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Development of First-Year Engineering Teams' Mathematical Models through Linked Modeling and Simulation Projects

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DEVELOPMENT OF FIRST-YEAR ENGINEERING TEAMS' MATHEMATICAL MODELS THROUGH LINKED MODELING AND SIMULATION PROJECTS

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ABSTRACT

Rodgers, Kelsey, J. PhD, Purdue University, August 2016. Development of First-Year Engineering Teams' Mathematical Models through Linked Modeling and Simulation Projects. Major Professor: Heidi Diefes-Dux.

The development and use of mathematical models and simulations underlies much of the work of engineers. Mathematical models describe a situation or system through mathematics, quantification, and pattern identification. Simulations enable users to interact with models through manipulation of input variables and visualization of model outputs. Although modeling skills are fundamental, they are rarely explicitly taught in engineering. Model-eliciting activities (MEAs) represent a pedagogical approach used in engineering to teach students mathematical modeling skills through the development of a model to solve an authentic problem.

This study is an investigation into the impact of linking a MEA and a simulation-building project on students' model development. The purpose of this research is to further address the need for developing effective curricula to teach students' mathematical modeling skills and begin to address the need to teach students about simulations. The data for this study were 122 first-year engineering student teams' solutions to both a MEA and a subsequent simulation-building project set in the context of a nanotechnology

topic, specifically quantum dot solar cells. The teams' mathematical models submitted at the end of the MEA and the simulation project were analyzed using two frameworks to assess the quality of the mathematical models and the level of simulation completeness. Three teams' works with the feedback they received were analyzed in a case study.

The analysis of the 122 teams' mathematical models showed that many teams selected particular aspects of their final MEA models for further development in their simulations. Based on the components of the models that were consistent in the MEA and project submissions, teams either improved, did not change, or weakened aspects of their models. Twenty-six teams improved the functionality of their model. Six teams increased the input variable handling of their models. Two teams improved the efficiency of their models; eight teams made their models less efficient through poor programming decisions. Based on an analysis of the 122 teams' simulations, 62 percent were complete simulations (i.e. backed by a model and front-ended with user-input and output visualization capabilities). The case study enabled a more detailed analysis of how select teams' mathematical models changed across their submissions and the evidence of potential deeper learning about their models across their submissions.

The findings of this study suggest that model development continued through simulation development enables student teams an opportunity to either further improve or explore their models. These sequential projects provide teams with low quality models with more time for development and application within a simulation. They provide teams with high quality models an opportunity to explore ideas beyond the original scope of the MEA.

CHAPTER 1. INTRODUCTION

1.1 Background

The development, use, and application of mathematical models are fundamental to virtually all engineering and engineered products (Hazelrigg, 2007). Hazelrigg (2007) discussed the importance of engineers' abilities to interpret models for their successful use in engineering design. Similar to models, as technology has developed, simulations have become indispensable tools in engineering (National Science Foundation [NSF], 2006). A report by the NSF (2006) stated the importance of simulations in engineering in resolving scientific and technological problems and identified numerous ways that simulations can play a vital role in increasing technological competiveness in the U.S.

As the development and use of models and simulations underlie much of the knowledge base and work of an engineer, teaching students to create and apply mathematical models and simulations is fundamental for student success in engineering. Lesh, Zawojewski, and Carmona (2003) explained that for students to succeed in our technology-based age they must be capable of creating and making sense of complex systems (i.e. models). Although modeling is a fundamental skill in engineering that underlies much of the content in many courses, it is rarely explicitly taught as its own skill for engineering students to develop (Carberry & McKenna, 2014).

Models are tools used to construct, interpret, understand, optimize, and/or predict another system or, in other words, a real-world phenomenon (Lesh & Doerr, 2003). Mathematical models are models developed utilizing mathematics (e.g., formulas, quantification, dimensions) (Lesh & Doerr, 2003). When challenged to identify models, many engineering students focus on physical models or prototypes (Carberry & McKenna, 2014). Mathematical models are less thought about and understood by engineering students (Carberry & McKenna, 2014; Rodgers, Diefes-Dux, Kong, & Madhavan, 2015; Zawojewski, Diefes-Dux, & Bowman, 2008).

Lesh and Doerr (2003) articulates the Models and Modeling Perspective (M&MP), which resulted from research in mathematics education to reform how students are taught mathematics to reflect how math is used by high-end users of mathematics (e.g. engineers, scientists, financiers). This research was harnessed and transformed in engineering education to create pedagogically sound problems that mimic real world engineering problems, while engaging students in mathematical modeling (Hamilton, Lesh, Lester, & Brilleslyper, 2008; Zawojewski et al., 2008).

Model-eliciting activities (MEAs) are a type of mathematical modeling problem utilized in engineering that stems from the M&MP (Diefes-Dux, Moore, Zawojewski, Imbrie, & Follman, 2004). Zawojewski et al. (2008) discussed the implementation of MEAs in engineering education as a means of advancing students' abilities to develop mathematical models. MEAs require students to analyze a mathematical problem, develop an understanding of the complexity of the problem through mathematizing (e.g., quantifying, dimensionalizing, organizing), and then communicate their model or process to address the problem, wherein their documentation of their model reveals their understanding of the attributes and limitation of the situation (Zawojewski et al., 2008). This is completed through an iterative process of refinement to further enhance model development (Lesh & Doerr, 2003).

MEAs are a well-researched pedagogy that help students develop mathematical thinking, model development skills, and other important professional skills (e.g. teaming, communication). Research around MEAs in engineering has been conducted since the development and implementation of the first MEAs in engineering classrooms; research topics have included the implementation of MEAs in engineering (e.g., Diefes-Dux & Imbrie, 2008; Hamilton et al., 2008), the MEA sequence (e.g., Diefes-Dux, Hjalmarson, Miller, & Lesh, 2008), investigations into the types of models students develop (e.g., Carnes, Cardella, & Diefes-Dux, 2010; Doerr & English, 2003; Doerr & Tripp, 1999; Diefes-Dux, Hjalmarson, & Zawojewski, 2013; Hjalmarson, Moore, & delMas, 2011), design of the MEAs given to students (e.g., Moore & Hjalmarson, 2010; Rodgers, Boudouris, Diefes-Dux, & Harris, 2015), the assessment criteria and methods (e.g., Diefes-Dux, Zawojewski, & Hjalmarson, 2010; Diefes-Dux, Zawojewski, Hjalmarson, & Cardella, 2012), and the types of feedback given to students during an MEA implementation (e.g., Diefes-Dux et al., 2012; Rodgers, Horvath, Jung, Fry, Diefes-Dux, & Cardella, 2015).

Prior research demonstrates that MEAs are an effective method of engaging students in an opportunity to build well-developed models; but there needs to be more opportunities for students to go beyond the model development that MEAs present. Model-adaptation activities also stem from the M&MP; they are another pedagogical method that enable further engagement with models through their application (Lesh & Doerr, 2003). There has been little research conducted on the implementation of model-adaptation activities in engineering education. One type of model-adaptation activity could challenge students to build simulations based on models; this would enable students to further interact with models, while presenting an opportunity to build simulations.

Simulations are user interfaces based on well-developed models with variable inputs and output visualizations (Alessi, 2000; Gould, Tocochnik, & Christian, 2007; Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). Simulations are crucial for the understanding and analysis of phenomena, processes, and products. They are especially important for investigating phenomena and processes that would be impossible to investigate through other modes of inquiry due to complexity, size, time, and/or safety considerations (Bell & Smetana, 2008; Stevens, Sutherland, & Krajcik, 2009). Size makes simulations especially important in nanotechnology, where nanotechnology is the understanding and control of matter at dimensions between approximately 1 and 100 nanometers, where unique phenomena enable novel applications (National Nanotechnology Initiative [NNI], 2009). According to the National Center for Learning and Teaching in Nanoscale Science and Engineering (NCLT) and the National Science Teachers Associations (NSTA), the use of computer simulations in nanotechnology is one of the eight “big ideas” of nanotechnology education (Stevens et al., 2009).

Simulations are implemented in education through either using them or building them (Alessi, 2000). Computer simulations are currently most used in engineering education as tools to enable communication or exploration of models through variable manipulation and visualization (Bell & Smetana, 2008). Using computer simulations makes learning meaningful through interactive, authentic opportunities to observe, explore, and recreate real objects, phenomena, and processes (Bell & Smentana, 2008). The implementation of simulations in the classroom has been shown to increase students' intuitive knowledge and skills more than traditional lectures (Swaak, van Joolingen, & de Jong, 1998).

While there is a need for continued research around using simulations in the classroom to help students understand phenomena, there is an even a greater need for research on building simulations in an exploratory learning environment. Within the M&MP, the implementation of simulation building in the classroom is a type of model-adaptation activity (Lesh & Doerr, 2003). There has been little research around model-adaptation activities. Most research around simulations in engineering education investigates the benefits of using expert-developed simulations in education settings (Alessi, 2000; Bell & Smetana, 2008). The development of simulations is typically taught through traditional prescribed methods (e.g., Gould, Tobochnik, & Christian, 2007; Leemis & Park, 2006), which do not enable the learning opportunities that well-constructed adaptation activities may present. Model-adaptation activities present a research-based pedagogy that can enable deeper learning of models and modeling through simulation development. Beaulieu, Ratto, and Scharnhorts (2013) noted the process of building simulations enabled developers to gain new perspectives and understandings of their problem and model, similar to what has been seen in model development.

Well-developed models are the foundation of simulations (Gould, Tocochnik, & Christian, 2007; Alessi, 2000). Rodgers, Diefes-Dux, Kong, and Madhavan (2015) conducted a study on student-developed simulations completed through a design project and found that many students submitted graphical-user interfaces (GUIs) that were not based on models and the majority of students did not submit complete simulations (a GUI overlaying an underlying model with user-input variables, and visualization of outputs). Engineering students seem to not understand the fundamental components of simulations, as well as the crucial connection between models and simulations.

MEAs result in well-developed models, which are the necessary foundation for simulation development, but do not continue the model development process with simulation development. Continuation of a model through simulation development can present students with the opportunity to better understand their original model, the concept of simulations, and the crucial relationship between models and simulations.

The M&MP can be used as a theoretical framework to develop a MEA and its continued development into a simulation tool in a model-adaptation activity. It can also be used to assess students' developed models through both the MEA and simulation.

Simulation development through the M&MP presents an opportunity to reform the current way of teaching students how to build simulations, while enabling further investigation into the impact of a model and simulation development sequence on the quality of students' models. Starting simulation development with MEAs also ensures that students understand their underlying model and have a sufficient foundation for building their simulations.

This study investigated how student-developed mathematical models changed as a result of student engagement in model building followed by a project to convert these models into usable simulations. This study also focused on the impact of feedback students received on their model and simulation development, particularly feedback regarding such aspects as the nature of their mathematical models, variable manipulations and selections, and visualizations. Research on creating learning environments around modeling development and simulation development acknowledges that feedback is a critical component for scaffolding students' learning and helping them progress in the development of their models and simulations (Alessi, 2000; Diefes-Dux et al., 2008).

1.2 Research Questions

The research questions of this study have evolved from previous studies that investigated student-developed simulations through grounded theory (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015), students' assessment of the presence of mathematical models and simulations in prototypical student work of student-developed simulations (Diefes-Dux, Rodgers, & Madhavan, 2015; Rodgers, Diefes-Dux, & Madhavan, 2014), and students' individual responses to questions that prompted them to define mathematical models and simulations (Rodgers, Diefes-Dux, Zielinski, & Madhavan, 2016). These studies are further discussed in the simulation section of the literature review.

Another consideration that inspired the research questions is the significance of feedback on developing student work. Alessi's (2000) research on the implementation of simulations in education and others' previous research on feedback (e.g., Rodgers et al., 2015) clearly identifies the importance of the role of feedback in exploratory learning environments. The feedback that influences change in students' mathematical models through model and simulation development needs to be further investigated to understand the types of feedback that prompt students to change their models and simulations.

This study was guided by the following research questions:

(1) What is the nature of student teams' mathematical models in the final submission of their model-eliciting activity and in the final submission of their design project?

(2) How do student teams' mathematical models change through model and simulation development over the course of the two linked projects?

(3) What type of feedback appears to contribute to changes found in the students' mathematical models and simulations?

The first question was investigated utilizing deductive analyses. The last question was investigated through a case study analysis. The second question was investigated using results from both of these analyses.

The MEA and design project created for this study were developed through the collaboration of technical experts in nanotechnology concepts, specifically the utilization of quantum dot solar cells, and engineering education research, specifically MEAs. Rodgers et al. (2016) described the development of this MEA and design project. The implementation of these projects was also supported by collaboration with the Network for Computational Nanotechnology (NCN). NCN is the team that developed and oversees the growth of nanoHUB.org. nanoHUB.org is an online community for researchers, educators, and learners to collaboratively develop, disseminate, and interact with simulations focused on nanotechnology (Klimeck, McLennan, Brophy, Adams, & Lundstrom, 2008).

1.3 Significance

The potential for creating a learning experience that links a mathematical modeling activity to a simulation development project for the purpose of strengthening students' model development skills, helping students build a connection between models and simulations, and fostering students' understanding of simulations were investigated in this study. This study involved investigating how students' mathematical models changed through simulation development. The research questions focused on exploring how continuation of model development through building a simulation impacts students' developed models. Investigations into how engineering students develop mathematical models contribute to the creation and improvement of instruction and curricula that focuses on mathematical model development skills (e.g. Carberry & McKenna, 2014; Zawojewski et al., 2008).

This research study contributes to building a better understanding of the opportunities that exploratory simulation development presents in engineering education. There is a need to continue this research to investigate the effects of simulation development on students' understanding of models, simulations, the relationship between models and simulations. This study also enables instructors to understand the potential successes and limitations of this promising approach of using simulations to further model development.

CHAPTER 2. LITERATURE REVIEW

The focus of this study was the process of development of first-year engineering students' mathematical models through both a model and a simulation discovery learning pedagogical approach, along with guidance the students received through instructor feedback. In this chapter, the relevant research on mathematical models, simulations, and feedback are reviewed. Then, the theoretical framework used in this study, M&MP, is discussed along with its connection to mathematical models and simulations.

2.1 Mathematical Models

Models are conceptual systems that are conveyed through symbolic systems (e.g., mathematical, physical, visual, computational) (Lesh & Doerr, 2003). Models are tools used to construct, interpret, understand, optimize, and/or predict another system - a real-world phenomenon (Lesh & Doerr, 2003). Models are fundamental to engineering and underlie much of the content in many courses, but modeling skills are rarely explicitly taught as a set of skills for engineering students to obtain (Carberry & McKenna, 2014). Carberry and McKenna (2014) found that when students were asked to "Describe different ways to model a design solution or idea" (p. 81), students that participated in design projects with explicit modeling modules versus implicit modeling activity embedded in the projects had varying responses. Prior to participation in either of these design projects, students referred most often to physical (94%) and computer drawing models (58%); only a few students referred to using mathematical models (19%). After the design projects, 32 percent of students that participated in implicit modeling activities discussed mathematical models and 98 percent of students that participated in the explicit modeling module discussed mathematical models (Carberry & McKenna, 2014). This highlights the need for curricula that explicitly addresses the nature and use of mathematical models in engineering design. The study conducted by Carberry and McKenna (2014) focused on students' concepts of models (i.e. types of models and purposes of models). The focus of this research and the remainder of this literature review are on students' modeling skills (e.g., ability to build and apply models).

Mathematical models focus on the use of mathematics to represent the structural characteristics of systems or real-world phenomena (Lesh & Doerr, 2003). Mathematical models are driven by real-world phenomena or data; understanding this and the underlying concepts (i.e. real-world phenomena or data) are crucial for building and modifying a model. Mathematical models are used to interpret situations or systems mathematically; this interpretation involves organizing, systematizing, and dimensionalizing systems (Lesh & Doerr, 2003). Mathematical models encompass calculations, quantification, and pattern identification. Mathematical models are further developed through a process of model refinement involving modifications, tests, and revisions (Lesh & Zawojewski, 2007). Mathematical models, like models more generally, are used to understand systems, make evidence-based decisions, and make predictions (Lesh & Doerr, 2003).

Investigations into how engineering students interact with, develop, and understand mathematical models contribute to the creation and improvement of instruction and curricula that focus on mathematical model development skills (e.g. Carberry & McKenna, 2014; Zawojewski et al., 2008). Much of the research that has investigated developing students' mathematical modeling skills was conducted through either the Models and Modeling Perspective (M&MP) or the computational adaptive expertise (CADEX) framework. Research efforts have focused on how students develop mathematical model solutions to model-eliciting activities (MEAs) (e.g., Diefes-Dux, Bowman, Zawojewski, & Hjalmarson, 2006), MEA implementation strategies within engineering courses (e.g., Diefes-Dux et al., 2008; Hamilton et al., 2008), and the improvement of MEA implementation strategies in large engineering courses (e.g., Diefes-Dux & Imbrie, 2008) within the M&MP (Lesh & Doerr, 2003). Other research has focused on enhancing students' mathematical modeling skills and developing computational adaptive expertise (e.g., Carberry & McKenna, 2014; McKenna & Carberry, 2012; Carberry, McKenna, Linsenmeier, & Cole, 2011) through the CADEX framework (Schwartz, Bransford, and Sears, 2005; McKenna, Linsenmeier, & Glucksberg, 2008).

The characteristics of a high-quality mathematical model are fundamental for the research conducted in this study involving the assessment of engineering students' mathematical models. High-quality models are determined based on the nature of the problem posed that requires a mathematical model and the type of data or phenomena the model is based on. A high-quality mathematical model requires selecting the appropriate mathematics and applying them to available and appropriate data to address the problem. For example, a high-quality model for the NanoRoughness model-eliciting activity (MEA) (MEA described by Moore & Hjalmarson, 2010) requires teams to have a component of spatial visualization, method of measurement or quantification of roughness, and successfully implemented statistics (i.e. sampling methods and measurements) (Hjalmarson, 2008). The development of high-quality mathematical models requires more than just computing though; it requires students have an ability to effectively interpret the problem and communicate the mathematics used within a model (Lesh, Zawojewski, & Carmona, 2003). The assessments of these different aspects of a high-quality model are further discussed within the methods chapter. The computing component is most relevant to this study.

For students to develop the computing aspect of high-quality models, they must have a broader, deeper, and higher-order thinking of more traditional, elementary mathematics topics (e.g., rational number, proportions) (Lesh, Zawojewski, & Carmona, 2003). Students must also have an understanding of pertinent mathematics (e.g., algebra, geometry, calculus, statistics, mathematics of motion) to successfully utilize them in their models (Lesh, Zawojewski, & Carmona, 2003).

The research conducted for this study utilized the M&MP, which is further discussed in a proceeding section (Section 2.4). Lesh, Cramer, Doerr, Post, and Zawojewski (2003) describe three types of modeling problems derived from the M&MP: (1) model-eliciting activities (MEAs), (2) model-adaptation activities, and (3) model-exploration activities.

MEAs are open-ended, realistic, client-driven problems that require the development of a mathematical model for a given situation within constraints that enable some solutions to be more successful than others (Diefes-Dux et al., 2008). Model-adaptation activities involve adapting a previously developed model to solve a problem that probably would have been too complex to start with (Lesh et al., 2003). Model-exploration activities are activities in which students compare and contrast alternative models (Hjalmarson, Diefes-Dux, & Moore, 2008).

MEAs were used in this study, so they are described in greater detail with emphasis on their application in engineering, more specifically first-year engineering. Model-adaptation activities are also further discussed, as these align with the idea of continuing a MEA into the development of a simulation tool, a form of applying the model to a more complex situation. Model-exploration activities are not discussed in greater detail because they were not relevant to this study.

2.1.1 Model-Eliciting Activities (MEAs)

MEAs were originally created and implemented in mathematics by Richard Lesh and colleagues (Lesh, Kelly, Hoover, Post, & Hole, 2000; Lesh & Doerr, 2003). They were later modified and implemented in engineering courses (Hamilton et al., 2008), including Purdue University's first-year engineering courses (Diefes-Dux & Imbrie, 2008). MEAs were designed as a means to allow students to continue to develop their conceptual understandings though problem solving, while revealing their evolving thinking through iterative problem solving. The implementation of MEAs requires students to work in teams and communicate within teams, across teams, and to clients (Diefes-Dux et al., 2008). Diefes-Dux and Imbrie (2008) explained the use of MEAs to enable a truly open-ended learning environment, promotes development of a broader range of skills, and rewards diverse thinking, allowing a more diverse set of students to emerge as talented than traditional pedagogies.

