ramvik) felt that problem implementation was the most beneficial learning component and one felt that all the problem solving steps were crucial for learning. Some comments quoted by the students in the response:

> Lone Ranger (Lone Ranger): “The problem framing phase made me understand all the equations thoroughly and their limitations”

> Rogue Elephant (Forest): “The problem framing phase required me to have a concrete understanding of the model”

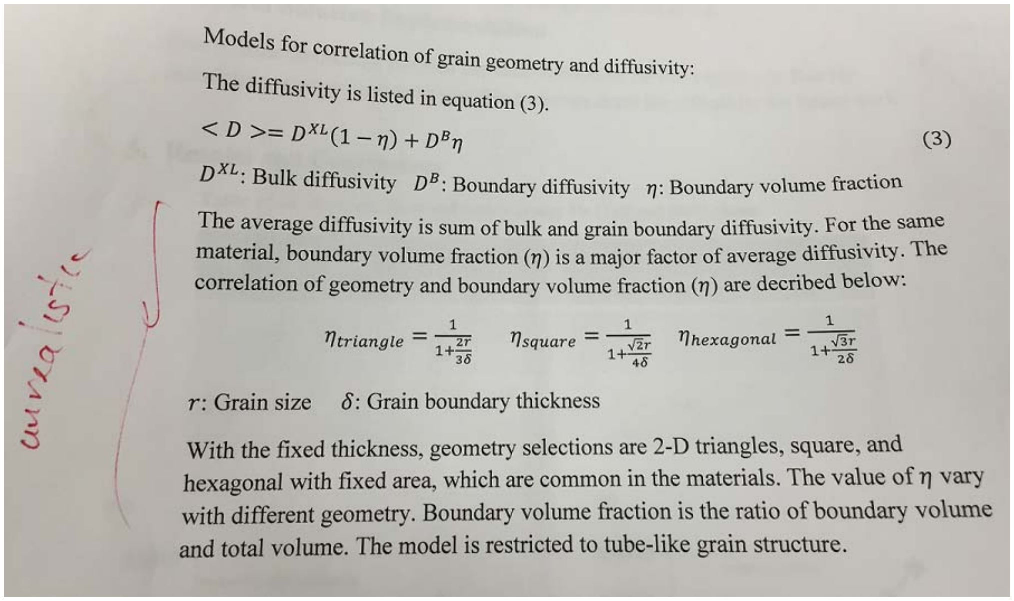
> Mittens (Kinetics): “Problem Framing. It made me go back and go through and use class knowledge and reinforce many concepts.”

> Squash (Squash): “I think all the steps helped. Starting from square I forced myself to relate all of the involved concepts into a cohesive framework. In doing so, I had a lot of questions as I went along and seeking answers along the way is one of the things I feel helped me the most.”

> Ramvik: “Problem solution implementation helped the most. Maybe we were not able to prepare a high volume fraction simulation, but even its low volume fraction, it looks promising. It helped us improve and learn something new.”

Problem Solutions from Low Performing Students

Three students, Tom, Harry and Sam, who scored low in the final project, belonged to the same team “Super Battery”. An analysis of the individual project documents reveals that they failed to define the problem clearly, were unable to identify a relevant conceptual model, and correspondingly delivered an unrealistic mathematical model. Figure 4 depicts that the students used three geometry selections namely triangle and square which are incorrect, rendering the mathematical model to be unrealistic. The students did not submit the homework summary, and hence missed the chance to understand and frame the problem. The main hurdle students experienced was their inability to fluently map between the conceptual and mathematical representations. They mention in the “Problem Solution” section that they were unable to find or build a valid simulation for the project due to time constraints. They defined and based their solution on the theoretical model and the fundamental concept of diffusivity with some mathematical analysis. Similarly, these students also exhibited a low confidence in their learning perceptions.