MEAs are an example of a cooperative learning pedagogy that enable students to gain personal experiences with the process of model development. MEAs ideally enable students to identify aspects of high-quality models and gain modeling skills, along with achievement of other learning objectives (Lesh & Doerr, 2003; Zawojewski et al., 2008). MEAs are open-ended problems that require students to work in teams to build and refine a mathematical model for a given realistic context with criteria that enables assessment leading to improved models. Student teams analyze a given mathematical problem, develop understanding through mathematizing (e.g., quantifying, dimensionalizing, organizing) the problem, and then communicate a model or process to address the problem (Diefes-Dux et al., 2008). An important attribute of model-eliciting activities is that they focus on the process rather than the product, in other words the important artifact is the model rather than the results that the model produces (Diefes-Dux et al., 2008; Lesh & Doerr, 2003).

This emphasis on the model rather than the results in these open-ended problems better enables a learning environment that allows for more diverse thinking than traditional mathematics problems that focus on a single answer (Diefes-Dux et al., 2008). While these activities are to an extent open-ended, they are not the type of open-ended problem where any solution is acceptable; there are criteria built into the problem that make some solutions better than others (aligning with the self-assessment principle of instructional design, as described in Section 2.4) (Lesh et al., 2000).

Models developed to solve MEAs are submitted through an iterative process where teams receive instructors' and/or peers' feedback to enable them to further improve their MEA solution (Rodgers et al., 2015). More discussion on feedback and assessment is within the feedback section of this literature review (Section 2.3). The model development process typically begins with teams presenting a hodgepodge of several disorganized and inconsistent ways of thinking about the problem context, given criteria, and possible solution steps (Lesh et al., 2000). The model refinement process involves moving from this initial chaotic model to an increasingly well-developed model through the iterative process. The process of model development requires students to communicate their ideas and continue to evolve their solutions to reflect their evolving ideas concerning the mathematical situation.

The process of solving MEAs reveals how students interpret a given mathematical situation and attempt to mathematize it; this allows researchers and/or instructors to investigate students' mathematical thinking (Lesh et al., 2000). Lesh and Doerr (2003) explain that solving MEAs can reveal "…what kind of quantities the students are thinking about, what kind of relationships they believe are important, and what kind of rules do they believe govern operations on these quantities and quantitative relationships."

(p. 9). In order to investigate these thoughts, teams' MEA solutions are submitted in the form of a written document that communicates their understanding of the context, the model itself, rationales behind model decisions, and some quantitative results from the application of the model (Zawojewski et al., 2008).

Hamilton et al. (2008) explained that the implementation of MEAs in undergraduate engineering has prompted a variety of research to further their use and intentionality of their use. Some of the research focuses they discuss are: (1) incorporating student reflection tools to capture the individuals' experiences throughout the teaming experience; (2) utilizing technology to facilitate teaming beyond local contexts; (3) identifying and addressing misconceptions; (4) emphasizing ethics; and (5) creating MEAs for advanced curricula. There are still many opportunities for further research around the use of MEAs in engineering.

Thus far this review of model-eliciting activities has been generalized to almost all engineering education contexts. Hjalmarson et al. (2008) and Diefes-Dux and Imbrie (2008) discuss some relevant struggles of early implementation of MEAs in Purdue University's first-year engineering courses, which is the setting of this study. One of the struggles was taking consideration of the primary course learning objectives to incorporate them in the modeling problems where appropriate. In early adoption of MEAs in the first-year engineering course it was crucial to incorporate the use of computer tools (e.g., Microsoft® Excel, MATLAB®) in the MEA problem solving process to fulfill a primary course goal (Diefes-Dux & Imbrie, 2008; Hjalmarson et al., 2008). The intertwining of the targeted learning objectives and skills with the implemented MEA allows the students to gain skills while applying them in an authentic, engineering context (Hjalmarson et al., 2008).

The details of one specific MEA used in Purdue University's first-year engineering course and its implementation sequence is discussed in the setting and participants section of the methods. Zawojewski et al. (2008) present examples of other MEAs that can be further investigated.

2.1.2 Model-Adaptation Activities

Model-adaptation activities, also sometimes called model-application activities or model-extension activities, focus on the practice of applying a model, most likely the model created in a MEA (Hjalmarson et al., 2008). The context for the model-adaptation activity can be the same as the MEA or it can require students to extend their model/s to a new problem situation. Lesh et al. (2003) explain that model-adaptation activities are essentially more complex versions of MEAs, but they add elements of problem framing and information gathering. The focus on problem framing (or posing) is an important attribute that is called for in *Educating Engineers: Designing for the Future of the Field* (Sheppard, Macatangay, Colby, and Sullivan, 2008). The model-adaptation activities still require concentrating on problem solving and information processing.

Similar to MEAs, model-adaptation activities emphasize high-order thinking and are based in realistic contexts. These activities are similar in many qualities, but the fundamental difference is that model-adaptation activities are more complex problems that begin after the process of the MEA; model-adaptation activity require modification to the model developed in the MEA. The process of developing a simulation based on a mathematical model that was developed through a MEA presents a similar situation where students are modifying an existing model for a more complex scenario that will require more information gathering and solution development.

2.2 Simulations

Beaulieu et al. (2013) explained that simulations are some partial re-creation of a phenomenon that can be developed through the use of mathematical models or re-enactment (e.g. war games, role playing games, virtual laboratories). Alessi (2000) describes educational simulations as any kind of simulation where a model can be manipulated. The focus of this study is on simulations based on models, specifically mathematical models. Alessi (2000) describes two major components of simulations: (a) the underlying model and (b) the programmed user interface. Rodgers, Diefes-Dux, Kong, and Madhavan (2015) describe three main components of simulations: (a) interactivity, (b) mathematical models, and (c) visualization. These two decompositions of simulations complement each other in that the programmed user interface that Alessi (2000) discussed encompasses the interactivity and visualization that Rodgers, Diefes-Dux, Kong, and Madhavan (2015) describe.

Simulations were investigated in this study and further discussed through the lens of preparing students for today's technology-based age. In preparing students to excel, we must understand the necessary abilities that students will need that they may have not previously needed. Future engineers must be capable of creating and making sense of technology-based, complex systems and growing from the opportunities they present. It is important we embrace the opportunities technology presents to continue to promote higher-order thinking and prepare students for this technology-based age (Lesh, Zawojewski, & Carmona, 2003).

Lesh, Zawojewski, and Carmona (2003) explain that technology-based tools are not just a "crutch" that simply enables people to do the same tasks that previously could be done by hand; they are tools that transform the way we can look at our reality and create new opportunities for learning about mathematics. In working through the development or interpretations of simulations there are new opportunities in the mathematical complexities (e.g., continuously changing quantities or input variables, iteration) and communication (e.g., representation, visualization) (Lesh & Doerr, 2003). For example, visualization enables students to further interact with models through a new mode of investigation. Lesh and Doerr (2003) discuss simulation visualizations, such as graphic, dynamic, and interactive displays, as presenting another mode of communicating conceptual understandings of mathematical models.

Gredler (1996) explains that educational simulations address a pedagogical need not addressed by other forms of instruction, but much more research is needed around how these impact students' learning. Computer simulations are important for making learning meaningful through interactive and authentic opportunities to observe, explore, and recreate real objects, phenomena, and processes (Bell & Smetana, 2008). Computer simulations are crucial for the analysis and understanding of physical properties and products, especially for nanoscale research (Stevens et al., 2009).

In education, students either investigate a concept through the use of an expert-developed simulation or build a simulation (Bell & Smetana, 2008; Gould et al., 2007; Leemis & Park, 2006; Alessi, 2000).

Alessi (2000) discusses some design considerations that should be explored when developing a simulation to use in the classroom. In using simulations, learners can have the opportunity to interact with simulations that target specific learning objectives (Alessi, 2000; Bell & Smetana, 2008) or are currently used in research and were not developed specifically for educational purposes (Magana, Brophy, & Bodner, 2012). Magana et al. (2012) discuss methods to incorporate expert-developed simulations for research purposes into classroom instruction for educational use.

Learners will benefit more from building simulations when the primary learning objective is general thinking and developing problem solving skills (Alessi, 2000). One of the benefits of building rather using simulations is students have more flexibility (e.g., room to pursue new directions, ability to explore their own set of assumptions). Alessi (2000) argues for the implementation of both using and building simulations to complement each other.

2.2.1 Using Simulations

Implementing expert-developed simulation tools in education settings enables learners to explore concepts. Simulations are important for making learning meaningful through interactive and authentic opportunities to observe, explore, and recreate real phenomena, processes, and objects (Bell & Smetana, 2008). They enable exploration that would otherwise be impossible to visually investigate due to complexity, size-constraints, time-consumption, and/or danger (Bell, & Smetana, 2008). For these reasons, simulations are especially important for nanoscale research and education (Stevens et al., 2009). nanoHUB.org is an online community for researchers, educators, and learners to develop, disseminate, and engage in simulations about nanotechnology (Klimeck et al., 2008).

There are various studies on the use of research-based simulation tools in education settings, use of simulation tools developed for learning environments (e.g., Alessi, 2000; Bell & Smetana, 2008; Reigeluth & Schwartz, 1989), what students learn from the use of simulation tools (e.g., Vasileska, Klimeck, Magana, & Goodnick, 2010), understanding instructor's learning objectives and intentions when implementing simulations into the curriculum (e.g., Douglas, Faltens, Diefes-Dux, & Madhavan, 2015; Magana et al., 2000), and plenty of other studies focused on using simulation tools – not building. There is a need for greater research on student-developed simulations to enable students to improve their modeling skills, which is the focus of this study.

2.2.2 Building Simulations

Activities that involve building simulations typically consist of prescriptive instruction on how to develop a given simulation (e.g., Gould et al., 2007; Leemis & Park, 2006); such instruction fosters passive learning (Bell & Smetana, 2008; Alessi, 2000). That is, simulation development is taught through directions and facts - a very traditional approach to teaching and learning (Rodgers et al., 2014). In the literature there is a lack of inquiry-based, simulation-building activities reported (Alessi, 2000).

Through self-reflection, Beaulieu et al. (2013) found that their own process of simulation-building resulted in insights that were beyond that of the simulation deliverables. There is a need to further investigate the potential insights that building simulations presents (Beaulieu et al., 2013) and bring these insights to bare in an educational setting. Little is known about how students progress from concept generation to a fully developed simulation or how instructors should design simulation development activities to achieve desired learning outcomes (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). This section emphasizes research around exploratory (not prescriptive) simulation building, where learning occurs through the process of developing simulations.

Before diving into research about building simulations in active learning settings, it is important to better understand the nature of simulations. Simulations are classified by the level of interactivity with the model, the visibility of the model, the types of variables, and the types of visualization. Gould et al. (2007) and Leemis and Park (2006) discussed these features in textbooks that instruct learners on how to build simulations and the purpose for building various types of simulations. Alessi (2000) discussed similar features in a paper that targets the development of effective simulation tools for educational purposes.

Gould et al. (2007) explain that the development of a computer simulation starts with the development of an idealized model of some physical system of interest. A procedure or algorithm is then developed to implement the model in a computer system. The components that are selected to be explored and measured are then chosen to be the variables of the model. Simulations are differentiated throughout the authors' book by the simulation presentation mode, the level of interactivity, the types of interfaces in the simulation, and the types of models used to develop the simulation. The two simulation presentation modes are (1) the actual simulation with user choice of variable inputs and (2) an animation or visualization of a simulation run with default variables. The authors explain that the latter is not simply a video, but a type of animation that presents a captured segment of a simulation. The level of interactivity is defined by the degrees of freedom present in the simulation, which is determined by the number of model variables the user can manipulate. The types of interfaces and models used in a simulation present a level of complexity in simulation differentiation that is not addressed in this study.

Leemis and Park (2006) described some complementing aspects that can be used to characterize simulations. The number of variable inputs indicates the level of interactivity provided by a simulation. The different types of variables involved in a simulation can be either discrete or continuous. The models that back simulations can be deterministic (not including random variables) or stochastic (including random variables). Finally, simulations can be either static or dynamic; dynamic models are time dependent.

Alessi (2000) described five different aspects of simulations that can be used to differentiate and categorize them. First, simulations can be used in educational settings for using or building. Second, simulations can have a black-box or glass-box approach. The black-box approach simply converts an input to an output through a model that is hidden from the user. The glass-box approach enables the user to see how the model works – it visualizes the process as the input changes to the output or details of the outputs allow the user to infer details about the model. Third, simulations are either procedural or conceptual – focus on a process or a concept. Fourth, the simulations are discovery or expository – used to learn new things or to communicate known ideas. Lastly, the degree of model visibility is a way to categorize simulations; this last part also aligns with the types of interfaces discussed by Gould, Tobochnick, and Christian (2007).

Although these books show various types of simulations for the purpose of helping students build effective simulations, there is a lack of research on the nature of simulations that students actually develop when they are first learning about simulations. Having students build simulations to solve open-ended problems presents a unique challenge for instructors. The pedagogical approach is not about giving clear directions of what to do, it is about scaffolding student learning through effective feedback. To give effective feedback, we need to better understand students' confusion regarding interactivity, mathematical models, and simulations. Alessi (2000) and Rodgers, Diefes-

Dux, Kong, and Madhavan (2015) state expert guidance, scaffolding, and feedback throughout challenges that involve building simulations are important for student success.

Rodgers, Diefes-Dux, Kong, and Madhavan (2015) identified and began to address some of the struggles in challenging students to build a simulation in a problem-based learning environment. The research identified types of student-developed simulations, projected stages that students passed through in simulation development, and presented a framework to scaffold students through these stages to enable them to develop a complete simulation tool. A complete simulation tool (Level 4: a Simulation in Table 2.1) contained a model that a user could interact with through manipulable input variables and visualized outputs. The four proposed stages of the framework were developed through a grounded theory analysis of student teams' graphical-user interfaces (GUIs) submitted for a simulation-building design project. The four types were: (Level 1) Basic Interaction, (Level 2) a Black-Box Model, (Level 3) an Animated Simulation, and (Level 4) a Simulation. Ideally, students should reach Level 4, where they have successfully completed a simulation. The scaffolding framework (Table 2.1) proposed student teams progress from Level 1 to Level 2 to Level 4. Level 3 requires a fully developed simulation, but with removed interactivity and converted into an animation of a simulation; this phenomenon of students thinking simulations must be animated has also been seen in investigation of other types of student data (e.g., Rodgers, Diefes-Dux, & Madhavan, 2014; Rodgers, Diefes-Dux, Zielinski, & Madhavan, 2016).

Table 2.1. Proposed Scaffolding Framework for Student-Developed Simulations

Levels	**Name of Level**	**Examples of Student Work**
1	Basic Interaction	These works would only consist of clicking, button selection, or other basic interaction.
2	Black-Box Mathematical Model	These works would have some type of mathematical model that the inputs could be changed on, but there would be no visualization or communication of how the mathematical model works.
4	Simulation	These have all three major components: (1) interaction – variable manipulation, (2) underlying mathematical model, and (3) visualization.
3	Animated Simulation	This would be an animation of one particular run of a simulation. There is not opportunity for the user to manipulate the input variables.

Level 1: Basic interaction. Generally GUIs at this level contain text content and clickable buttons that lead to more text or quiz-like content, both without meaningful interaction with a mathematical model (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). *Level 2: Black-box model.* This level requires some underlying mathematical model, but there is no visual representation of the nature of the model or relationship/s between the input/s and output/s (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). The lack of visibility of the model fulfills the definition of black-box (Alessi, 2000). *Level 3: Animated simulation.* This level requires a visual presentation of a model, but users can only play the simulation with default variables; there are no input variables that the user can set. This level has a higher level of model visibility than *Level 2* and fulfills the definition of glass-box, but does not present user choice (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). *Level 4: Simulation.* At this level, the user can change input variables to explore the nature of the mathematical model behind the simulation (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). This level fulfills the definition of glass-box (Alessi, 2000).

Rodgers, Diefes-Dux, Kong, and Madhavan (2015) found that only about a third of first-year engineering students developed simulations (i.e. Level 4) for a required simulation-building project, about 20 percent of students did not include a mathematical model in their GUI tools, and every student incorporated some type of GUI that only had simple interactions with click buttons to pull up more information or quizzes (i.e. Level 1). Scaffolding and assessment should focus on students' development of three key elements of a simulation: an underlying mathematical model, interactivity (user choice) for exploring the model, and visualization of the model (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015; Rodgers, Diefes-Dux, & Madhavan, 2014).

Rodgers, Diefes-Dux, and Madhavan (2014) created an assessment tool based on the four types of student-developed "simulations" and found that first-year engineering students are able to assess interactivity, but struggle to identify the presence of models and simulations. One aspect of interactivity that students may not understand is the difference between Basic Interaction interactivity (e.g. clicking buttons for information) and Simulation interactivity (i.e. variable inputs that enable meaningful user exploration of a model) (Rodgers, Diefes-Dux, & Madhavan, 2014). Rodgers, Diefes-Dux, and Madhavan (2014) found that students have a lack of understanding of the connection between models and simulations, with some students even indicating simulations are not based on models and there is no connection between them.

Many first-year engineering students do not understand that simulations are based on mathematical models (Rodgers, Diefes-Dux, Kong, & Madhavan, 2014; Rodgers, Diefes-

Dux, & Madhavan, 2014; Rodgers, Diefes-Dux, Zielinski, & Madhavan, 2016). The foundation for building a simulation is a well-developed model (Alessi, 2000; Rodgers, Diefes-Dux, Kong, Madhavan, 2015). Alessi (2000) explains that the model development process is the most complex component of simulation development, over visualization and variable (i.e. input and output) generation. This fundamental connection suggests an opportunity to learn from extensive research within the models and modeling perspective (Lesh & Doerr, 2003) about model-building pedagogical approaches for simulation-building learning environments, along with other research about developing students' understanding of models.

As previously stated, Alessi (2000) points to scaffolding, guidance, and being embedded in cooperative learning as key aspects to creating a successful learning environment for building simulations. The next section of this review discusses effective feedback and techniques to more effectively scaffold students' understandings.

2.3 Feedback

Hattie and Timperley (2007) describe feedback as a "consequence" of performance, since feedback is any type of response to some piece of work. More specifically, feedback is the process of identifying a gap between current and optimal solutions; then determining methods to advance the current work (Hattie & Timperley, 2007; Sadler, 1989). Feedback is a crucial aspect of helping students learn science, technology, engineering, and mathematics (STEM) concepts, especially in problem-based learning environments (Rodgers et al., 2015). In STEM education, effective teacher feedback is largely acknowledged to be one of the most important aspects to student success and also one of the most lacking areas (Carless, Slater, Yang, & Lam, 2010). This section focuses on some types of ineffective and effective feedback.

There are many challenges that students face in receiving feedback (Higgins, Hartley, & Skelton, 2001; Weaver, 2006; Gibbs, 2006; Nelson & Schuun, 2009). Ineffective feedback is difficult to comprehend (Weaver, 2006), lacks details on how to improve (Higgins et al., 2001), and is difficult to use for advancing work (Gibbs, 2006). Effective feedback is focused, well communicated, or relevant. Ineffective feedback is described in greater detail first and then followed by a discussion about effective feedback.

A common feedback technique that is utilized and sometimes taught that is ineffective is praise and mitigation. Praise is any feedback that provides a positive statement of someone's work (e.g. good job). Mitigation is feedback that presents a positive statement followed by a call for change (e.g. good job, but add more details). It is found that praise and mitigation in feedback almost never leads to improvement or change in students' works, especially mitigation because it is confusing feedback (Nelson & Schuun, 2009). Praise is a technique that can be used in feedback to positively influence the student's view of the reviewer/s and potentially lead to changes on other aspects of feedback (Nelson & Schuun 2009). Giving a positive view of the reviewer to the person receiving feedback through praise can be helpful, but mitigation should be completely avoided, especially when giving feedback to non-native English speakers (Nelson & Schuun, 2009). These are the two specific types of feedback that should be avoided to encourage change, but praise can be used to establish trust with the person receiving feedback.

According to research, feedback must be understandable, applicable, and ideally continue through an iterative process to be effective (Alexander, Schallert, & Hare, 1991; Carless et al., 2010; Dale, 2007; Hattie & Timperley, 2007; Nelson & Schuun, 2009; Nicol & Milligan, 2006; Sadler, 1989; Shute, 2007). To prompt change, feedback should be constructive (Rodgers et al., 2015; Shute, 2007).

Nelson and Schuun (2009) explained the most important aspect of effective feedback is ensuring the person receiving the feedback understands the advice for addressing the identified problem. The person receiving feedback must be able to rethink, verify, or build upon the feedback to comprehend it (Alexander, Schallert, & Hare, 1991). This can be done through giving a possible solution, specifically pointing out the location of the problem, and giving a summary of the problem without a further explanation of why to keep focus directed on the actual problem (Nelson & Schuun 2009).

Once feedback is understandable, it must progress to a greater level of effectiveness by being applicable. Instructional feedback should address a gap between current work and an ideal form of the work (established by criteria for success) and then propose alternative solutions or methods to reduce this gap (Nelson & Schuun, 2009; Dale, 2007; Sadler, 1989). Specifically addressing a problem with advice enables a person to address the current shortcomings, which is determined to typically be much easier to utilize than feedback that only identifies a problem (Nelson & Schuun; 2009). Specifically addressing the work being evaluated entails summarizing the concept of the standard or goal being aimed for, comparing the current level of performance to the standard or goal, and giving information that will help enable the creator of the original work to engage in the necessary action to progress the current work closer to the target (Dale, 2007; Sadler, 1989). This feedback may consist of providing more information that may help address the shortcoming, pointing to potential directions to further the work, or indicating alternative strategies to understand relevant information (Hattie & Timperley, 2007).

In order for feedback to be understandable and applicable, it should not be vague or generic (Shute, 2007). Feedback should target the work being evaluated. It is important when using a rubric to evaluate work that the rubric not just be quoted, but feedback is tailored to the work (Rodgers et al., 2015).

Not only is it important that the content of the feedback be effective; it is vital that the mode of giving feedback is effective. The most effective feedback is completed in a closed-loop process, as follows: (1) the person who is receiving feedback submits the work with an explanation of what they feel they need most help on, (2) the reviewer gives understandable and applicable feedback that addresses the work's shortcomings and encourages thinking of the overall concept, (3) the submitter reviews the advice, and finally (4) post reviewing and comprehending the feedback, the submitter makes any necessary revisions (Sadler, 1989). This close-loop process should then be cycled as many times as necessary to progress the work to meet all of the criteria for success

(Sadler, 1989). Iterative feedback should be timely to keep the students motivated, ensure any faulty or misconceived directions are caught early on and mitigated (Lesh & Doerr, 2003). It has also been suggested that transforming this feedback process to a more dialogue conversation rather than written feedback can further enhance it (Nicol & Milligan, 2006; Carless et al., 2010).

Once feedback is provided in an effective manner, it is important to think about the content focus of provided feedback. The most effective feedback prompts change through constructive feedback (Rodgers et al., 2015; Shute, 2007). Constructive feedback can be given through direct or indirect recommendations for change (Rodgers et al., 2015; Shute, 2007). Rodgers et al. (2015) suggested using direct or indirect feedback depending on the type of problem that needs to be addressed; the type of feedback needed may also vary based on context. For example, communication problems and incorrect information usually require direct feedback. Design decisions and logic used in mathematical models should be addressed with indirect feedback to prompt change, while enabling someone to think on their own (Rodgers et al., 2015; Marbouti, Diefes-Dux, & Cardella, 2015). Shute (2007) suggested that indirect feedback, such as cues, hints, and prompts, is more effective for high-achieving learners, but recommends more direct feedback for low-achieving learners.

It is beneficial to keep in mind that the scope of feedback is likely to affect the changes made in response to feedback. Feedback should contain both problems that are localized (typically addressed through direct feedback) and globalized (typically addressed through indirect feedback) (Nelson & Schuun, 2009). Specific feedback is more likely to be implemented in revised works, but global feedback presents a greater possibility to affect the overall quality of the work (Nelson & Schuun, 2009; Matsumura, Patthey-Chaves, Valdes, & Garnier, 2002).

Although feedback may be written in an effective manner, this does not ensure it will be understood or all of the suggested changes will be made. Students response differently to peer feedback than feedback from their instructors (Lin & Chien, 2009; Rodgers et al., 2015). Rodgers et al. (2015) found, in a case study, that a student team made all changes their instructor suggested in the feedback they received during the development of their solutions in model-eliciting activities, even when they did not understand the instructor feedback or the purpose of the changes they made (beyond hopefully getting a better grade). The student team members explained in individual interviews that the instructor knew the answer and controlled their grade, so they always tried to do what the instructor suggested. The studied team improved their mathematical model and received a higher score on their solution, but was not aware of how or why. The same team also did not make changes to their mathematical models based on potentially helpful feedback from their peers. This study presented an example of how students weight of importance of feedback from peers and instructors differently.

Effective, constructive feedback is a critical interaction in model development (e.g., MEAs) for instructors to help guide students away from low-quality models towards high-quality models (Lesh & Doerr, 2003). It is also critical in the simulation building process (Alessi, 2000). This study investigates the types of feedback that teams received during model and simulation development to determine the kind of feedback that students respond to and how they respond to it.

2.4 Theoretical Framework – Models and Modeling Perspective (M&MP)

Constructivism is a learning theory that argues students build knowledge upon previous understandings based on experiences and social interactions (Duffy & Cunningham, 1996; Ferguson, 2007; Straver, 1998). The M&MP goes beyond constructivism in that it emphasizes students' construction of knowledge about mathematical models through interactions with modeling activities through the model development process (Lesh & Doerr, 2003). M&MP is the framework that describes how students learn through the process of building their models both in the studied MEA and design project.

An important aspect of M&MP, similar to constructivism, is connectedness of concepts learned; knowledge is not fragmented segments of ideas (Driver, Asoko, Leach, Mortimer, & Scott, 1994; Kelly & Lesh, 2000; Lesh & Doerr, 2003). The M&MP promotes higher-order thinking by working under the belief that learning is a complicated system that requires refining unstable systems and is not just a simple process of gradually adding and deleting understandings from a novice to make an expert (Lesh & Doerr, 2003; Zawojewski, Hjlamarson, Bowman, & Lesh, 2008). The M&MP focuses on creating meticulously planned experiences for the students rather than transferring facts and skills to students through regulation – traditional perspectives (Lesh & Doerr, 2003). Lesh and Doerr (2003) explain that learning environments utilizing the M&MP prepares students for the future by teaching them vital skills, such as communication, project management, teaming, adaptability to advancing technology, and problem solving (e.g. solving complex problems through simplified interpretations). These skills align with abilities called for by the Accreditation Board of Engineering and Technology (ABET) Accreditation Department (2015) and the National Academy of Engineering (NAE) in *The Engineer of 2020* (2004).

The M&MP focuses on teaching and learning through the use of modeling to reward diversity in thinking, while promoting learning (English, 2003; Lesh & Doerr, 2003). The M&MP focuses on students' models that are developed to solve given modeling problems (e.g. model-eliciting activities). The M&MP focuses on a cycle of growth, a process of development, and mathematical models to describe situations rather than solutions, finite paths, and input-output condition-action rules that are seen in traditional perspectives (Lesh & Doerr, 2003). Since students' models are the primary source of data used to understand students' mathematical thinking, it is crucial that the modeling problems are developed with great scrutiny.

To ensure that the modeling problems are realistic and designed to recognize a broader range of mathematics potential, six principles of instructional design were created. The six principles are: (1) *the personal meaningfulness principle ("reality" principle)*, (2) *the model construction principle*, (3) *the self-evaluation principle*, (4) *the model-externalization principle (model-documentation principle)*, (5) *the simple prototype principle*, and (6) *the model generalization principle* (Lesh et al., 2003). Lesh et al. (2000)

describe these six principles in greater depth; they are summarized here. The *reality principle* enables students to make sense of the situation by ensuring the scenario could happen in real life. The *model construction principle* requires the modeling activity incorporate the development of an explicit construction, description, explanation, or justification of a mathematical situation. The *self-evaluation principle* (or *self-assessment principle*) focuses on the appropriateness of the given criteria to ensure the students can understand improvement of their model. The *model-externalization principle* (or *construct documentation principle*) emphasizes making students' ideas visible for the purpose of self-reflection and researchers' investigation into their understanding. The *simple prototype principle* (or *effective prototype principle*) ensures the context is memorable and requires the development of a significant construct, while still eliciting as simple a solution as possible. The *model generalization principle* (or *construct shareability and reusability principle*) means students' models should work with other data sets and have the potential for modification for similar scenarios.

Through development of modeling problems, these six principles emphasize the importance of having adequate complexity, ensuring the problem is open-ended – meaning the solution does not have one single right answer, and while there is not a single answer, not every solution can be a good solution. The principles also ensure the modeling problem are set in a realistic context that is believable and presents opportunity for a solution that is generalizable (Lesh et al., 2003).

According to the M&MP, solving the modeling problems facilitates a social enterprise for students. This means the development of models requires students to work as a team to utilize their varied perspectives, diverse thinking, and unique abilities. It also means they must develop their model thinking with different modes of communication (e.g., symbols, numbers, graphs, verbal, written). Lastly, it means they must consult within teams and outside of teams (e.g., peers, instructors, superiors, customers, stakeholders) to further refine their models (Lesh & Doerr, 2003). Lesh and Doerr (2003) discuss visualization, such as graphic, dynamic, and interactive displays, as presenting another mode of communicating conceptual understandings of models – further contributing to the social enterprise. This presents opportunity to consider the influence that new modes of communication may have on students' models; this is investigated in this study.

CHAPTER 3. METHODS

Lesh (2008) explains the importance of using qualitative methods within the constructivism paradigm to investigate how people learn by getting in their heads. Qualitative approaches acknowledge students are constantly changing individuals with varying perspectives and previous experiences, whereas more traditionally accepted "scientific research" methods are more suited to subject matter where variables can be controlled (Gall, Gall, & Borg, 2007; Johnson & Christensen, 2002). To do rigorous research investigating "how" one must understand that investigating an environment with people presents a complex set of assumptions and models that are inconsistent with the phenomena established in traditional laboratory settings. In the development and assessment of curriculum innovations it is vital to understand how and why the curriculum is impacting the students' understandings, not just simply demonstrating that it is working (Lesh, 2008). Aligning with this, the research questions, data collection, and data analysis are rooted in a qualitative perspective and utilize case studies to gain in-depth understanding of mathematical models and simulation tools students developed.

The purpose of a case study is to gain an in-depth understanding of a phenomenon (Yin, 2011). Case studies enable investigation of students' project work under authentic classroom conditions, insight into the views of the students in the study, understanding of the contextual conditions, assessment of the emerging perceptions that may explain what the students did in their projects, and allowance for multiple sources of evidence rather than reliance on a single source (Yin, 2011). Yin (2011) discusses eight distinct decisions that should be made prior to data collection. These decisions require a researcher to start a research design at the beginning of a study, determine what measures will be taken to strengthen the validity of a study (e.g. integrity in data collection), clarify the complexity of data collection units, attend to sampling, incorporate concepts and theories into a study, plan at an early stage to obtain participant feedback, be concerned with generalizing a study's findings, and prepare a research protocol. One option is to determine not to make any of these decisions, but either way it should be a conscious decision made prior to the beginning the study. These steps are discussed in greater detail where pertinent in the data collection and data analysis subsections (Sections 3.2 and 3.3).

This study is set within a first-year engineering (FYE) course at Purdue University in Spring 2015. The setting and participants are discussed in greater detail in the first subsection. This study consists of three major steps: (1) a quantitative analysis of the nature of all teams' mathematical models and simulations and how they changed, (2) identification and selection of teams for case study based on their mathematical models, simulations, and changes, and (3) the case study analysis. These three steps are discussed in the data collection and data analysis subsections.

3.1 Setting and Participants

At Purdue University all engineering students are required to complete the First-Year Engineering (FYE) Program before they can matriculate into their field of study in engineering and take discipline-specific courses. The students are required to take the FYE courses ENGR 131 and ENGR 132, Ideas to Innovations I and II, respectively. ENGR 132 is the subsequent course to ENGR 131. ENGR 131 is most commonly taken in the fall and ENGR 132 in the spring. Both courses are two credit hours and require students to meet in-class twice each week for 110 minutes. Both of these courses focus on helping students develop fundamental skills for engineering, such as problem-solving, mathematical modeling, design, using computer tools, teaming, and communication. This study was set in the ENGR 132 course in Spring 2015.

The ENGR 132 course facilitates students' achievement of four primary course goals. The goals, as stated on the syllabus, are to:

1. Practice making evidence-based engineering decisions on diverse teams, guided by professional habits,
2. Develop problem-solving, modeling, and design skills of an engineer,
3. Learn how to use computer tools to solve fundamental engineering problems, where the emphasis will be on MATLAB®, and
4. Develop teaming and technical communication skills.

In Spring 2015, 1,563 students continued in the FYE Program and completed ENGR 132: Ideas to Innovations II. These students were enrolled in 15 sections of ENGR 132 taught by 11 different instructors (with 2 instructors teaching 2 sections and 1 instructor teaching 3 sections).

The curriculum of ENGR 132 includes two projects: a model-eliciting activity (MEA) and a design project. Students completed both of these projects in teams that were assigned through CATME (Ohland, Loughry, Carter, & Schmucker, 2006). These projects contribute to the students attaining the course goals. In spring 2015, all of the students were required to complete the quantum dot solar cell (QDSC) MEA. Upon completion of the MEA, 11 of the 15 sections required students to develop their QDSC MEA model into a simulation for the QDSC design project, while the other 4 sections completed design projects that were not connected to the QDSC MEA. The students in these 11 sections that complete both QDSC projects are the participants of this study. The ENGR 132 course structure, materials, and these two discovery-learning projects are described in detail in the subsequent sections.

Since the development of computational tool skills to solve fundamental engineering problems is an important learning objective in this FYE course, students are prompted to use Microsoft® Excel and/or MATLAB® to build their mathematical models in response to the MEA (Diefes-Dux & Imbrie, 2008). Students are also required to use MATLAB® for their design project.

3.1.1 ENGR 132 Course Structure and Curricular Elements

Since there are a large number of students in the FYE program, ENGR 131 and ENGR 132 are strategically structured. There are up to 120 students in a class (or section), and students work in teams of ideally four students (resulting in up to 30 teams per a section). To give students facilitator support and timely feedback, each course has an instructional team consisting of one instructor, one graduate teaching assistant (GTA), four undergraduate teaching assistants (UTAs), and an undergraduate grader. The instructors determine how their course is facilitated. GTAs and UTAs are responsible for giving students verbal feedback in class during activities and written feedback to teams on their submitted projects (i.e. MEA or design project); graders do not interact with students and are solely responsible for helping the TAs outside of class time with grading homework assignments and submitted in-class activities. This structure is presented in Figure 3.1 with the numbers of students, sections, and TAs for ENGR 132 in Spring 2015.

With a large instructional team consisting of both GTAs and UTAs who play an important role in scaffolding student learning through feedback, training and professional development are an important part of TA preparation. There are some required trainings that focus on their responsibilities and interacting with students. In addition the TAs participated in the formalized MEA training – the training relevant to this study (Verleger & Diefes-Dux, 2013). There was no formal training related to the design project.

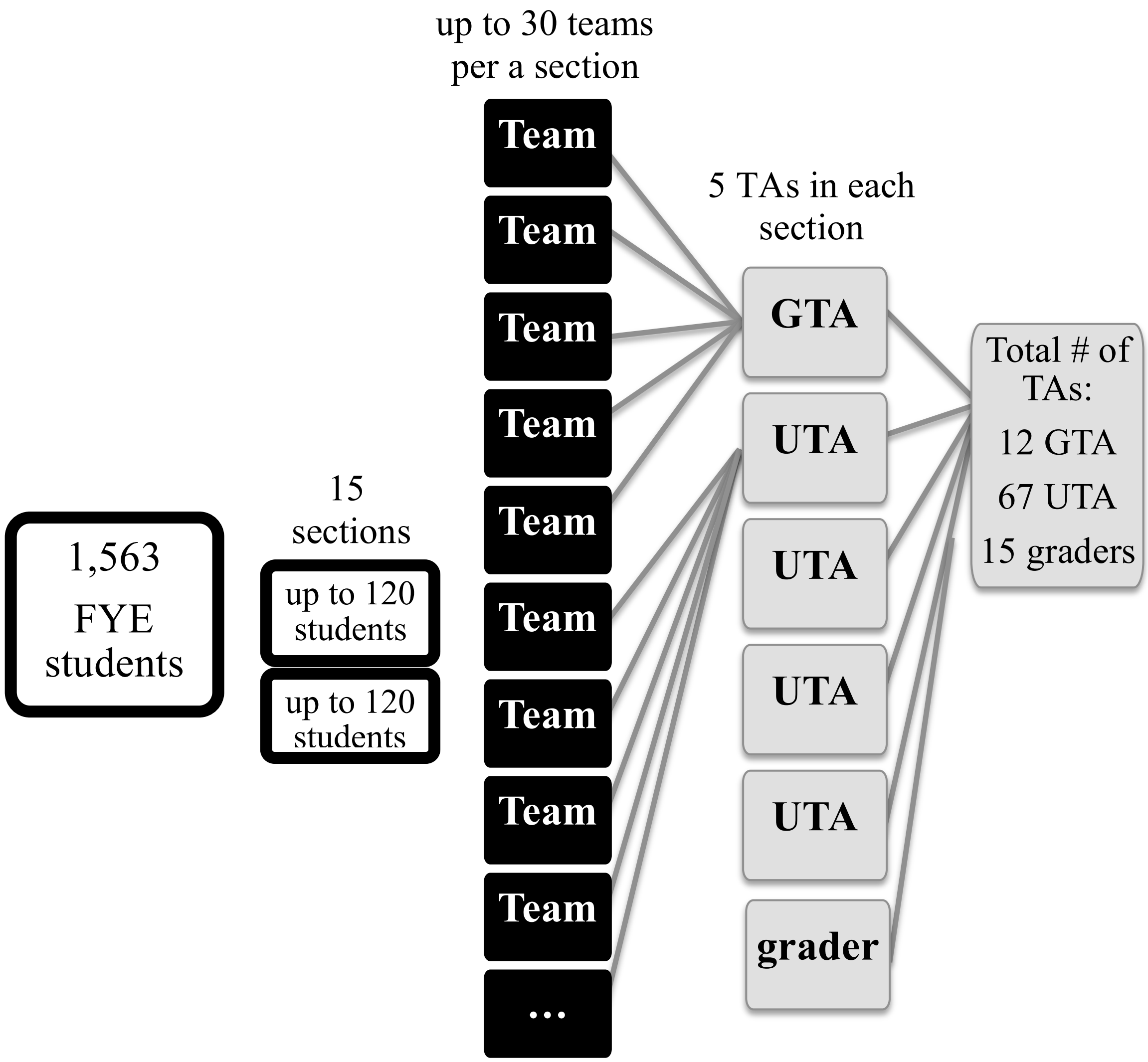

Figure 3.1. Structure of ENGR 132 in Spring 2015

The class itself is run in studio mode, meaning the bulk of class time is reserved for teams to work on exploratory activities, problem sets, and projects. Each class typically began by summarizing material that the students struggled with in the previous class and the new material they reviewed prior class. Prior to attending class students are required to watch online modules covering the basics of the content for the upcoming day. The course topics include teaming, basic statistics topics (e.g., descriptive statistics, introductory linear regression), and programming skills (e.g., flowcharting, user defined function, for loops, while loops, GUI development). A full list of topics can be seen in the course schedule, as printed in the syllabus (Appendix A). Students are also required to pass online module learning-objective driven assessments, complete unfinished in-class activities, and do homework assignments focused on the current lecture topic. The course content enables the students to acquire course goals and develop their project solutions.

The curricular elements most pertinent to this study are the QDSC projects that the students completed. Both of these projects had a nanotechnology context. Prior to working on these projects, students were prompted to individually explore how nanotechnology impacts their anticipated field of study to help them personally connect to the topic of nanotechnology (Rodgers, Diefes-Dux, & Madhavan, 2013). To help them further engage with the nanotechnology context, students were prompted to participate in an online nanotechnology community (i.e. nanoHUB.org) throughout their projects. Some of the project content was provided to the students through group pages developed specifically for these projects on nanoHUB.org (nanoHUB.org/groups/qdsc_fyeproject and nanoHUB.org/groups/qdsc_fyedesignproject). To help explain the context of these projects, the science relevant to these projects and the simplifications that were made to make this subject accessible to first-year engineering students is discussed below.

3.1.2 Quantum Dot Solar Cell (QDSC) Context

To establish how nanotechnology impacted solar energy conversion in QDSCs, the students were introduced to the physical phenomena associated with semiconducting materials and, specifically, quantum dots. For example, due to the electronic band structure provided by the materials and atomistic order associated with semiconductors, these electronically-active quantum dot materials are capable of converting photons to electrons in a rather direct manner. That is, the absorption of a photon with an energy greater than or equal to that of the band gap energy (E_g) of the semiconducting material allows for the promotion of a valence electron of the semiconducting material to the conduction band of the semiconductor (Sze & Ng, 2006). Once in the conduction band, the electron is able to move with a relatively high degree of freedom (i.e., in a manner that is fairly decoupled from the nuclei of the crystal lattice). These charges can then be extracted from the semiconductor and used to power external devices. In this way, the solar energy is converted to the higher value electrical energy in a direct manner.