Models for correlation of grain geometry and diffusivity:

The diffusivity is listed in equation (3).

$$< D >= D^{XL}(1-\eta) + D^{B}\eta \quad (3)$$

D^{XL}: Bulk diffusivity D^{B}: Boundary diffusivity η: Boundary volume fraction

The average diffusivity is sum of bulk and grain boundary diffusivity. For the same material, boundary volume fraction (η) is a major factor of average diffusivity. The correlation of geometry and boundary volume fraction (η) are decribed below:

$$\eta_{triangle} = \frac{1}{1+\frac{2r}{3\delta}} \quad \eta_{square} = \frac{1}{1+\frac{\sqrt{2}r}{4\delta}} \quad \eta_{hexagonal} = \frac{1}{1+\frac{\sqrt{3}r}{2\delta}}$$

r: Grain size δ: Grain boundary thickness

With the fixed thickness, geometry selections are 2-D triangles, square, and hexagonal with fixed area, which are common in the materials. The value of η vary with different geometry. Boundary volume fraction is the ratio of boundary volume and total volume. The model is restricted to tube-like grain structure.

Figure 4. An unrealistic Mathematical Model in the final project document submitted by Tom.

Perceptions of Low Performing Students

Most Challenging Component

Two members of the low scoring team, Tom and Harry, faced challenges in the problem description phase. Their responses depict a low level of confidence:

> Tom (Super Battery): "Problem Description was the most challenging. I panicked and almost did not talk about it. Project as a whole was challenging. Proposed problem solution was hard to validate."

Strategies/Resources to overcome challenges

Tom, Sam and Harry agreed that they worked as a team to discuss the problem. They used class notes and online resources to overcome the challenges they faced.

Most Beneficial Learning Component

Tom felt that he learnt the most in the problem framing phase, while Sam and Harry believed they benefitted the most in the problem description phase.

> Tom (Super Battery): "Creating the models in the problem framing phase help me learn, because it let me understand more of the basics before solving the problem"

> Sam (Super Battery): "Problem Description. Reading literature"

Harry (Super Battery): “Reading relevant papers and google.”

Discussion

This study explored how modeling and simulation practices can support or hinder the problem solving process in the context of a kinetics of materials advanced course. Overall, computational modeling and simulation practices applied to real-world problems supported student learning, at least for most of the students. Regarding the pedagogical strategy, students considered all the problem solving phases useful for their learning process. This finding is consistent with previous research in engineering education that identifies the value of the use of modeling and simulation for supporting learning of advanced topics [16].

Many engineering schools are moving towards structuring their curriculum to simulate the work of real world engineering practices [30]. One of objectives of the term project assigned to the students in the course was to stimulate their use of concepts learnt in class to real world research problems. The students were able to successfully apply the theoretical constructs to identify potential solutions to the problem.

Three high performer students highlighted *problem framing* as the most challenging phase. The reasons they exposed suggest that relevant literature and data may have helped them to create these initial models. As described above, previous knowledge is an important factor in the student ability to solve problems[13]. Interestingly, one of the students who highlighted this was Lone Ranger, who chose a topic related to her thesis. She had previous knowledge in the area and some basis to complete this phase and yet, she struggled to find enough resources to create her model. The availability of these resources for the context of the projects should be taken into consideration when defining the topics for these modeling and simulation activities. For instance, Magana and collaborators proposed that students learning from simulations are able to overcome challenges through sample data, demonstrations and executing test cases [21].

Also, at least four high performers mentioned they struggled during the problem synthesis phase. The main issue in this phase was building or adapting a computer simulation using a programming language that was new for them. Researchers have consistently found that integrating a programming component with the practices of modeling and simulation poses some challenges for novice and advanced learners equally [23, 21]. Since some students did not have previous experiences with some of the simulation tools, building new simulations or adapting existing ones became a challenge to complete the project. Even though Ramvik and Solo struggled with the simulations initially, they both agreed that it was the most beneficial learning step for them.

In spite of these hindering effects of the lack of resources and previous knowledge, most of these students also mentioned that the identified challenging phases were also the most helpful ones for their learning. They were able to overcome the challenges using different strategies, and then benefited from being exposed to them. This could be explained from the lens of *productive failure*: “when students generate solutions to problems that target concepts novel to them, it often leads to failure" [22]. Students take advantage of this failure by looking for resources and instructional support that will benefit their learning.