Because the band gap energy of the material is critical in determining if an incoming photon will promote a valence electron to the conduction band, systematic tuning of the band gap energy to match the solar spectrum is a heavily-studied field (Boudouris, 2013). On a more macroscopic, device level, an increase in the number of photogenerated charge carriers typically (all though not always) leads to an increase in the short-circuit current density (J_{sc}) of a photovoltaic device. Any increase in the short-circuit current density leads to a proportional increase in the power conversion efficiency of the solar cell; therefore, adjusting the band gap energy in a well-conceived manner can lead to marked solar cell device improvements.

Quantum dot materials offer a direct means by which to provide this tuning as their absorption (and emission) spectra can be tuned by simply changing the size of the materials according to well-known principles that account for the size of the nanoparticle and the band gap energy of the bulk inorganic semiconductor. In general, this is a rather remarkable feat for inorganic materials as altering the band gap energy of these materials through chemical means is rather challenging.

Therefore, significant effort has been placed in designing, synthesizing, and implementing quantum dot semiconductors in photovoltaic applications. This has led to a combination of computational design investigations by physicists, advanced synthetic procedures by chemists, and fabrication and testing of quantum dot solar cells by engineers. As such, significant progress has been made with respect to achieving relatively high power conversion efficiency values at the laboratory scale. However, the ability to scale the production of quantum dot semiconductors to larger values and the potential toxicity (e.g., adverse effects felt by the fabrication engineers and concerns regarding run-off and ground water contamination of toxic quantum dot materials in the event of a catastrophic failure of the solar panels) concerns of some of the semiconducting nanomaterials has been of concern to the alternative energy community.

In this effort, one key underlying assumption is made in the project to keep the complexity of the problem manageable for the FYE students. This assumption is that the average band gap energy value of the quantum dot mixture is the summation of the band gap energy values of the individual components weighted by their relative abundance in the mixture (by mass). In reality, the combination of materials would likely result in some sort of alloyed material structure (i.e., a material that would have different chemistry and crystal structure arrangements relative to any of the pure components) that would have a band gap energy that would not necessarily be related to the band gap energy values of the pure materials. As such, we stress that the assumption made to simplify this MEA does not fully address the complex chemistry and materials science of actual quantum dot combinations. While this assumption is non-physical in nature, it provides a clear means by which to allow the student teams to optimize the quantum dot mixture. Furthermore, it does not remove the key nanotechnology design idea that relates the band gap energy of a quantum dot material to the radius of the semiconducting particle.

By making this assumption, the student teams are able to optimize the performance of the quantum dot solar cells as a function of overall efficiency and the tradeoff between cost and the potential human and environmental impact of the materials used in the production of the quantum dot solar cell for various efficiencies. In this way, the MEA allows students to connect nanotechnology concepts with economic and environmental health and safety concerns in a direct and tangible manner.

3.1.3 Quantum Dots Solar Cells (QDSC) Model-Eliciting Activity (MEA)

The QDSC MEA was designed in accordance to the six principles of instructional design (Lesh et al., 2003). This ensures that the modeling problem is realistic and designed to recognize a broad range of students' mathematics ability (Rodgers et al., 2016). Rodgers et al. (2016) describe the process of developing, testing, and fully implementing the

QDSC MEA in greater detail. This section focuses on the QDSC MEA and its implementation sequence in Spring 2015.

In the QDSC MEA, the student teams are tasked with developing algorithms to optimize a mixture of quantum dot materials for cost and toxicity using the actual science of quantum dot solar cells. Given five materials, and their relevant properties, student teams must develop a method to mix the materials such that the mixture contains at least two percent by composition each of the five materials. The material properties of importance are: (1) bulk band gap energy value; (2) quantum dot radius; (3) cost per unit mass; and (4) toxicity per unit mass. The resulting optimization strategies must achieve a specified band gap energy ($E_{g,eff}$). The students must demonstrate functionality of their algorithm for two different band gap energies (1.33 eV and 1.65 eV), but their algorithms should allow the direct user to change the desired band gap energy. Again, the assumption is that the average band gap energy value of the quantum dot mixture is the summation of the band gap energy values of the individual components weighted by their relative abundance in the mixture (by mass). The teams used theoretical equations to compute effective band gap energy ($E_{g,eff}$) and band gap energy (E_g) and sample QDSC materials' properties data provided in the MEA materials to develop their mathematical models.

Prior to developing their mathematical models for the QDSC MEA, students individually explored the relevant theoretical equations in the quantum dot solar cells computational homework assignments (Appendix B). Based on the initial requests for the MEA (Appendix D), students also investigated the problem context through the individual questions homework assignment (i.e. problem scoping, shown in Appendix C). Once the students were familiar with the background information, teams work together to address the initial MEA requests (Appendix D).

The project information was provided to teams in the form of memorandums (memos) written by the Vice President of Research of a fictitious company (i.e., Power-by-Nano Technologies) (provided in Appendix D, Appendix E, and Appendix F). To align with the model-externalization principle (Rodgers et al., 2016; Lesh et al., 2003), all of the MEA submissions (i.e. MEA Draft 1, MEA Draft 2, and MEA Final Response) were submitted in the form of a technical brief. Some of the teams' solutions also included additional data or their calculations in attached document(s) (e.g., MATLAB programs, Microsoft® Excel files), but all aspects of their solution were required in the written document.

The iterative solution process and feedback were crucial to the implementation of the QDSC MEA sequence. Table 3.1 lists all of the major submissions for the MEA. The name of assignment of task, the corresponding documentation in the appendix, the main purpose for the submission, how the submission was completed (i.e., individually or in teams), the week due, and who gave feedback are described in the table. For example, the first submission was the homework assignment – quantum dot solar cell computations. This assignment was completed individually, submitted by the second class of the first week (1B), and students received feedback on this assignment from their TA.

Table 3.1. QDSC MEA Implementation Sequence

Assignment or Task	Docum-entation	Primary Function/Focus	Completed by:		Week Due	Feedback
			Indiv-idual	**Team**		
Quantum Dot Solar Cell Computations	Appendix B	Introduction to equations and their application	**X**		1B	TAs
Individual Questions	Appendix C	Problem scoping	**X**		2B	TAs
Initial Requests	not included	More practice using relevant equations		**X**	2B	TAs
MEA Draft 1	Appendix D	First iteration of MEA		**X**	3A	peers
MEA Draft 2	Appendix E	Second iteration of MEA		**X**	5A	TAs *(based on I-MAP)*
Data Generation	not included	Create data set to test modifiability dimension of MEA	**X**	**X**	6A	TA
MEA Final Response	Appendix F	Third iteration of MEA		**X**	7A	TA *(based on I-MAP)*

The QDSC MEA submissions (i.e. MEA Draft 1, MEA Draft 2, and MEA Final Response) are most relevant to this study and are described in greater detail below. Upon completion of each of these MEA team submissions, the team also submitted a documentation of changes that described how the team responded to the feedback they received and the changes that they made. The documentation of changes portion prompted students to reflect on their feedback by asking six questions. Four of these questions prompted students to think about changes along the four MEA dimensions. (Example: "Identify 1 or more things for the Mathematical Model dimension that your team needs to address in order to improve your work. Write out how you can / will address these things.") The other two questions asked the teams if there was feedback they disagreed with or did not understand, respectively.

The teams submitted their first attempt at solving the QDSC MEA in Draft 1. This attempt focused on the development of algorithms to optimize mixtures for cost or toxicity only. Students provided feedback on teams' Draft 1 submissions through a double-blind peer review process after completing a required calibration exercise (Verleger, Rodgers, & Diefes-Dux, in press; Verleger, Diefes-Dux, Ohland, Besterfield-Sacre, & Brophy, 2010). Each of the teams then revised their memos by responding to the peer feedback they received. The team documented the changes they made to their solution based on the peer feedback and turned in this documentation. The teams also revised their solutions to address the additional request given in the Draft 2 memo to provide additional demonstrations of the functionality of the algorithms using the extended QD materials list and to create an algorithm to minimize both cost and toxicity.

The revised solution (i.e. Draft 2) was then submitted for TA grading. Each team received feedback from a TA. The TAs assessed the teams' solutions and gave feedback based on their training and use of the instructor MEA feedback and assessment package (*I-MAP*) (Appendix G). The teams made revisions based on the TA feedback and again documented the changes made in response to the feedback. The teams demonstrated the functionality of their algorithms on their solutions to incorporate the new QD materials they created in the data generation in-class activity and homework assignment.

The revised solution (i.e. the Final Response) was then submitted for a final round of TA grading. Each team received feedback and a grade from their TA based on the *I-MAP*. For this submission, TAs were trained to give feedback on the changes that students made for this submission and re-iterate feedback that was given on Draft 2 and that was not addressed in this submission.

As aforementioned, the TAs used the *I-MAP* (Appendix G) to give feedback to teams on their MEAs. The *I-MAP* addressed four dimensions of the MEA solutions (i.e. *Mathematical Model*, *Re-Usability*, *Modifiability*, and *Share-Ability*). The *Mathematical Model* dimension addressed the soundness of the mathematics underlying the model and the selection of the data sources incorporate into the model; this dimension focused on the actual model. The *Re-Usability* dimension focused on the stakeholders, constraints, and assumptions; this dimension addressed how well the teams' solutions are situated in the problem context. The *Modifiability* dimension addressed the malleability of the model and focused on the teams' justifications for decisions about their model development. The *Share-Ability* dimension focused on the audience and ensured effective communication to the given audience (i.e. fellow engineers – Power-by-Nano Technologies). The team response portion of the *I-MAP* gives guidelines to TAs on how to score teams' work along all four of these dimensions. There was some guidance for the TAs in the *I-MAP* about what solution content to focus on and how to give the most effective feedback when responding to teams' submissions, but the majority of preparation for giving feedback was received in TA training.

For the MEA training, all of the TAs were required to participate in an online and face-to-face session. First the TAs had to develop their own solution to the QDSC MEA to better understand the challenge the student teams were going to face. Then the TAs had to assess and give feedback on prototypical pieces of team solutions. They were then prompted to compare their feedback to the feedback of an expert. After they completed these portions of their online training, they attended a 2.5-hr face-to-face training. During this training the TAs were taught how to assess and give feedback on various types of team solutions. The face-to-face training consisted of lecture content about typical teams' solutions and assessment techniques, discussions about lecture content and veteran TAs' past experiences, and time for asking clarifying questions.

Since the mathematical model was the focus of this study, this is the only dimension described in greater detail. The *Mathematical Model* dimension required TAs to assess the teams' mathematical models along nine items (Table 3.2).

These items were based on the requirements for a high quality model. This table of items to assess for scoring teams' mathematical models was only given to the TAs and instructors to enable them to both assess teams' models and provide feedback to guide teams to produce higher quality models. The students did not receive this list, but most of these items were explicitly communicated in the memos (e.g., material quantities sum to 100 grams, minimum material quantity is two grams, required mechanisms). The assessment of all these items resulted in a score of 0 to 18 points.

Table 3.2. Mathematical Model Elements Assessed for Scoring

Mathematical Model Elements	Fully Addressed (2 pt)	Somewhat Addressed (1 pt)	Missing or Inadequately Addressed (0 pt)
1. Material quantities sum to 100 g			
2. Minimum material quantity is 2% (2 g)			
3. $E_{g,quantum\ dot}$ for each material is correctly computed			
4. $(E_{g,quantum\ dot})_{eff}$ is correctly computed			
5. There is a mechanism for achieving the desired $(E_{g,quantum\ dot})_{eff}$			
6. There are mechanism for minimizing cost			
7. There are mechanism for minimizing toxicity			
8. There are mechanism for minimizing cost and toxicity			
9. The solution space is searched with some attention to minimizing the number of iterations.			

3.1.4 Quantum Dots Solar Cells (QDSC) Design Project

While the teams completed their QDSC MEA Final Response, they began their QDSC design project (i.e. Milestone 1). The QDSC design project required the same student teams to continue developing their QDSC models by building them into simulations with GUIs generated through MATLAB®'s GUIDE (graphical user interface design environment). The MATLAB® environment enabled students to create visually appealing interfaces to overlay their computational work using predominantly programming techniques they learned in the course. Thus, students could practice their design and teaming skills while reinforcing their newly acquired programming skills.

Previous nanotechnology-based GUI design projects implemented in the FYE course emphasized building simulations (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015), because this is one of the big ideas of nanotechnology (Stevens et al., 2009). Previous research investigating students' solutions to these projects found that many students did not understand that simulations are based on models (Rodgers, Diefes-Dux, & Madhavan, 2014; Rodgers, Diefes-Dux, & Madhavan, 2013; Rodgers, Diefes-Dux, Kong, & Madhavan, 2015; Rodgers, Diefes-Dux, Madhavan, & Oakes, 2013). To ensure this misunderstanding or disconnected thinking was addressed, the development of students' QDSC models was extended into the development of one or more simulations through the QDSC design project (Rodgers, Diefes-Dux, & Madhavan, 2015).

The QDSC design project required the teams to build simulation suites consisting of at least one simulation based on the QDSC mathematical model and two or three additional simulations. The teams were required to develop at least one simulation per team member to ensure that each student was responsible for some MATLAB® coding. The simulations had to be packaged together along a common theme about solar energy to a team-determined audience (e.g., residential consumer looking to install a solar panel, a cost analysis calculator for consumers wanting to install a solar panel, and a manufacturing company mass producing solar panels). The teams were given potential ideas, mathematical models, and data that they could use in their simulation suites in class and through the nanoHUB group page created for their design project (nanoHUB.org/groups/qdsc_fyedesignproject).

Teams' projects were assessed using the following five criteria: (1) targets a well-defined direct user and presents clear goals around planning PV solar panel fabrication, (2) contains at least one mathematical model per student team member on which a simulation is based, (3) each mathematical model should be made into a simulation that enables the direct user to explore and visualize the relationship(s) between inputs and outputs of the mathematical model, (4) is highly interactive, and (5) is easy to use and operate. These criteria were assessed using the *Project Rubric* (Appendix H), as applicable to particular project milestones.

The project began with Milestone 0, where the students were prompted to ask questions of a nanoHUB representative about the project, nanotechnology, and nanoHUB to better prepare the students to develop their solutions through nine proceeding milestones. Teams' projects were developed through an iterative process of project submissions, and TAs, instructors, and nanoHUB.org representatives provided feedback. These milestones are summarized in Table 3.3, which details the learning objectives associated with the milestone (i.e. Documentation), the purpose of each milestone (i.e. Primary Focus/Function), if the milestone was completed by teams or individual students (i.e. Completed By), the week the milestone was due (i.e. Week Due), and who the team received feedback from (i.e. Feedback). This implementation sequence follows a typical design process starting with problem scoping, followed by concept generation, leading to concept reduction and prototyping, and ending with detailed projects.

Table 3.3. QDSC Design Project Milestones (M) Implementation Sequence

M	Documen-tation	Primary Focus/Function	Completed by: Indiv-idual	Team	Week Due	Feedback
0	Appendix I	Project Introduction	**X**		6A	In-class
1	Appendix J	Problem scoping	**X**		7A	TAs
2	Appendix K	User profile and GUI evaluation	**X**		8B	TAs and automated
3A	Appendix L	Concept generation		**X**	9A	TAs
3B	Appendix L	Concept reduction		**X**	11A	TAs
4	Appendix M	Navigation map and rapid prototype (PowerPoint of potential GUI)		**X**	12A	nanoHUB *(based on Project Rubric)*
5	Appendix M	Final proposal (final PowerPoint submission of potential GUI)		**X**	13A	TAs *(based on Project Rubric)*
6	Appendix N	Draft GUI (interfaces completed, but coding behind functionality not yet developed)		**X**	14B	TAs
7	Appendix O	Beta 1.0 demonstration for instructional team (full GUI)		**X**	15B	TAs
8	none	Beta 2.0 demonstration for nanoHUB (full GUI)		**X**	16A	nanoHUB *(based on Project Rubric)*
9	Appendix P	Final demonstration for instructional team (full GUI)		**X**	16B	TAs *(based on Project Rubric)*

For each of these milestone submissions, the team documented how they addressed the feedback they received on their previous milestone by responding to two questions (e.g., in Milestone 2 they wrote about feedback they received on Milestone 1). The questions prompted the teams to summarize the feedback they received and how they were responding to the feedback. (Example: "In your own words, what feedback have you received on M1?" and "How are you addressing this feedback in M2?")

The type of feedback the teams received focused on the objectives for the particular milestone. For Milestones 4, 5, 8, and 9, the feedback focused on the five established project criteria (Appendix H). The criteria for the other milestones were associated with their particular learning objectives (found in their corresponding "Documentation" listed in Table 3.3). Students only received feedback on those aspects of their milestones for which they did not receive a perfect score.

Unlike the MEA assessment, there was no formalized training to prepare TAs and instructors to give feedback to student teams on their design project (Rodgers et al., 2016). While there was no rigorous process to prepare the instructors to implement the projects in their sections, the projects were introduced during the pre-semester retreat and discussed periodically in the instructors' weekly meeting. Each instructor was responsible for organizing how feedback was given and overseeing their TAs that gave feedback. This was the current practice for previous design projects implemented in the course. Prior to giving written feedback to teams on Milestone 4, the nanoHUB representatives did participate in a 1-hr training to understand the nature of the students' projects via prototypical student solutions and how to use the rubric through explanations and examples of how to apply the *Project Rubric* to prototypical solutions. This was the only project-related training that any nanoHUB representatives received.

3.2 Data Collection

The previous sections described the setting of this ENGR 132 course and the QDSC projects embedded in the course; this provides the big picture view of the data collected for this study. This section discusses the pertinent details of the data collected.

It is important to acknowledge that the research questions were established prior this study. Some qualitative researchers argue that questions should emerge from field experiences rather than be predetermined, so the initial questions do not influence the study's direction (Hatch, 2002; Yin, 2011). Since this study's questions were pre-established, it was important to maintain integrity during data collection so as not to influence the findings, such as adjusting the data collection or learning environment during the semester based on preliminary findings. When changes are made during the data collection, they must be well-documented and made transparent (Yin, 2011). There were no mid-stream changes made in reaction to this study's research questions to the course or projects to influence the findings of the research questions. There also was not any data analysis conducted prior completion of the course. Some instructors did make changes in their sections based on personal decisions unrelated to this research. These changes were not documented but are discussed by Rodgers et al. (2016).

The data collected for this study consisted of the project submissions, the feedback teams received, and the teams' documented changes based on their feedback. The project submissions consisted of all of the content submitted for the team MEA submissions (i.e.

Draft 1, Draft 2, and Final Response; Table 3.1) and the design project milestones (i.e. all nine milestone project submissions; Table 3.3).

All of the data from the MEA were collected through mealearning.com© (Verleger & Diefes-Dux, 2010). The MEA submissions were submitted as uploaded files of Microsoft® Word, Microsoft® Excel, and/or MATLAB® files, based on the teams on discretion. The MEA feedback from the peers and TAs was collected through textbox inputs associated with the *I-MAP*. The documentation of changes were collected through six textbox inputs that corresponded to the six questions about the feedback they received and how the team responded to it.

All of the data from the design project were collected through Blackboard©. The design project submissions were submitted as file uploads in the form of word documents, presentations, Microsoft® Excel files, and MATLAB® files (both GUI figure and code files). The design project feedback from the instructional team was collected through rubrics that covered the pertinent project criteria or learning objectives. The design project feedback from nanoHUB representatives was documented by student teams and uploaded in the form of a Microsoft® Word document. The documentation of changes were submitted within uploaded Microsoft® Word document, as part of their milestones. Observations and field notes pertaining to the students' learning environment were also collected. To ensure an accurate portrayal of the setting and participants, the researcher documented observations while attending the majority of classes for one ENGR 132 section, watching the online video lectures, and while attending all of the training sessions. These field notes were documented from a post-positivist, ethnographic perspective since the sole purpose of these observations was to document what happened and not to capture the environment, social interaction, or any other interpretative aspect.

In addition to these field notes, research notes were documented to capture impressions, reactions, reflections, and tentative interpretations throughout the collection and analysis of data. Hatch (2002) explains analysis happens as soon as data collection begins, so it is important for researchers to document their thoughts and reflections throughout the process of data collection. These notes influenced the discussion about limitations of this study and future research directions (CHAPTER 4).

The variety of data collected for this study enabled results to be triangulated to verify particular findings pertinent to the research questions about how students' mathematical models changed and the factors that influenced those changes. Triangulation strengthens the validity of claims in a study (Yin, 2011). An example of triangulation is analyzing a team's project submissions to see how their mathematical model changed, the feedback the team received to see what may have influenced the change, and the team's documentation of changes to understand what the team stated influenced their change.

3.2.1 ENGR 132 Course Instructors

In Spring 2015, both of these projects were implemented in 11 sections of the FYE course that were taught by eight different instructors (Table 3.4), which did not include all of the 15 sections from the original data set. Three instructors taught four of the 15 sections and chose to do different design projects, and therefore did not participate in this study. The lecture materials, projects, and evaluation criteria were all developed by the ENGR 132 development team and supplied to the instructors. The instructional materials provided to the students were consistent. The variation of instruction given in the classroom was not documented through observations. The eight instructors for the 11 sections had varying backgrounds and experiences. Two of the instructors were advanced graduate student instructors; four of the instructors were tenured professors within the same department (two associate and two full); and two of the instructors were full-time lecturers for the department. The educational backgrounds for the instructors were an assortment of engineering disciplines (e.g., engineering education, mechanical engineering, civil engineering). The amount of experience with nanotechnology both within and outside of the course varied amongst the instructors. One of the eight instructors was part of the team that developed the two projects. Five of the eight instructors had previously implemented a nanotechnology-based MEA (i.e. NanoRoughness MEA – described by Moore & Hjalmarson, 2010) in ENGR 132 (Table 3.4). Two of the instructors (including the one that helped develop the QDSC projects) had been involved in previous implementations of nanotechnology-based design projects in ENGR 132 (Table 3.4).

Table 3.4. Instructor Information

Instructor	**Sections**	**Nano-Roughness MEA**	**Nanotechnology-based Design Project**
A	1	No	No
B	2	Yes	Yes
C	3	Yes	No
D	4	Yes	No
E	5	No	No
F	6 – 8	Yes	Yes
G	9, 10	No	No
H	11	Yes	No

3.2.2 ENGR 132 Student Participation

Out of the 303 student teams from the 11 sections, teams with poor class participation were removed to ensure the lack of student participation was not the primary reason for a team missing components of the assigned projects. Lack of student participation was determined by class attendance and scores on their individual assignments completed for the course. Seventy (70) teams were eliminated from this study because at least one student on the team had 6 or more class absences and/or earned less than 50 out of a possible 150 points on individual assignments. In addition to these 70 teams, three more teams were removed due to significantly incomplete data. One team from Section 1 did not submit the required documentation for their MEA Final Response; they only submitted an excel file and not the required technical brief. One team from Section 6 did not submit the required documentation for their Milestone 9 submission. One team from Section 2 that completed the design project was actually just an individual student that was removed from their original team after the MEA.

Seventy-three (73) teams were eliminated from the analysis (Table 3.5). The remaining 230 teams were included in this study (Table 3.5). Marbouti, Diefes-Dux, and Strobel (2014) found FYE students in 7:30 am sections had lower grades than other sections. Sections 1, 6, and 8 were 7:30 am classes; this may be connected to Sections 1 and 6 having the highest percentages of teams removed for low participation – 50 percent and 44 percent, respectively.

Table 3.5. Number of Student Teams in the Study

Instructor	**Section**	**No. of Students**	**Total No. of Teams**	**No. of Teams removed**	**No. of Teams in the study**
A	1	90	26	13	13
B	2	111	30	2	28
C	3	112	29	6	23
D	4	111	29	9	20
E	5	112	29	2	27
F	6	95	25	12	13
	7	116	29	5	24
	8	76	20	5	15
G	9	115	29	4	25
	10	112	28	6	22
H	11	115	29	9	20
ALL – total		**1165**	**303**	**73**	**230**

3.3 Data Analysis

The purposive sampling method discussed throughout this analysis is to ensure meaningful cases are selected to yield relevant and abundant data, while still capturing a broad range of information and perspectives (Yin, 2011). Typically in qualitative studies there is a single unit for analysis at the broader level and a number of units for analysis at the narrower level (Yin, 2011). In this study, the single unit at the broader level was the first-year engineering course (ENGR 132), which is a representation of Purdue's FYE

Program – the entry level for undergraduate students into Purdue's College of Engineering, which is the equivalent of an organization that can be compared to other universities' engineering programs. In this study, the units at the narrower level are the participants- the students and their teams within the course. This study involved analysis of the majority of the teams' works to represent a broader perspective and a case study analysis to capture a more in-depth perspective of a few teams.

All of the 230 teams' final submissions of their QDSC design projects (i.e. Milestone 9) were analyzed to categorize the type of simulations submitted and determine the presence of their QDSC models. All of the 230 teams that had QDSC models in at least one of their simulations in their design projects were further analyzed. All of theses teams' QDSC models within both their final submissions of their QDSC MEAs (i.e. Final Response) and QDSC design projects (i.e. Milestone 9) were also analyzed to categorize and score the quality of their mathematical models. Deductive analysis was selected to efficiently analyze all of the 230 teams' projects to provide a high-level picture of the teams' models (Hatch, 2002). Some qualitative observations were also documented through both of these analyses to further categorize types of models and changes. All of these analyses were used to identify meaningful cases. The final selection of cases is based on the numeric change and qualitative notes.

In planning for a case study there were a few decisions made to strengthen the creditability of the study. One of the first decisions made about the case selection was to target teams with progress in their model. This study emphasizes the how and why of student teams' improvement in this learning environment. The purpose of selecting cases that show advancement is to harness the identified successes of their experience to enable more teams to improve in the future. It is common practice to target cases with change, either negative or positive, for the purpose of identifying hindering or helpful factors, respectively (Yin, 2011). Teams with stagnation present opportunities for investigating students' experiences, but student work alone does not present a good data set for understanding this type of experience; no stagnant teams were selected for this study. This began with categorizing teams that improved, regressed, or were stagnant from their final QDSC MEA submission to their final QDSC design project submission.

The data analyzed for the case study used both inductive and deductive analysis. Hatch (2002) recommends a combination of both deductive and inductive analyses to best understand the data. The set of data analyzed for the final teams selected for the case study consisted of all of the content described in the data collection (Section 3.3) – every submission of the teams' project work, all the feedback students received on their MEA drafts and project milestones, and their documentation of changes.

3.3.1 Analysis of Simulations in QDSC Projects

The 230 teams' Milestone 9 submissions for the QDSC design project were analyzed using a typological analysis (Denzin & Lincoln, 2011; Hatch, 2002; Johnson & Christensen, 2002), also sometimes referred to as a deductive analysis. Along with the typological analysis, some additional coding was completed to identify the number of simulations submitted by the teams and the number of teams that incorporated the QDSC mathematical model into at least one of their simulations. The basic interaction to complete simulation framework developed by Rodgers, Diefes-Dux, Kong, and Madhavan (2015) was used to divide the data into categories based on the level of completeness of students developed simulations. This coding scheme has four possible categories or typologies that were developed through grounded theory on a similar data set and inter-rater reliability was obtained after the framework was developed (Strauss & Corbin, 1990; Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). The four code categories are: simple, interactive user-interface (i.e. Level 1), black-box mathematical model (i.e. Level 2), animation of simulations (i.e. Level 3), or complete simulation (i.e. Level 4) (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015; Rodgers, Diefes-Dux, & Madhavan, 2014).

3.3.2 Analysis of Mathematical Models and Types of Changes

All of the 230 teams' design projects that included the QDSC mathematical model were further analyzed through deductive analysis resulting in a scoring method (Denzin & Lincoln, 2011; Hatch, 2002; Johnson & Christensen, 2002). The QDSC models in both the QDSC MEA and design project final submissions were analyzed based on the nine items used to evaluate student teams' mathematical models (Table 3.2).

The purpose of applying the QDSC MEA *I-MAP Mathematical Model* dimension is to identify improvements in teams' mathematical models from the MEA Final Response to the Milestone 9 submission of the project. This analysis was previously completed with an acceptable inter-rater reliability of 0.83 across the nine items (Rodgers, Diefes-Dux, & Madhavan, 2015). Table 3.6 presents the detailed coding scheme used for this analysis. The nine items analyzed were divided into five categories that describe the main types of mathematical model elements analyzed. The categories *Material Constraints* and *Given Equations Included* were only used for analyzing teams' QDSC mathematical models in their MEA Final Responses since previous research by Rodgers, Diefes-Dux, and Madhavan (2015) pointed to the lack of relevance to the simulation version of their models. The design project did not require the students to maintain the same constraints and purposes, so it was no longer relevant to assess the teams on the *Material Constraints* category. While it was good for the teams to venture away from the original material constraints to further explore their model, it would have resulted in a low score making the score difficult to interpret. Changes to the material constraints in the design project does not present valuable information that cannot be captured in the analysis of the *Optimization Strategy* category. The mode of communication was changed from a written memo in the MEA to MATLAB® GUIs with underlying code in the design project; this eliminated the need for the teams to communicate the equations used in their simulations. Therefore, the *Given Equations Included* category was not used to assess teams' underlying QDSC models in their simulations as all of the teams that had a component to calculate the effective band gap energy had to include this equation in their model for it to function; assessing the inclusion of this equation was repetitive to assessing the functionality of it in the *Given Equations Functions* category. It is not informative to see a range of scores without understanding the context.

The three remaining categories – *Given Equation Functions*, *Optimization*, and *Search Space* – were assessed in both the MEA Final Response and design project Milestone 9. The change in each of these three categories was calculated by subtracting the teams' scores on their MEA from their scores on the design project. The resulting change could range from positive ten to negative ten. Improvement was identified by a positive change in the numeric score.

The remainder of the analysis was inductive (Hatch, 2002; Yin, 2011) for the purpose of documenting the types of mathematical models and simulations teams completed. The purpose of this portion of the analysis was to investigate the mathematical models teams developed, how the models changed, and to select cases that presented a variety of mathematical models and simulations in the solutions teams developed.

Table 3.6. *I-MAP* applied to Teams' QDSC Mathematical Models

Divided into categories	**MM Elements Assessed**	**Fully Addressed (2 pt)**	**Somewhat Addressed (1 pt)**	**Missing or Inadequately Addressed (0 pt)**
Material Constraints (2 elements, up to 4 points)	1. Material quantities sum to 100 g	There is a mechanism to constrain the material total (100 g)	The sum is mentioned in the model, but there is no mechanism to constrain it.	There is no mention of the total material quantity in their model.
	2. Minimum material quantity is 2% (2 g)	There is a mechanism to constrain the material minimums (at least 2 g per material)	The minimum is mentioned in the model, but there is no mechanism to constrain it.	There is no mention of the material minimum quantities in their model.
Given Equations Included (2 elements, up to 4 points)	3. $E_{g,quantum\ dot}$ for each material is correctly computed	E_g equation provided Sample values are not necessary.	Sample E_g values No E_g equation	E_g mentioned or not No sample values No equation
	4. $(E_{g,quantum\ dot})_{eff}$ is correctly computed	$E_{g,eff}$ equation is provided. Sample values are not necessary.	Sample $E_{g,eff}$ values. No $E_{g,eff}$ equation.	$E_{g,eff}$ mentioned or not No sample values No equation
Given Equation Functions (1 element, up to 2 points)	5. There is a mechanism for achieving the desired $(E_{g,quantum\ dot})_{eff}$	There is a clear explanation of how the mechanism works.	$E_{g,eff}$ is mentioned in model. No mechanism for attainment.	There is no mention of $E_{g,eff}$ No mechanism for attainment.
Optimization Strategy (for minimizing cost only, toxicity only, and both cost & toxicity) (3 elements, up to 6 points)	6. There are mechanism for minimizing cost		Mechanism requires every possible combination be found, then select for minimum cost out of all possible combinations.	There is no mechanism for minimizing cost.
	7. There are mechanism for minimizing toxicity	Non-iterative mechanism for minimizing cost only or toxicity only. Math details are complete	OR Mechanism shows thought about reducing iteration, but math details are incomplete.	There is no solution for minimizing toxicity.
	8. There are mechanism for minimizing cost and toxicity	The mechanism for minimizing cost and toxicity allows the direct user to select the cost and/or toxicity weighting.	There is a mechanism for minimizing cost and toxicity with a preset weighting of importance.	There is no mechanism for minimizing cost and toxicity.
Search Space (1 element, up to 2 points)	9. The solution space is searched with some attention to minimizing the number of iterations.	There is clear acknowledgement that limiting the number of iterations it important. Models embed measures to limit the number of iterations.	There is either (a) an acknowledgement that there is a need to limit the number of iterations or (b) algorithm(s) do not employ iteration.	There is an excessive amount of iterations required to find a result and there is no acknowledgement that this is a problem.

3.3.3 Case Study Analysis

The final step of the analysis was the case study of the selected teams. The cases were analyzed using both typological and inductive analyses (Hatch, 2002; Yin, 2011). The analysis is similar to the one conducted by Rodgers et al. (2015) in that a case study analysis was used to understand changes to students' mathematical modeling solutions and the feedback that influenced those changes.

The analysis began with a typological analysis of all students' MEA submissions and pertinent design project submissions that incorporate the QDSC mathematical model (i.e. Milestones 4 through 9) through the lens of the *Mathematical Model* dimension of the MEA I-MAP to assign scores. The QDSC design project milestones that focused on problem scoping and brainstorming (i.e. Milestones 1-3) were not assessed using the QDSC *I-MAP* because they did not contain a model sufficient to assess. This initial analysis resulted in numeric values that showed significant changes to the mathematical model throughout the course of both projects.

Each of the nine items assessed (e.g., *I-MAP* Items 1 and 2 in *Material Constraints* category), based on the QDSC *I-MAP* (Table 3.6.), was assessed with a score or binary yes or no. A score of zero or a no (N) indicated that the team did not address the corresponding item (e.g., *I-MAP* Item 1, *I-MAP* Item 2). A yes (Y) indicated the team either somewhat addressed (i.e. a score of 1) or fully addressed (i.e. a score of 2) the corresponding item. All of the QDSC MEA submissions and QDSC design project milestones with a functioning simulation were assessed with 0, 1, or 2 scores. The QDSC design project milestones that were prototype versions of the simulation (i.e. Milestones 4-6) were assessed with yes (Y) or no (N) because it was only possible to assess if the team discussed including different items, not how they functioned. This process resulted in quantitatively captured changes. The *I-MAP* hit on key features that were required for a successful model in the MEA, but was limited in its ability to assess concepts beyond the MEA requirements. The summary helped highlight some changes, but more changes are discussed in the detailed descriptions of how the team's mathematical model and simulation/s changed.

In addition to the deductive analysis of the projects, an inductive analysis of the projects was conducted to identify other changes to the mathematical models and simulations throughout the projects that were not captured in the deductive analysis. This process resulted in qualitatively captured changes. These notes consisted of information about the direct user, types of inputs, types of output visualizations, and nature of the underlying models. Some of these changes included incorporating new variables and types of visualization in the QDSC simulation, and approaches to the QDSC mathematical model.

After all of the teams' projects were analyzed for change, each case was analyzed independently to ensure that the cases were not confused with each other. Each case was viewed independently to ensure its data told its own story and bias from other cases was minimized. This process of becoming familiar with the data was an important step of the analysis to best represent the students' learning experiences through the projects (Yin, 2011). This process involved exploring the teams' project submissions individually and collectively to determine their model development process, investigating the teams' changes independently of the feedback and with the feedback to recognize potential influential information, and approaching the data from various perspectives to grasp each case. This familiarizing process is much more critical in interpretive analysis than inductive analysis, but still an important part of the process (Hatch, 2002).

In analyzing the teams, each identified change was further investigated to understand what could have influenced the change. The documentation of changes was the main source of student data analyzed to help explain the changes that occurred. The feedback the students received within the appropriate time frame of the change was the primary data source that may have influenced the change. All of these data sources were used to triangulate the events that happened and tell a story of what may have caused the identified change. This process was completed for each instance of change. After all of the instances of change were explained for the team, a full story was written to explain the entire case across the course of the semester.

The findings presents each case by first describing how the team's QDSC model developed across the three MEA submissions based on the three groupings of *I-MAP* categories: (A) *Material Constraints* (*I-MAP* Items 1 and 2 in Table 3.6), (B) *Given Equations Included* and *Given Equation Functions* (*I-MAP* Items 3 – 5 in Table 3.6), and (C) *Optimization Strategy* and *Search Space* (*I-MAP* Items 6 – 9 in Table 3.6). After the discussion of the team's MEA, there is a discussion about their QDSC model within their simulation/s along the same five *I-MAP* categories (i.e. *Material Constraints*, *Given*

Equations Included, *Given Equation Functions*, *Optimization Strategy*, and *Search Space*). Then the nature of the team's QDSC model throughout the QDSC design project milestones is discussed, along with pertinent external factors that may have affected their model. The team's QDSC design project solution is discussed in a linear fashion through milestones from 1 to 9; though some milestones are grouped together when appropriate. Their simulation development, is concluded with a discussion about the transformation of the model based on the input and output variables. Changing the types of variables for inputs and outputs changed the nature of how the model was implemented. The design project permitted students to determine their own purposing of the model, which enabled them to change these variables. This discussion focused on Milestones 4 through 9 because the team presented their simulations in either a prototype or finalized version; these milestones more clearly presented the models they used and the input and output variables they selected for their simulation/s.

After each case was analyzed individually, a cross-study case analysis was conducted to identify themes, issues, or phenomena that tied the cases together (Stake, 2006). It was critical to tell the story of each case individually first so as to maintain its unique experience, but the identification of similarities helps lead to identification of commonalities and can lead to more generalizable conclusions. These similarities are explored where relevant in the discussion (CHAPTER 5).

CHAPTER 4. FINDINGS

The findings presented in this chapter are the results from each of three steps of this study: (1) applying the two frameworks to analyze the teams' MEAs and design projects, (2) selecting the teams for the case study, and (3) the case study.

First, the level of completeness of the 230 teams' simulations is shown. During this analysis, 108 teams were identified as being incomplete sources of data for this study; these teams did not include their MEA QDSC model in their design projects. Next, the quality of the remaining 122 teams' mathematical models as the appeared in this final MEA and design project submissions are shown. Second, the selection of teams for the case study is described. Finally, the works of the three teams selected for the case study, the development of their mathematical models and potential influential factors in that development, are presented.

4.1 Analysis of Simulations in the QDSC Design Projects (M9)

One of the requirements of the project stated that each team member must create their own simulation. Ideally, each team was to have three or four simulations depending on the number of students on their team. Table 4.1 shows the number of teams in each section, the number of students on these teams, the number of simulations these teams developed, and the average number of simulations per a student. No team had more simulations than the number of students on the team, but some teams did not meet the requirement of having one simulation per team member.

Table 4.1. Number of Simulations

Instructor	**Section**	**No. of Teams**	**No. of Students**	**No. of Simulations**	**Avg. No. of Simulations per Student**
A	1	13	50	48	0.96
B	2	28	106	100	0.94
C	3	23	84	84	1.00
D	4	20	77	74	0.96
E	5	27	103	99	0.96
F	6	13	53	43	0.81
F	7	24	95	68	0.72
F	8	22	57	52	0.91
G	9	15	99	91	0.92
G	10	25	88	88	1.00
H	11	20	79	75	0.95
Overall		**230**	**891**	**822**	**0.95**

The sections taught by Instructor F had the lowest number of simulations per student. The sections taught by Instructor F typically had the same three simulations: (1) a simulation based on the QDSC mathematical model, (2) a simulation based on a model that determined the feasibility of a solar panel in different geographical locations, and (3) a simulation based on a model that calculated efficiency of the solar panel. Some teams still fulfilled the original requirement of one simulation per student by including two simulations based on the QDSC mathematical model.

The design project challenged teams to select their own direct user and design a simulation suite tailored to their direct user, while also incorporating their QDSC model into at least one of their simulations. With this freedom, there was variability across teams' direct users, models, and simulations in most sections. Instructor F's sections were the only ones where all the teams used the same models and context for their simulations.

Another one of the requirements of the project stated that each team must have at least one simulation based on the QDSC model from their MEA. Of the 230 teams' projects that were analyzed in this study, 122 teams (53.9%) incorporated the QDSC model in their design project; the other teams dropped this model. Table 4.2 shows the number of teams that incorporated some aspect of their QDSC mathematical model from the MEA in their simulation suite. Sections A, C, G, and H had less than the average percent of teams with QDSC mathematical models in their design project solutions.