For the low performers, a similar finding can be reported. Students failed to submit the first homework delivery that comprised the problem representation. That fact became a major issue for them to complete the project. They presented an "unrealistic" model, probably because they did not understand the problem in the first place. In spite of that, the problem description was the most useful phase for two of them. Furthermore, the employed strategies to overcome the challenges did not include the instructor assistant or other experts involved.

Overall, the participants succeed to follow the problem solving phases to complete a computational modeling and simulation project. Students who struggled the most (i.e., low performers) failed to understand description the problem at the beginning, which led them to consequent inaccurate solutions. Additional scaffolding and available resources may have an impact on student learning process [33].

Conclusion and Implications

In this paper, an approach to integrate problem solving methods with modeling and simulation was presented. The results suggest that engineering students solving computational problems should first work on abstract representations and then work gradually into further problem solving stages[29]. We interpret the results to indicate the four primary phases that can assist the learners (a) allow learners to focus on the understanding the problem by reading conceptually relevant literature, (b) frame the problem using appropriate conceptual and mathematical models, (c) use a simulation or model to define the solution approach and validate the approach and (d) allow learners to use the simulation to implement a solution to the problem. From the students' opinions, it can be inferred that the students appreciated the importance of the different problem solving steps in guiding their learning. They also appreciated the use of simulations to represent the concepts of the posed challenges and solving problems. This kind of experimentation is crucial in the development of engineers along with a strong conceptual foundation [34].

The results suggest that the IPMS model was able to adequately guide the students through the analysis process, which is consistent with the results of the study which proposed the IPMS model [9]. Additionally, the results suggest the importance of the *problem framing* phase in solving a problem, which concurs with the TDS model [10].

The implications of our study relate to (a) the design of problem solving learning experiences that engage learners in authentic practices contextualized in real world problems and that at the same time develop modeling and simulation skills and (b) the integration of different constructs associated with workplace engineering practices that can enable us to propose an analytical framework to investigate them concurrently. Curriculum at engineering schools should be balanced with theoretical knowledge and promote the idea of coupling the content with real word situations[30]. Computational modeling and simulations are now highly relevant to solve these real world complex problems.

The results suggest that the use of computer simulations can be helpful in the process of problem solving enabling students to validate theoretical constructs. We recognize that other types of intervention, for example, the instructor guiding the students with the problem, demonstrating the software packages and tools, or the students working together in teams, might have been equally effective, but the issue here was to identify whether a particular approach (modeling and simulations) would be feasible.

The contribution of our study centers in the joint investigation of complex problem solving and modeling and simulation, which in discipline-based education research have commonly been studied separately. However, the combination of these practices and tools are now widely acknowledged and desired in engineering workplaces. Even though there is a proliferation of computer-based education in engineering, there is still a deep need for more systematic research that explores the aspects of improving problem solving and its larger implications to learning. This research is an attempt to investigate one aspect of this pursuit.

Limitations

The limitation of this study includes the small sample size and the use of only project documents and written survey data completed by the students without collecting any interview data. . Since the graduate class had a small strength of 14 students, only one instructor was assigned to the course. The course instructor alone graded the term project documents and hence inter-rater reliability was not accounted for in this research. However, an exploratory study of this nature provides evidence of students' processes for using modeling and simulations as part of their problem solving processes in engineering design. At the same time, this study also provides a basis for future studies using a larger sample size and additional aspects of problem solving using modeling and simulation that can be explored further using interview or think-out-loud protocols.

Although the findings of the present study are preliminary and need to be replicated using diverse engineering topics and student groups, they indicate that engineering education instruction may benefit from these different problem representations and simulation practices. The results of the study also suggest that modeling and simulation can help graduate engineering students to improve their problem solving abilities, particularly in the analytical stages of the problem solving process. Simulations enable active manipulation and reinforced practice supporting students to learn the concepts better.