Table 4.2. Number of Teams with QDSC Mathematical Models in Design Projects

Instructor	Section	No. of Teams in the Study	No. of Teams with QDSC Model	Percent of Teams with QDSC Model
A	1	13	4	30.7%
B	2	28	23	82.1%
C	3	23	11	47.8%
D	4	20	11	55.0%
E	5	27	15	55.5%
F	6	13	13	100.0%
F	7	24	19	79.2%
F	8	15	15	100.0%
G	9	25	7	28.0%
G	10	22	4	18.2%
H	11	20	0	0.0%
Overall		**230**	**122**	**54.7%**

The percentage of teams that continued to develop their QDSC mathematical model in their design projects varied across instructors' sections – from 0% in Instructor H's section to an average of 90% across Instructor F's three sections (Table 4.2). Instructors B and F had the highest percentage of student teams that maintained the QDSC context in their design projects; these were also the only two instructors that had previous experience with implementing nanotechnology-based design projects in the FYE course.

The 230 teams' 822 simulations were analyzed for completeness using the basic-to-complete simulation framework (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). Simulations were categorized as complete (L4. Simulation), simple black-box models that include a mathematical model but no visualization component (L2. Black-box Model), or GUIs that lack any mathematical model (L1. Interactive only). There were no examples of L3. Animated Simulations in these teams' projects.

Table 4.3 shows the results of this analysis by instructor (In) and section (Se). The simulations are broken into three groups. The first group are those simulations appearing in projects without a single QDSC model (Simulations in the non-QDSC Projects). These are the 383 simulations developed by the 108 teams that did not include the QDSC model in their simulations (see Table 4.2). The second and third group together comprise the 439 simulations that were developed by the 122 teams that incorporated the QDSC model into their design projects (see Table 4.2). The second group are those simulations not including the QDSC-based simulations (Simulations not based on QDSC Projects). The third group are the QDSC model simulations (Simulations based on the QDSC Model).

Table 4.3. Levels of Teams' Simulations

In.	Se.	Simulations in non-QDSC Projects				Simulations in QDSC Projects: Simulations not based on QDSC Model				Simulations in QDSC Projects: Simulations based on QDSC Model			
		No. of Sims.	L1	L2	L4	No. of Sims.	L1	L2	L4	No. of Sims.	L1	L2	L4
A	1	35	8.6%	37.1%	54.3%	5	0.0%	20.0%	80.0%	8	0.0%	12.5%	87.5%
B	2	13	0.0%	38.5%	61.5%	55	7.3%	21.8%	70.9%	32	0.0%	37.5%	62.5%
C	3	41	0.0%	4.9%	95.1%	28	0.0%	17.9%	82.1%	15	0.0%	13.3%	86.7%
D	4	35	0.0%	48.6%	51.4%	25	0.0%	40.0%	60.0%	14	0.0%	42.9%	57.1%
E	5	42	0.0%	23.8%	76.2%	23	4.3%	13.0%	82.6%	34	0.0%	26.5%	73.5%
F	6	0	-	-	-	23	8.7%	82.6%	8.7%	20	0.0%	30.0%	70.0%
F	7	6	0.0%	50.0%	50.0%	35	5.7%	85.7%	8.6%	27	0.0%	11.1%	88.9%
F	8	0	-	-	-	28	0.0%	100.0%	0.0%	24	0.0%	16.7%	83.3%
G	9	64	1.6%	23.4%	75.0%	18	5.6%	33.3%	61.1%	9	0.0%	22.2%	77.8%
G	10	72	0.0%	43.1%	56.9%	12	0.0%	50.0%	50.0%	4	0.0%	25.0%	75.0%
H	11	75	0.0%	24.0%	76.0%	0	-	-	-	0	-	-	-
All Sections		**383**	**1.0%**	**29.8%**	**69.2%**	**252**	**4.0%**	**47.6%**	**48.4%**	**187**	**0.0%**	**24.6%**	**75.4%**

Out of all 230 teams' 822 simulations, the majority (64.2%) were complete simulations with variable inputs, visualized outputs, and based on an underlying model (L4). Fourteen students developed GUIs not backed by a mathematical model (L1). Students from the Simulations in QDSC Projects group developed ten of these GUIs.

Across the 9 sections that had at least one team from the Simulations in non-QDSC Projects group, the majority (69.2%) of the 383 simulations developed by the 108 teams were complete simulations (Table 4.3). Across the 10 sections that had at least one team from the Simulations in QDSC Projects, the majority (59.9%) of the 439 simulations developed by the 122 teams were complete simulations (L4) (Table 4.3).

All of the 187 simulations from the Simulations based on QDSC Model group contained an underlying model (i.e. the QDSC model) and therefore none of these were L1. Basic Interaction. The 187 simulations were predominantly complete simulations (L4) (75.4%, Table 4.3), which was not true for the other two groups. For example, all of Instructor F's sections only had a majority of complete simulations (L4) within the Simulations based on the QDSC Model group (Table 4.3). Within the Simulations in QDSC Projects group, the teams from Instructor F's sections most commonly developed black-box models (L2) for the simulations not based on the QDSC model and typically developed complete simulations (L4) for the simulations based on the QDSC model (Table 4.3).

The 187 simulations completed by the 122 teams that were based on their QDSC mathematical models were further analyzed and compared to the models submitted in their MEAs. The results of this analysis are discussed in the next section.

4.2 Analysis of QSDSC Mathematical Models (based on *I-MAP*)

The 122 teams' QDSC mathematical models submitted in their final submission for the MEA (i.e. Final Response) and design project (i.e. M9) were analyzed using the *I-MAP* categories (Table 3.6). These results and the teams' changes are presented in Table 4.4.

All 122 teams ensured their model resulted in a material composition comprised of 100 grams with at least 2 grams of each material (see *Material Constraints* scores in Table 4.4). That said, there was one additional material constraint provided in the MEA that was not assessed in the QDSC I-MAP Rubric – teams were required to include five QDSC materials in each mixture. Through evaluation of all 122 teams' MEAs, it was discovered that a couple of teams did not meet this requirement. It was also observed that a few teams included all of the sample materials in each mixture (i.e. 5 in Draft 1, 10 in Draft 2, and 12 in Final Response). The required number of materials in the mixture is another aspect of their mathematical models that could have been assessed for in the *Material Constraints* category.

Table 4.4. *I-MAP* applied to Teams' QDSC Mathematical Models

In.	Sec.	# of Teams	MEA (Final Response)					Design Project (M9)			Change (M9 – Final Response)			
			Mat. Con.	Given Eqs.	Eq. Func.	Optim-ization	Search Space	Eq. Func.	Optim-ization	Search Space	Eq. Func.	Optim-ization	Search Space	SUM
A	1	4	4.00	4.00	1.75	4.00	1.00	1.00	1.25	0.00	-0.75	-2.75	-1.00	-4.50
B	2	23	4.00	3.09	1.57	4.00	0.57	1.65	2.74	0.39	0.09	-1.26	-0.17	-1.35
C	3	11	4.00	3.55	1.73	3.91	0.64	1.36	1.82	0.09	-0.36	-2.09	-0.55	-3.00
D	4	11	4.00	3.91	1.73	3.91	0.73	1.27	1.55	0.27	-0.45	-2.36	-0.45	-3.27
E	5	15	4.00	3.13	1.60	3.80	0.60	1.27	1.60	0.27	-0.33	-2.20	-0.33	-2.87
F	6	13	4.00	3.46	1.54	4.08	0.77	1.62	3.23	0.31	0.08	-0.85	-0.46	-1.23
F	7	19	4.00	3.47	1.74	3.74	0.63	1.53	3.58	0.42	-0.21	-0.16	-0.21	-0.58
F	8	15	4.00	3.27	1.60	3.33	0.47	2.00	3.27	0.07	0.40	-0.07	-0.40	-0.07
G	9	7	4.00	3.86	2.00	4.29	0.86	1.57	2.14	0.29	-0.43	-2.14	-0.57	-3.14
G	10	4	4.00	3.75	2.00	4.00	0.75	2.00	1.00	0.00	0.00	-3.00	-0.75	-3.75
Teams' Average			**4.00**	**3.43**	**4.00**	**3.86**	**0.65**	**1.55**	**2.52**	**0.26**	**-0.12**	**-1.34**	**-0.39**	**-1.85**
Teams' St. Dev.			**0.00**	**0.77**	**0.00**	**1.02**	**0.62**	**0.77**	**1.68**	**0.44**	**0.89**	**1.79**	**0.60**	**2.64**

The majority of teams (70 out of 122) included both the equation to calculate the band gap energy of QDSC materials and the equation to calculate the target or effective band gap energy in their model (see *Given Equations Included* score in Table 4.4). Throughout the teams' memos, all but four teams provided evidence that they incorporated the theoretical equations for the individual materials' band gap energies and the target band gap energy in their models by either stating the equation or providing band gap energy values obtained from the equation or target band gap energy values used for the equation. When the teams included sample data or an equation, it did not mean they explained how they acquired the sample data or how to implement the equation in their memo. The first step to building the QDSC model required teams to use the band gap energy equation to determine the band gap energy for each of the given materials. Some teams skipped this step and began their model with the calculated band gap energies, which assumes the user already has these values. Since calculating the target band gap energy was a major function of the model, all but one team included the target band gap energy equation and/or sample target band gap energy values required to apply the equation.

The 122 teams made decisions about changing and repurposing their QDSC model in their simulations for the design project. This meant many teams did not carry all components of the model that were assessed from their MEAs to their design projects; this contributed to the low scores in changes shown in Table 4.4. Table 4.5 shows the number of teams that maintained various assessed aspects of their QDSC models in their simulations and the change in scores based on teams that upheld the respective elements.

Table 4.5. *I-MAP* applied to Teams' QDSC Mathematical Models (limited projects)

Ins.	Sec.	Equation function No.	Equation function Δ	Optimization Cost only No.	Optimization Cost only Δ	Toxicity only No.	Toxicity only Δ	Both No.	Both Δ	Search space No.	Search space Δ
A	1	2	0.00	2	0.00	1	0.00	1	1.00	3	-1.00
B	2	20	0.30	18	-0.06	16	-0.06	15	0.07	19	-0.11
C	3	8	0.25	6	0.00	6	0.00	6	-0.17	8	-0.25
D	4	7	0.00	6	0.00	3	0.00	2	0.00	7	-0.43
E	5	10	0.30	7	0.14	6	0.17	4	0.25	8	-0.13
F	6	12	0.25	11	-0.18	11	-0.09	13	0.00	13	-0.46
F	7	17	0.00	19	-0.11	19	-0.11	19	0.05	19	-0.21
F	8	15	0.40	15	-0.07	15	-0.07	15	0.07	15	-0.40
G	9	6	-0.17	5	0.00	4	0.00	2	-0.50	6	-0.50
G	10	4	0.00	1	-1.00	1	-1.00	1	1.00	1	-1.00
Overall		**101**	**0.19**	**90**	**-0.07**	**82**	**-0.06**	**78**	**0.05**	**99**	**-0.31**
St. Dev.		–	**0.58**	–	**0.33**	–	**0.33**	–	**0.32**	–	**0.55**

Note: **No.** = number of teams with corresponding *I-MAP* item in their simulations
Δ = Average Change (Design Project M9 – MEA Final Response)

Most of the teams (83 out of 122) included a procedure to obtain the target band gap energy that they clearly explained (see *Given Equation Functions* score in Table 4.4). Some teams (38) only somewhat addressed the criteria by including a procedure to obtain the target band gap energy, but not clearly explaining how to use it. Only one team did not address the criteria for this category at all. This team set the material composition to 92% for the material with the lowest cost, toxicity, or both (depending on the mechanism) and 2% for each of the remaining 4 materials; this team clearly missed the need to obtain the target band gap energy for their mixture.

The average change in teams' scores on the *Given Equation Functions* category from their MEA Final Response submissions to design project Milestone 9 submissions is negative (-0.20, see Table 4.4), but 21 teams also did not include the effective band gap energy in their QDSC models for their simulations (see Table 4.5). Teams were encouraged to repurpose their QDSC models in their simulations, so removing this equation was acceptable. The majority of teams (88 out of 101) that did include the band gap energy function in their design projects ensured that it was fully functioning, meeting the criteria for the *Given Equation Functions* category. Out of the 101 teams that did include the effective band gap energy equation in their model, there was an average positive change of 0.19 points (Table 4.5), with eight teams' scores decreasing and 26 teams' scores increasing. It is possible that the eight teams that struggled to implement their equation with full success in their design project had difficulty programming in MATLAB®. Some of the 26 teams with improved scores likely improved their score because they did not have to communicate how to implement the equation through written text and others may have improved their understanding of the equation through the simulation development process.

It was most common for teams (70 out of 122 teams) to use iteration in their models to find the mixtures with the lowest cost or toxicity in their MEA Final Response (see *Optimization Strategy* score in Table 4.4). Many teams (51 teams) fully addressed the criteria for the minimize cost only and toxicity only mechanisms with a QDSC model that used systems of equations. Only one team did not at all address the criteria for the minimize cost only and toxicity only mechanisms by failing to submit a QDSC model to address these mechanisms. Only five teams fully addressed the criteria for minimizing both cost and toxicity by incorporating a weighting dependent on the direct user's needs; the other 117 teams somewhat addressed the criteria for this mechanism.

Since there were no requirements to maintain all three optimization mechanisms, the teams' average change in score was the most negative for this category. Based on the analysis of all 122 teams' QDSC models for the three different optimization strategies, the team average score from the MEA Final Response submission to the design project Milestone 9 submission decreased by 1.69 points (see Table 4.4). With the freedom to define their own direct user and purpose for their simulations, many teams did not include all three of the optimization criteria that were required in their MEA. The teams incorporated all three, two, only one, or none of the model/s with the goal/s of only minimizing cost, only minimizing toxicity, and/or only minimizing both cost and toxicity. Of the 122 teams, 90 teams included a model to minimize cost only in their QDSC model (see Table 4.5). Of the 90 teams, 25 teams fully addressed the criteria for this optimization strategy by utilizing a non-iterative solution. Of the 122 teams, 82 teams included a model to minimize toxicity only in their QDSC model (see Table 4.5). Of the 82 teams, 25 teams fully addressed the criteria for this optimization strategy by utilizing a non-iterative solution. There were a total of 26 teams that used non-iterative solutions for their models to minimize cost only and/or minimize toxicity only. (One of these 26 teams only implemented a model to minimize cost only and another team only implemented a model minimize toxicity only.) Of the 122 teams, 78 teams included a model to minimize both cost and toxicity in their QDSC model (see Table 4.5). Seven of these teams fully addressed the criteria for this optimization strategy by enabling the user to select the importance of cost versus toxicity.

Based on the analysis of only these teams that incorporated each type of model, the average changes were much closer to 0 (-0.07, -0.06, and 0.05 in Table 4.5). Through the simulation development process, two teams that had iterative solutions changed their QDSC model to be a non-iterative solution and eight teams that had non-iterative solutions changed their models to iterative solutions. In the teams' MEA Final Response submissions, five teams proposed an importance weighting method that was dependent on the direct user for their model to minimize both cost and toxicity; only one of these teams successfully implemented this model in their simulation. Six additional teams that did not propose this solution in their MEA implemented this method in their design project QDSC model.

The majority of the teams somewhat addressed the criteria for the *Search Space* category in their Final Response MEA Submissions. In the MEA Final Response, nine teams fully addressed the criteria for the *Search Space* category by reducing the search space and discussing the need to reduce the search space. A total of 19 teams discussed the need to reduce the search space in their memos, but some of these teams did not attempt to reduce the search space in their solution.

No teams fully addressed the *Search Space* criteria in their design project submissions. Based on the QDSC *I-MAP* assessment, the majority of the teams did not address the criteria for the *Search Space* category in their Milestone 9 design project submissions. The average scores decreased from the MEA to the design project on this category (-0.49, see Table 4.4). This score still decreased when comparing only the 99 teams that had some type of optimization strategy, where the *Search Space* criteria was relevant (-0.31, see Table 4.5).

4.3 Selecting Teams

Based on the above findings of the applied QDSC I-MAP and simulation framework and the qualitative notes, three teams were selected for the case study. The reason for selecting each team is discussed in this section.

Team A was selected because this team improved their optimization strategy element of their models to minimize cost only or toxicity only. For their QDSC MEA, they submitted an iterative solution that tried every possible combination of materials. For their QDSC design project, they wrote a non-iterative solution using systems of equations to significantly reduced the search space (i.e. I-MAP Item 9) and improve their optimization strategy (i.e. I-MAP Items 6 and 7).

Team B was selected because this team enabled users to select the weighting for cost and toxicity in their optimization model in the QDSC design project. This was an improvement over their QDSC MEA solution.

Team C was selected based on the high score (i.e. 16 out of 18) they received on their QDSC MEA and the two different approaches they took to incorporating their QDSC model in the design project. In their first QDSC-based simulation, the team extended their model with an additional mathematical model that was not part of the MEA. Their second QDSC-based simulation allowed users to investigate how changing the band gap energy of their solar panel affects the total cost and/or toxicity

4.4 Case Studies

The case study analysis (Yin, 2011) of these three teams is described in this section. For each team, the scores the team received on their QDSC mathematical model for each pertinent submission of the MEA and the QDSC design project are summarized and discussed. This is followed by a rich description of the team's mathematical model and how it changed across the MEA and then the design project. Throughout this narrative, any peer, instructional team member, or nanoHUB representative feedback that may have prompted the changes to the team's models or simulations are presented.

4.4.1 Team A

Team A's ability to meet the mathematical model requirements, as assessed by the QDSC *I-MAP*, for each pertinent submission is summarized in Table 4.6. Team A received the same final score on Draft 1 and Draft 2, thought there were two changes based on the *I-MAP* rubric items. Their score slightly increased from Draft 2 to Final Response due to the addition and modified implementation of the effective band gap energy equation. They significantly improved their QDSC model from their MEA to their design project by improving the optimization strategy for minimizing cost or toxicity only (see Final Response to Milestone 7 in Table 4.6). Based on the *I-MAP* rubric items, it would appear that the team's mathematical model did not change throughout their design project.

However, through a more detailed description of their simulation development changes will reveal change that this team made to their model.

Table 4.6. MEA and Design Project Submissions for Team A

MEA or Design Project Sub-mission	**Mathematical Model Analyzed: QDSC *I-MAP* (from** Table 3.6**)**									
	Material Constraints		**Given Equations Included**		**Given Equation Functions**	**Optimization Strategy**			**Search Space**	**Final Score (out of 18)**
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	
Draft 1	2	2	0	2	1	1	1	n/a	0	10
Draft 2	2	2	0	1	1	1	1	1	0	10
Final Response	2	2	2	1	2	1	1	1	0	13
Milestone 4	Y	Y	Y	Y	Y	N	N	Y	n/a	n/a
Milestone 5	Y	Y	Y	Y	Y	N	N	Y	n/a	n/a
Milestone 6	N	N	N	N	N	Y	Y	N	n/a	n/a
Milestone 7	2	2	2	2	2	2	2	0	1	15
Milestone 8	2	2	2	2	2	2	2	0	1	15
Milestone 9	2	2	2	2	2	2	2	0	1	15

4.4.1.1 Team A's QDSC MEA

Throughout MEA Draft 1, Draft 2, and Final Response, Team A's QDSC mathematical model fully addressed the material constraints of there being a minimum of two grams of each material (*I-MAP* Item 2 in Table 4.6) and a total of 100 grams in the mixture (*I-MAP* Item 1 in Table 4.6). The procedure sets three materials to 2 grams to ensure this material constraint is met. The remaining two materials equal 94 grams to ensure the mixture has 100 grams. The team maintains this same material composition throughout their MEA. The only other material related changes were related to the requirements of the MEA sequence; the team had five materials to use in their Draft 1, 10 possible materials for the mixtures in their Draft 2, and 12 possible materials for the mixtures in their Final Response (incorporating the two materials from their Data Generation Table 3.1).

Team A included one of the required equations (*I-MAP* Item 4) in their MEA Draft 1 and included the other required equation (*I-MAP* Item 3) in MEA Final Response, but they did not include both equations in any of their MEA submissions. In MEA Draft 1, the team did not include the use of the equation for computing the band gap energies of individual quantum dot materials (*I-MAP* Item 3 in Table 4.6) and briefly mentions that each material has a band gap energy in their discussion about an "index" to help them determine which materials to use in their QDSC model. The team did include the equation needed to determine the effective band gap energy (*I-MAP* Item 4 in Table 4.6), but did not describe how to apply this equation in their model with enough detail for the direct user to use it (*I-MAP* Item 5 in Table 4.6). The team did not receive any peer feedback addressing this. In MEA Draft 2, the team removed the effective band gap energy equation and only provided sample target band gap energy values; resulting in a lower score (*I-MAP* Item 4 in Table 4.6). The revised model described their method of approaching the target band gap energy, but not how to calculate it; they merely pointed to their MATLAB® file to do it (*I-MAP* Item 5 in Table 4.6). The team did not receive any TA feedback directly pointing to this error, but the TA did mention that their procedure did not describe any calculations. In MEA Final Response, the team included the equation to calculate the band gap energy for each material (*I-MAP* Item 5 in Table 4.6) and better described their procedure to obtain the target band gap energy (*I-MAP* Item 3 in Table 4.6). The procedure was to look at every resulting material composition and determine which one had the resulting target band gap energy. The team received one piece of feedback from the TA to prompt them to think about their method for selecting the material composition with the target band gap energy. The TA wrote, “Method for enforcing band gap energy constraint is never described. This clearly needs some sort of tolerance built in, but this is never mentioned.”

Throughout MEA Draft 1, Draft 2, and Final Response, Team A used an iterative approach for their optimization strategy in their QDSC Model (*I-MAP* Items 6-9). In Draft 1 MEA, the team somewhat addressed the two required mechanisms for their QDSC model – one for minimizing cost and the other toxicity (*I-MAP* Items 6 and 7 in Table 4.6). The team provided an equation in their memo, which is the resulting equation based on systems of equations (Eq. 1); they failed to use this strategy in their models. In their equation they mislabeled some variables (e.g. material 1 and material 2 should be clarified as the band gap energies for these material), but their application of it appears they understand the correct variables. They did not explain how to use this equation in their written memo, but their supplemental excel files clearly shows they used an iterative solution, inputting all possible percentage values (p in Eq. 1) from 2 to 92 (increasing by 1), to find the material composition with the effective band gap energy closest to the target band gap energy. The team did not discuss limiting their search space and did not have a non-iterative solution (*I-MAP* Item 9 in Table 4.6).

$$E_{g,eff} = 2\%(sum\ of\ E_g of\ 3\ mats.) + p(mat.1) + (94\% - p)(mat.2) \qquad (Eq.1)$$

The team received feedback from their peers that addressed the lack of detail in their memo. One peer stated, "The description on the calculations is lacking. It is hard to tell which numbers to calculate in which step of the procedure. The only way I could replicate the results was using my knowledge of [already] doing the problem." They also received some feedback about their current way of approaching the problem. Two peers made comments about MATLAB® in regards to their approach, even though the team only submitted supplemental excel files. One peer wrote, "But I think an [illustration] of what method you choose (i.e [MATLAB®], [Microsoft® Excel]) to get the answer is necessary. Also the difference [between] each possible answer is 1, which I think might be not so accurate. A smaller difference of percentage [between] each [possible] combination like 0.1 will be [better]… Only provide a list of calculation data, no [MATLAB®] file for the formula which would be one of the best way to [achieve] share-ability." This peer guided the team to consider both using MATLAB® and discussing the program they select in greater detail in their memo. This peer also prompted the team to consider changing the grams of the two changing materials in smaller increments.

In MEA Draft 2, Team A removed their equation (Eq. 1) and changed their memo to only describe their supplemental MATLAB® file. The team also incorporated a procedure for minimizing both cost and toxicity, as required. The team somewhat addressed the criteria for their models to minimize cost only, minimize toxicity only, and minimize both (*I-MAP* Items 6-8 in Table 4.6). The team used the same iterative procedure from Draft 2, but incorporated it into MATLAB®. The team explained the program would select the two best materials based on the selected mechanism and then iterate through every possible combination to find the target band gap energy. This same method was used for all three mechanisms. The team still did not discuss limiting their search space and did not have a non-iterative solution (*I-MAP* Item 9 in Table 4.6). The TA gave the team three different direct feedback statements telling them to explain their model not a supplemental file. In one example of this, the TA stated, “Practically nothing was described in the memo. Remember, we are NOT grading your [MATLAB®] script!” The TA did not give the team any constructive feedback on their optimization strategies or the need to limit the search space.

In MEA Final Response, Team A better described their QDSC model without pointing to their MATLAB® file. The team still only somewhat addressed the criteria for their models to minimize cost only, minimize toxicity only, and minimize both (*I-MAP* Items 6-8 in Table 4.6). They used a similar iterative solution, but with an even less limited search space (*I-MAP* Item 9 in Table 4.6). The model no longer selected two materials to change for each selected mechanism, the model iterative changed two materials at a time by 1 percent to find every possible material combination. The program would then identify all of the combinations with the target band gap energy and then the material composition with the lowest cost, lowest toxicity, or lowest both cost and toxicity (based on the desired mechanism). Based on their Final Response, the TA gave the team some feedback about the optimization strategy used in their QDSC model, while focusing on the need to limit their search space. The TA explained that their “brute force method” (i.e. loop structure that tests every possible combination, while changing two of the five materials) did not adhere to minimizing the search space to more effectively address the problem. The TA wrote, "Algorithm barely even tries to reduce the number of iterations. It took over 20 minutes for my computer to run all these test cases."

4.4.1.2 Team A's QDSC Design Project

In the QDSC Design Project, Team A approached implementing their QDSC model into one simulation (i.e. QDSC Model). This simulation had different ways of changing their features within the *Material Constraints*, *Given Equations Included*, *Given Equation Functions*, *Optimization Strategy*, and *Search Space* categories.

The QDSC Model simulation maintained the same material constraints in their model (i.e. *I-MAP* Items 1 and 2). The final simulation they designed removed opportunities for user input related to the materials (see inputs in Table 4.7). The underlying model for their simulation contained both the given equations (i.e. *I-MAP* Items 3 and 4). Their simulation allowed the user to input any target band gap energy within the range of possible effective band gap energies and functioned properly (i.e. *I-MAP* Item 5). The team did not present any further exploration of this equation. The team improved their QDSC model through simulation development by developing a non-iterative solution for their minimizing cost only and toxicity only mechanisms (i.e. *I-MAP* Items 6-7 and 9). The team did not do much exploration beyond the MEA challenge, but the team demonstrated a better understanding of their model through their design project.

In Milestone 1, the team established their understanding of the problem and potential stakeholders without an explanation of how the stakeholders related to the problem. The team selected their direct user to be SolarCity, "an American provider of energy services." The team explained, "We want to work with SolarCity because it is the number one residential solar installer in the U.S." The team received feedback that they did not identify how each stakeholder is related to the problem The team wrote that they would address this feedback by identifying how each stakeholder is related to the problem and how they would benefit from their solution, but they did not present any of this information in their Milestone 2 to show this updated.

As part of the team's submission for Milestone 1, the team members had an individual assignment in which they had to evaluate prototypical student-completed GUIs. All four students on this team completed this assignment. They all correctly identified the GUIs that were a demonstration of a black-box model (i.e. was a model, but not a simulation) and a demonstration of a simulation (i.e. was a model and a simulation). Two of the students correctly identified the animated simulation, as both a model and a simulation. The other of two students thought the animated simulation was only a simulation (without a model present). None of the students correctly identified the GUI that was only interactive (i.e. no models or simulations). Two of the students thought it had both a model and a simulation; the other two students thought it was a simulation, but it did not contain a model. Overall the students presented some understandings of the presence of models and simulations. The students received auto-generated feedback on this assignment based on their individual responses, but the team did not refer to this feedback in their Milestone 2 documentation.

In Milestone 2, this team proposed 19 out of the 20 required ideas. Three of the ideas were based on the QDSC model. The three ideas were: 1 – QDSC Model) “Input of the model: Number of materials and its properties, cost of different materials, toxicity of different materials. Output of the model: Three optimized combinations of different materials. The first one is only for cost, the second one is only for toxicity and the third one is for both cost and toxicity.” 2 – Cost vs. Toxicity) “Graphs of cost vs. toxicity for each QD material.” and 3 – QDSC Properties) “Graph that changes as properties of QD materials are changed.”

In Milestone 3, the team acknowledged the feedback on their previous submission about their vagueness and stated they would more clearly explain their ideas. The team only considered one of their QDSC ideas in their concept reduction (i.e. QDSC Model). The team selected this idea because they determined it would be “very modifiable”, have “shareability”, and “gives the user three different options”. The cons that they foresaw for their simulation were it “could be very cluttered”, “could have a large range of materials”, and “hard to achieve both optimized results”. The team received feedback that pointed out their submission was lacking evidence-based decisions throughout.

In Milestone 4, the team presented their proposed QDSC Model simulation. The proposed simulation allowed the user to input material information for five QDSC materials then outputs the cost, toxicity, and material composition based on their minimized cost and toxicity model. The presentation only presented the output for one aim (minimize both cost and toxicity) in this model instead of allowing the user to select their desired aim, as proposed in Milestones 2 and 3. There is no discussion about the target band gap energy, so it is assumed at this point that it would be a defaulted input in the underlying model. The main constructive feedback the team received on this milestone was to more clearly communicate their mathematical models.

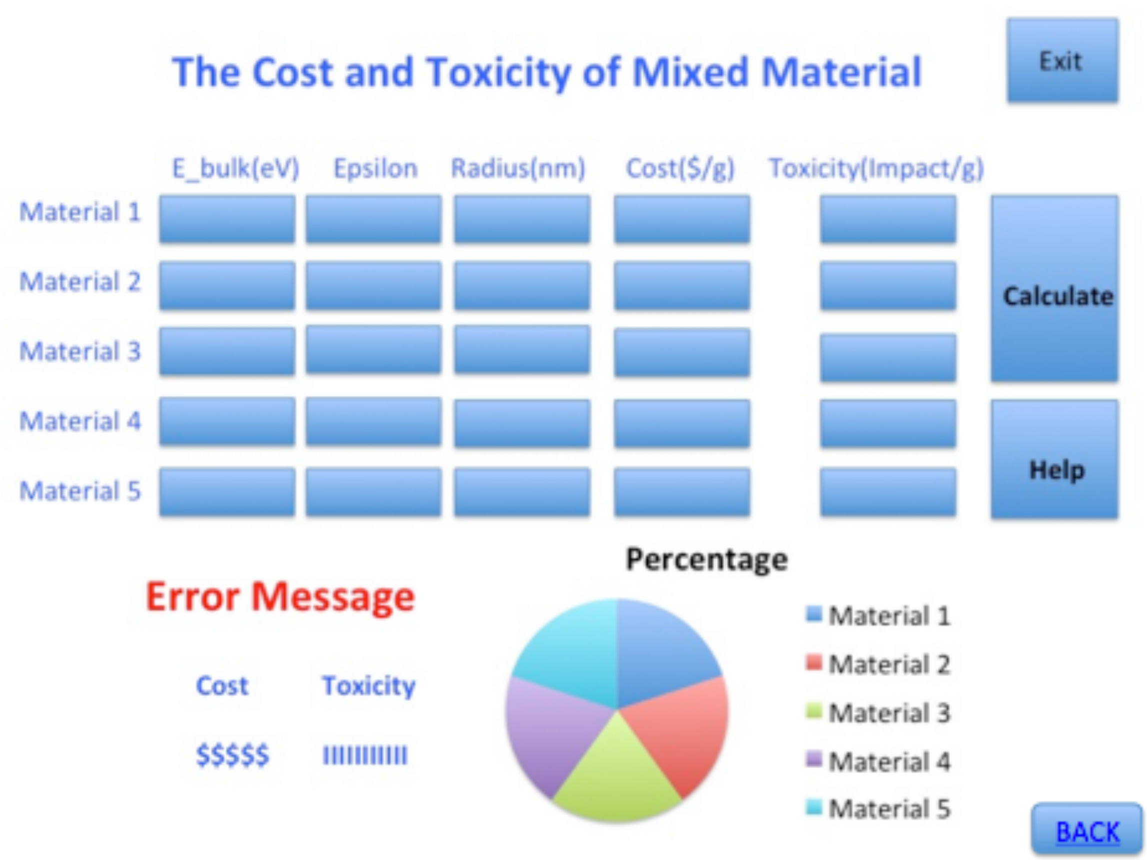

Figure 4.1. Team A's QDSC M4 Simulation Prototype – QDSC Model

In Milestone 5, the team changed their proposed QDSC Model simulation (Figure 4.2) to no longer have material property inputs. The QDSC materials were boxes to select five of the ten preset materials. The team still had no mention of the effective band gap energy in the presented information. The team did not receive any constructive feedback related to this simulation on this milestone.

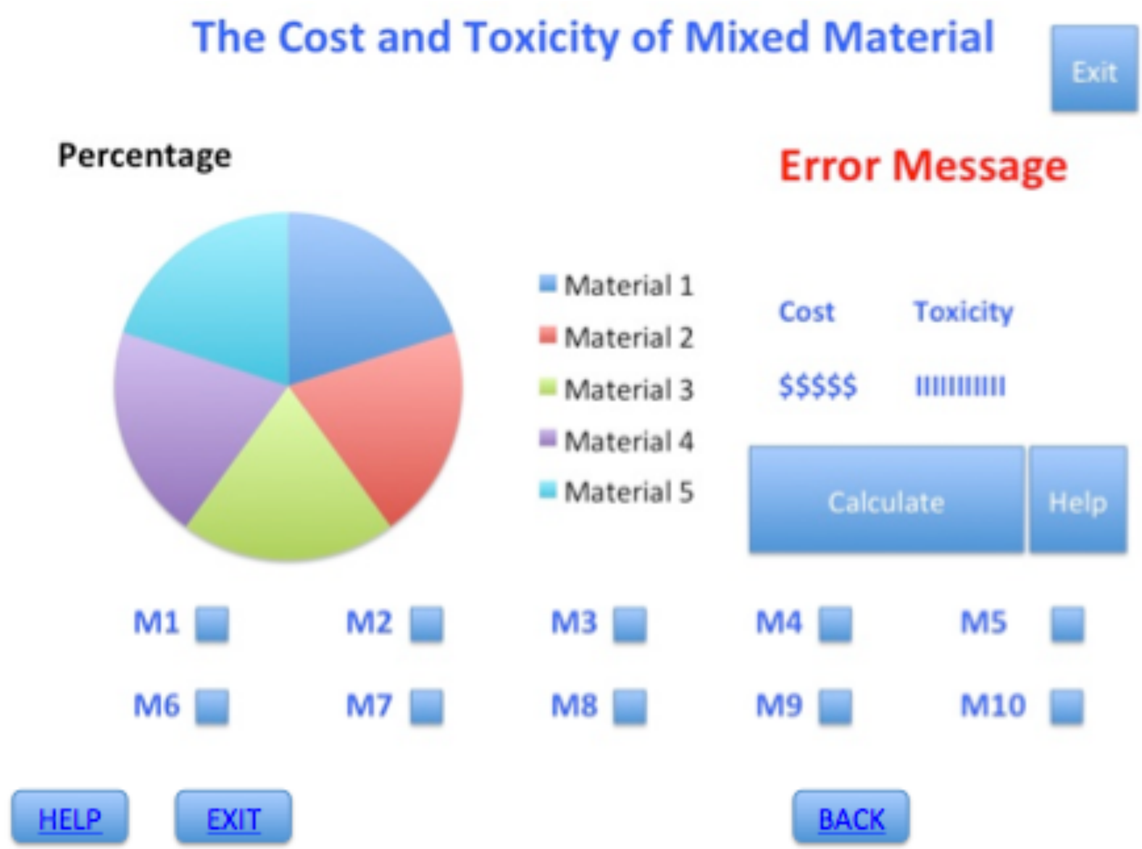

Figure 4.2. Team A's QDSC M5 Simulation Prototype – QDSC Model

In Milestone 6, the proposed QDSC Model simulation (Figure 4.3) changed to present only the minimize cost only or toxicity only mechanisms and no longer included the aim for minimizing both. The GUI did not yet include the materials or input for target band gap energy; it was difficult to determine if these inputs were included. The team received feedback that they needed to specify the acceptable ranges of inputs on their GUIs.

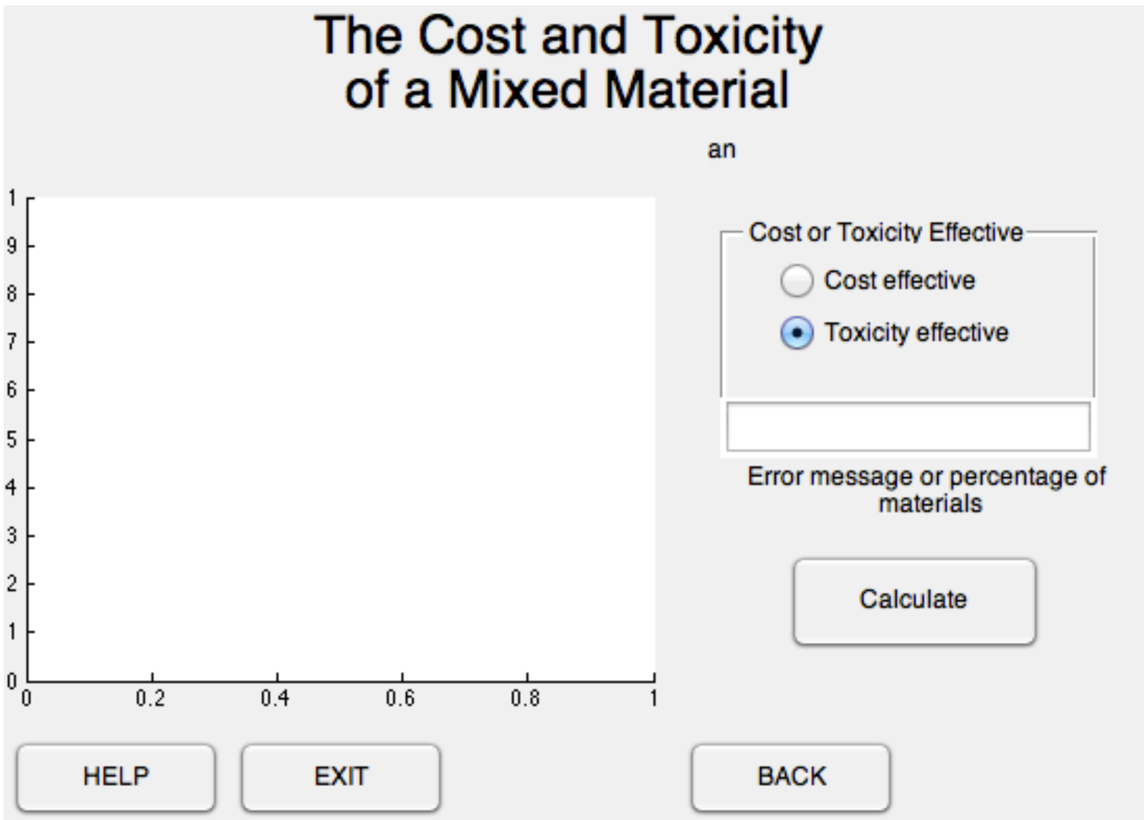

Figure 4.3. Team A's QDSC M6 Simulation Prototype – QDSC Model

In Milestone 7, the QDSC Model simulation (Figure 4.4) functioned, as required. The QDSC materials were defaulted to the same five materials for all of the compositions. The model for minimizing cost only or toxicity only used if statements and system of equations to determine the material composition for the target band gap energy for each aim; the model no longer used an iterative process (*I-MAP* Items 6 and 7 in Table 4.6). The MATLAB® code also included the given material constraints and equations to calculate the band gap energy of each material and effective band gap energy (*I-MAP* Items 1-5 in Table 4.6). The resulting material composition is presented in a pie chart along with either the found toxicity or cost (depending on the model selected). The team received constructive feedback to include units throughout their GUIs.