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Appendix A

Assessment Rubric

Student ID:	Unsatisfactory(1)	Needs Improvement (2)	Meets Expectation (3)	Exceeds Expectation (4)
Problem Description (20%) Description the problem that is proposed to be solved and provide a justification using literature from relevant research papers.	An unclear description of the problem statement and no relevant research backing provided.	Description of the problem statement needs refinement. Inadequate research relevance.	The problem is defined appropriately, but will need a little more refinement in terms of relevant literature.	The problem is very well defined and the literature from relevant research work builds a perfect case for the problem.
Problem Framing **Conceptual (10%)** **Mathematical (10%)** Building of both a conceptual and mathematical model to solve the problem. Interpret the problem (goals, information, limitations, and assumptions) in terms of relevant models, concepts or theories.	-No conceptual or mathematical model included in the report.	- A conceptual and mathematical model is provided, but it is incorrect.	- A conceptual model is provided, but needs minor improvisation. - A mathematical model is provided, but needs minor improvisation.	-Both the conceptual and mathematical models provided accurately frame the problem.
Problem Synthesis **Build (15%)** **Validate (10%)** Evaluates the quality of the solution approach built to solve the problem. The simulation or program needs to be validated thoroughly with either experimental data or test cases. Predictively compare and contrast alternate solution processes in terms of relevant metrics (e.g., accuracy, precision, efficiency, reliability, feasibility, risk, impact, etc.) Use a simulation or build your own program that will help you solve the problem.	-The implementation of the solution approach is incorrect. -The solution approach is not validated	-The implementation of the solution approach serves the purpose, but needs refinement. -The validation process for the solution approach needs to be improved.	-The implementation of the solution approach provides the approach to solve the problem, but needs minor improvements. -The validation process for the solution approach needs minor improvements,	-The implementation of the solution approach is accurate. - The solution approach is validated appropriately.
Problem Implementation and Deployment of Disciplinary Concepts (30%) Evaluates whether the student can use the model they build to solve the problem. Can the student use their code to address the disciplinary issue or to solve a related problem?	-No solution provided to the problem. -Does not discuss the application of solution for a related problem.	- A solution is provided, but it is incorrect or does not adequately address the issue or problem. -Not a clear description of how the solution can be used to resolve a related problem.	-A solution is provided that would adequately address the issue or problem, but it is presented in a way that is unclear, or improperly documented. -A discussion is included which describes the use of the current approach to solve related problems.	- A solution is provided that is correct, clear and well documented. -A very clear description is included which describes the use of the current approach to solve related problems.
Organization of the Report (5%) An important aspect of a project report is its appropriateness in terms of structure, sentence construction and grammar.	Report is not well structured and contains more than 10 grammatical and sentence construction errors.	Report contains more than 5 grammatical and sentence construction errors.	Report is structured well, but contains less than 5 grammatical and sentence construction errors.	Report contents are well structured. The report contains no grammatical and sentence construction errors.

Appendix B

Project Topics and Challenges

Project Topic Description	Description of Problem Solving Challenge
Hydrogen Storage: Size Effects in MgH_2	**What is the optimal operation temperature and particle size combination?** The objective of the project was to find an optimal temperature operation and particle size combination to maximize hydrogen storage in metal hydrides.
Analytical Model of O^{2-} Transport in Thermal Battery Coatings	**Design (or propose) deposition operation that will lead to a microstructure that more resistant to thermally grown oxide layer (TGO).** The objective of this project was to use the models learnt in the course to evaluate the oxygen transport through thermal barrier of coatings (TBC) with the purpose of determining the optimized microstructures which inhibits oxygen diffusion, yet allows the coating to have a high temperature gradient.
Optimal Combination of Grain Microstructures and Film Thickness for Thin Film $LiCoCO_2$ batteries	**What is the optimal grain microstructure and film thickness combination?** In most batteries, charging and discharging them is a chemical reaction. Charging of L-ion batteries if ion-diffusion dominated. By increasing ionic diffusion, a shorter recharge time of the batteries can be obtained. The diffusion is affected by the grain microstructure and film thickness. The problem is to find the best combination of grain microstructure and film thickness for highest ionic diffusion, or shortest battery recharge time.
Non-Ideal Coarsening Kinetics	**Propose a model that describes the 90% volume fraction.** The kinetics of Ostwald ripening and grain growth of two phase systems has a broad range of implications in metallic systems and composites. The driving force for these processes is to reduce total interfacial surface area, which results in coarsening of one phase in the matrix of other. The object of this project was to propose a model that describes 90% volume fraction regime.