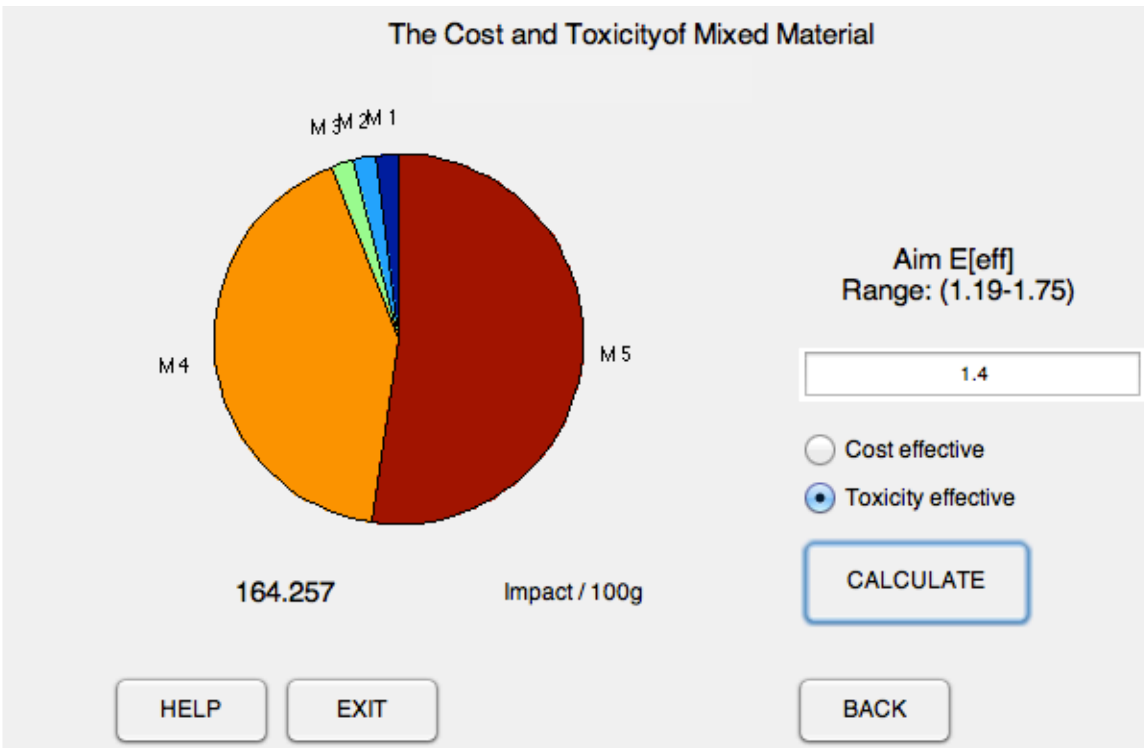

Figure 4.4. Team A's QDSC M7 Simulation – QDSC Model

The QDSC Model simulation functioned and looked the same in Milestone 8 as Milestone 7. The team received one piece of constructive feedback about their QDSC simulation in Milestone 8. The nanoHUB representative wrote, “The cost/toxicity GUI needs to be clearer on what it is calculating.”

In Milestone 9, the QDSC Model simulation (Figure 4.5) functioned the same as in Milestone 8. The only two differences in their Milestone 9 submission were an added statement on the GUI that explained the use of the GUI (the text in the top right of Figure 4.5) and both the cost and toxicity were displayed for both mechanisms (instead of cost only for minimizing cost or toxicity only for minimizing toxicity).

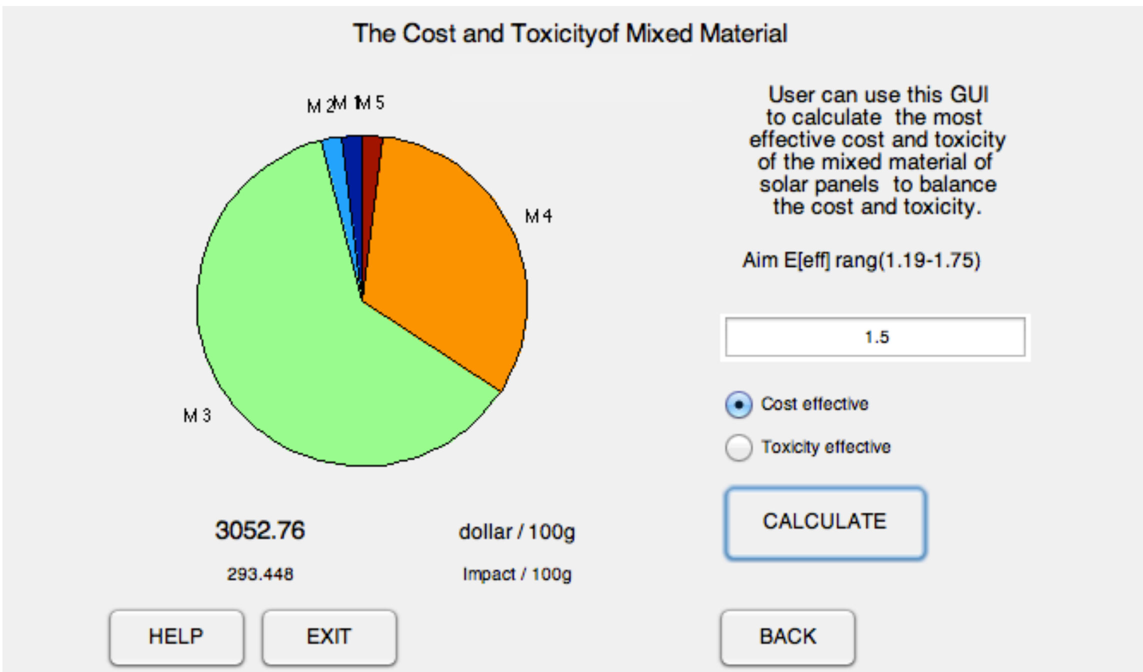

Figure 4.5. Team A's QDSC M9 Simulation – QDSC Model

The input and output variables for their QDSC model within their MEA and simulation are shown in Table 4.7. The inputs and outputs stayed constant through the MEA since this was a requirement, but the input options for the 5 QDSC Material input varied across the submissions (i.e. only 5 given materials in Draft 1, 10 given materials in Draft 2, and 12 possible materials in the Final Response).

Table 4.7 described the input and output variables of the QDSC Model simulation. The team used five QDSC materials in their underlying model throughout all the milestones. These materials changed throughout the course of their simulation development. In their first prototype (Milestone 4), the team proposed having the user input material properties for five QDSC materials of their choice. This method would increase the modifiability of their QDSC model. In their next submission, they changed this input to 10 preset materials that the user had to select five from. This was the same input as the MEA Draft 2 submission. In the next milestone, the team completely removed this input. In Milestones 7 through 9, the team's model was based on five default materials that the user could not change. This made their QDSC model less modifiable. In their Milestone 4 submission, the team only used the model to minimize both cost and toxicity; they did not give the user an option to select a mechanism. In Milestone 6, they brought back the Type of mechanism input with the option to minimize cost only or toxicity only. They kept this input for the remainder of their simulation development. In Milestone 7, the team implemented a second input (i.e. Target band gap energy). Their simulation input had more flexibility than this input in their MEA because the MEA was only based on two sample data points, although ideally their MEA should have been capable of this. The outputs for their simulation remained fairly constant throughout the milestones and consistent to the MEA version of the outputs. The simulation contained the same two outputs (i.e. QDSC material composition and Total cost and toxicity). The Total cost and toxicity output was changed in Milestone 7 to be only the total for cost or toxicity (depending on the aim selected). This was changed back to both totals in Milestone 9.

Table 4.7. Team A's Variables for QDSC Simulation – QDSC Model

Sub.	**Input**	**Possible Inputs**	**Output**
MEA FR	5 QDSC materials Target band gap energy Type of mechanism	12 possible (preset) materials 1.33 ev or 1.65 ev Min. cost, toxicity, or both	QDSC material mixture composition (%) Total cost and toxicity
M4	5 QDSC materials	User inputs 5 materials	QDSC material mixture composition (%) Total cost and toxicity
M5	5 QDSC materials	10 possible (preset) materials	Same as M4
M6	Type of mechanism	Min. cost or toxicity	Same as M4
M7	Type of mechanism Target band gap energy	Min. cost or toxicity 1.19 ev to 1.75 ev	QDSC material mixture composition (%) Total cost or toxicity (depending on the selected mechanism)
M8	Same as M7	Same as M7	Same as M7
M9	Same as M7	Same as M7	QDSC material mixture composition (%) Total cost and toxicity

4.4.2 Team B

Team B's ability to meet the mathematical model requirements, as assessed by the QDSC *I-MAP*, for each pertinent submission is summarized in Table 4.8. Team B slightly improved their QDSC model from Draft 1 to Draft 2, Final Response to Milestone 7, and Milestone 8 to Milestone 9 based on the *I-MAP* rubric items (see respective Scores in Table 4.8). This team had slight changes in their scores through their design project, but the change to their *Optimization Strategy* (*I-MAP* Item 8) enabled a user to select their own weighting of importance for cost and toxicity. This presents a new opportunity they created in their simulation that was not in their MEA model. This significant change along with the process of development is further described in this section. The formation of the QDSC model through the MEA is explained first; followed by an explanation of how their model was transformed to enable its use in their simulation suite.

Table 4.8. MEA and Design Project Submissions for Team B

MEA or Design Project Sub-mission	**Mathematical Model Analyzed: QDSC *I-MAP* (from** Table 3.6**)**									
	Material Constraints		**Given Equations Included**		**Given Equation Functions**	**Optimization Strategy**			**Search Space**	**Final Score (out of 18)**
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	
Draft 1	2	2	0	2	2	2	2	n/a	1	13
Draft 2	2	2	1	2	2	2	2	1	1	15
Final Response	2	2	1	2	2	2	2	1	1	15
Milestone 4	Y	Y	Y	Y	Y	Y	Y	Y	n/a	n/a
Milestone 5	Y	Y	Y	Y	Y	Y	Y	Y	n/a	n/a
Milestone 6	Y	Y	Y	Y	Y	Y	Y	Y	n/a	n/a
Milestone 7	2	2	2	2	2	2	2	1	1	16
Milestone 8	2	2	2	2	2	2	2	1	1	16
Milestone 9	2	2	2	2	2	2	2	2	1	17

4.4.2.1 Team B’s QDSC MEA

Throughout MEA Draft 1, Draft 2, and Final Response, Team B’’s QDSC mathematical model fully addressed the material constraints of there being a minimum of two grams of each material (*I-MAP* Item 2 in Table 4.8) and a total of 100 grams in the mixture (*I-MAP* Item 1 in Table 4.8). In MEA Draft 1, the direct user was required to select two materials to change (dependent on band gap energy and mechanism) and set the other three materials to two percent or two grams (accounting for this material requirement – *I-MAP* Item 2 in Table 4.8). The two changing materials added up to 94 grams to ensure a total of 100 grams was maintained (*I-MAP* Item 1 in Table 4.8). In their equations the team wrote the materials had to equal 1 (meaning 100%), but a peer gave feedback stating that this may be confusing. The peer wrote, “Additionally mentioning the units for every variable would be of great help, just to keep the user on track. I was confused about the unit of "=1" in the first equation.” The team changed their equation in Draft 2 to state the sum of the materials had to equal 100 grams. This further clarified the requirement of the mixture equaling 100 grams (*I-MAP* Item 1). There were no other changes throughout their MEA related to the *Material Constraints* category. The only other material related changes were related to the requirements of the MEA sequence.

Team B included the given equation to calculate the target band gap energy (*I-MAP* Item 4) throughout all three MEA submissions, but they did not ever include the given equation to calculate the band gap energy of individual quantum dots (*I-MAP* Item 3). In MEA Draft 1, the team did not include the equation for computing the band gap energies of individual quantum dot materials (*I-MAP* Item 3 in Table 4.8). The team only told the direct user to use MATLAB®, but the team did not include any MATLAB® file with their submission. The team did include the equation needed to determine the effective band gap energy (*I-MAP* Item 4 in Table 4.8) and did clearly describe how to apply this equation in their model (*I-MAP* Item 5 in Table 4.8). The target band gap energy was obtained through systems of equations. Two of the four peers gave the team feedback about their model missing any discussion and calculations for the band gap energies for the QDSC materials. One peer wrote, "This mathematical model … ignore the process of calculating Eg and have no explain for this issue." The other peer wrote, "I do not think that the mathematical take into account the quantum dot equation given to us in the beginning of the problem set."

The team responded to this feedback in MEA Draft 2 by adding a discussion about the need to calculate the band gap energy for each given quantum dot at the beginning of their procedure and providing sample band gap energies of materials in their memo. They still did not include the equation (*I-MAP* Item 3 in Table 4.8). They did not receive any feedback about this from the TA and did not make any more changes related to the *Given Equations Included* and *Given Equation Functions* categories.

Team B maintained a non-iterative solution, using systems of equations, for their optimization strategy throughout all three MEA submissions (*I-MAP* Items 6-9). In MEA Draft 1, the team fully addressed the two required mechanisms for their QDSC model – one for minimizing cost and the other for minimizing toxicity (*I-MAP* Items 6 and 7 in Table 4.8). Both procedures began with identifying one material with the lowest cost or toxicity (depending on the selected mechanism) that had a band gap energy above the desired band gap energy and another one with the lowest cost or toxicity (also depending on the selected mechanism) with a band gap energy below the desired band gap energy. The amount to include for these two materials is determined through systems of equations. They provide two equations that have two variables and tell the user to "solve two variables". They provide more details through an example of one demonstration. The team received full points on the *Optimization Strategy* category of their model (*I-MAP* Items 6 and 7 in Table 4.8). The team somewhat addressed the criteria for the *Search Space* category by providing a non-iterative solution, but they did not discuss the effects of limiting the search space through a non-iterative solution (*I-MAP* Item 9 in Table 4.8). The team did not receive any peer feedback related to either of these categories.

For MEA Draft 2, Team B was further challenged and required to add a mechanism to minimize both cost and toxicity. Their revised procedure accounted for all three goals – minimizing cost only, toxicity only, and both (*I-MAP* Items 6 – 8 in Table 4.8). There were no changes to their models to minimize cost only and minimize toxicity only. The team only somewhat addressed the criteria for their model to minimize both cost and toxicity because they did not have an option for user-input to set the weighting for the importance of cost versus toxicity (*I-MAP* Item 8 in Table 4.8). The QDSC model for minimizing both cost and toxicity also used systems of equations. The two materials were selected based on a cost-toxicity factor that the team developed (i.e. cost divided by the average cost plus toxicity divided by the average toxicity). There were no major changes in the team's mathematical model from the team's MEA Draft 2 to Final Response. This makes sense taking the TA's feedback into account because the TA simply stated, "The model addresses the complexity of the problem." The team changed the cost-toxicity factor to be dependent on median and standard deviation instead of mean in their Final Response. With their MEA Draft 2 and Final Response MEA submissions, the team also included three MATLAB® files that consisted of their QDSC models to minimize cost, toxicity, and both cost and toxicity.

It is common for TAs to focus their feedback on the *I-MAP* dimensions or items on which a team has low scores. As the team did not have low mathematical model scores for their Draft 2 and Final Response, the TA's feedback focused on other dimensions. The TA gave the same feedback about the team's QDSC model on the Final Response as Draft 2.

4.4.2.2 Team B's QDSC Design Project

Team B approached implementing their QDSC model into a simulation through five GUIs (i.e. Material Selection, QDSC Model, QDSC Weighted Model, Material Mixing, and Material Composition). Each GUI had a different way of changing their features within the *Material Constraints*, *Given Equations Included*, *Given Equation Functions*, *Optimization Strategy*, and *Search Space* categories.

The Material Selection GUI contained one of the given equations (i.e. band gap energy – *I-MAP* Item 3) and content pertinent to the *Material Constraints* category (i.e. *I-MAP*

Items 1 and 2). This GUI enabled the user to input any QDSC material that they wanted; this made their model much more modifiable to other scenarios.

The QDSC Model simulation used the same non-iterative QDSC model for minimizing both cost and toxicity that the team submitted in their MEA Final Response submission (i.e. *I-MAP* Items 8 and 9). Throughout the milestone submissions this model did not present any new opportunities in their simulation because it was only a black-box model that calculated the same information. In their last submission, Milestone 9, the team added a visual to this model that enabled them to further explore the total cost and toxicity based on different target band gap energies selected (i.e. *I-MAP* Items 4 and 5).

The QDSC Weighted Model simulation presented an idea to improve the optimization strategy of their model for minimizing both cost and toxicity (i.e. *I-MAP* Item 8). The underlying model used the same non-iterative QDSC model through the initial submissions, which resulted in only the minimize toxicity only and minimize cost only solutions functioning at first (i.e. *I-MAP* Items 6 and 7). In their Milestone 9 submission they changed the optimization strategy used for their model to minimize both cost and toxicity to an iterative model enabling the user to change the weighting of importance for cost and toxicity (i.e. *I-MAP* Item 8). Although their iterative model did not minimize the search space (i.e. *I-MAP* Item 9), it enabled new functionality to their model.

The Material Mixing simulation presented new opportunities beyond the original material constraints (i.e. *I-MAP* Items 1 and 2) and another perspective for the effective band gap energy (i.e. *I-MAP* Items 4 and 5). The model enabled the user to select varying percentages (i.e. minimum material constraint of 1 percent) for material composition, as shown through the inputs in Table 4.11. The model enabled the user to calculate the band gap energy for any material composition instead of starting with the band gap energy as a goal (i.e. *I-MAP* Items 4 and 5). This simulation removed the models to minimize cost, toxicity, and both, so this simulation did not enable any new functionality to this aspect of the QDSC model.

The Material Composition simulation enabled the user to view the resulting material composition for the QDSC Model, QDSC Weighted Model, and Material Mixing simulations. This visual may have presented a different way to view the resulting material composition, but it did not enable any new functionality to any of the *I-MAP* categories.

In Milestone 1, Team B communicated the given project deliverables, function, criteria for success, and constraints. The team also discussed potential stakeholders and the direct users for their simulation suite. The team selected the US Federal Highway Administration as their direct user. They explained that they should take advantage of the opportunities that solar energy presents; they decided to make their simulation suite to encourage advancing the roadway systems. The team described their motive to select their direct user, "We want to work with them because we feel as though converting components of the roadway system to make full use of PV solar panels is critical to improving our current energy issues and will be highly beneficial in the future." The team received feedback on the lack of description in this Milestone and acknowledged this feedback in their documentation in the beginning of their Milestone 2 documentation by listing out three more potential stakeholders and their relationship to the deliverable.

As part of the team's submission for Milestone 1, the team members had an individual assignment in which they had to evaluate prototypical student-completed GUIs. All four students on this team completed this assignment. They all correctly identified the GUIs that were a demonstration of a black-box model (i.e. was a model, but not a simulation) and a demonstration of a simulation (i.e. was a model and a simulation). None of the students correctly identified the animated simulation, as both a model and a simulation. Three of the students thought the animated simulation was only a simulation (without a model present). The other student thought it was neither a model nor simulation. Two of the students correctly identified the GUI that was only interactive (i.e. no models or simulations). One of the other students thought it had both a model and a simulation. The last student thought there was a model present, but it was not a simulation. Overall the students presented some understandings of the presence of models and simulations. The students received auto-generated feedback on this assignment based on their individual responses, but the team did not refer to this feedback in their Milestone 2 documentation.

In Milestone 2, the team proposed 20 ideas that all involved their QDSC model. Not all of these ideas were simulations. Some of the ideas were GUIs that would only present users with the opportunity to select QDSC materials that potentially could be used as inputs. Some of the ideas were only different methods to visually display results of their QDSC models. Most of the proposed models involved the original QDSC model, but a few used the results form the model with another model added on to give new information (e.g., display durability of various QDSC mixtures). The major constructive feedback the team received on this milestone was that some of their ideas were not fully developed enough to constitute as acceptable for their simulations.

In Milestone 3, they addressed the feedback by eliminating any ideas that did not benefit their final simulation suite. The team then selected four ideas for their simulations that all had to do with the QDSC model. The ideas were: 1 – Material Selection) "Display to the user all of the materials on the GUI screen, and let them select the exact materials that they want from there." 2 – QDSC Model) "Display to the user the minimum cost, the minimum toxicity, and the optimized mixture given certain materials to mix." 3 – Weighted QDSC Model) "Give the users flexibility in what they prefer in terms of maximizing cost and toxicity (i.e. we've always done either only looking at cost, only looking at toxicity, or looking at both equally; we would give the user more flexibility)." and 4 – Material Mixing) "Allow the user to specify how much of the materials they want used and output the cost, toxicity, and final Eg." The Material Selection idea would only enable the user to select materials, which would only constitute as input selection for a model. The QDSC Model idea would consist of presenting the original three mechanisms. The Weighted QDSC Model idea would allow the user to weight the importance of cost and toxicity on their own, which would enable them to fully address the optimization strategy for their mechanism to minimize both cost and toxicity (*I-MAP* Item 8) based on the assessment tool. The Material Mixing idea would allow the user to interact with their QDSC model in a different manner – selecting the material composition instead of the target band gap energy. The team received feedback that they did not provide at least 3 reasons pro and con for each idea through their concept reduction process.

In their Milestone 4 presentation, the team presented four proposed GUIs with three models and one visual. All of three ideas from the previous milestone were included in their prototype with an addition of a graph of the material composition (i.e. Material Composition). The navigation map, presentation slides, and written text further explained their simulation suite. Their proposed simulation suite began with a material selection GUI (Material Selection – in Figure 4.6). The user selects the materials on this GUI; from here the user can select one of four different simulations (i.e. QDSC Model, QDSC Weighted Model, Material Mixing, or Material Composition).

On the Material Selection GUI (Figure 4.6) the direct user can choose from the ten given materials or input their own materials. The team explained that the user must select a total of five materials. They do not count this as one of their simulations; this is only used to select the material inputs for their four simulations. Even though they did not label this as a model or simulation, this is an example of a black-box model. The band gap energy equation was the underlying model for this GUI to calculate the band gap energy for any new materials that the user inputs (i.e. M11 – M15).

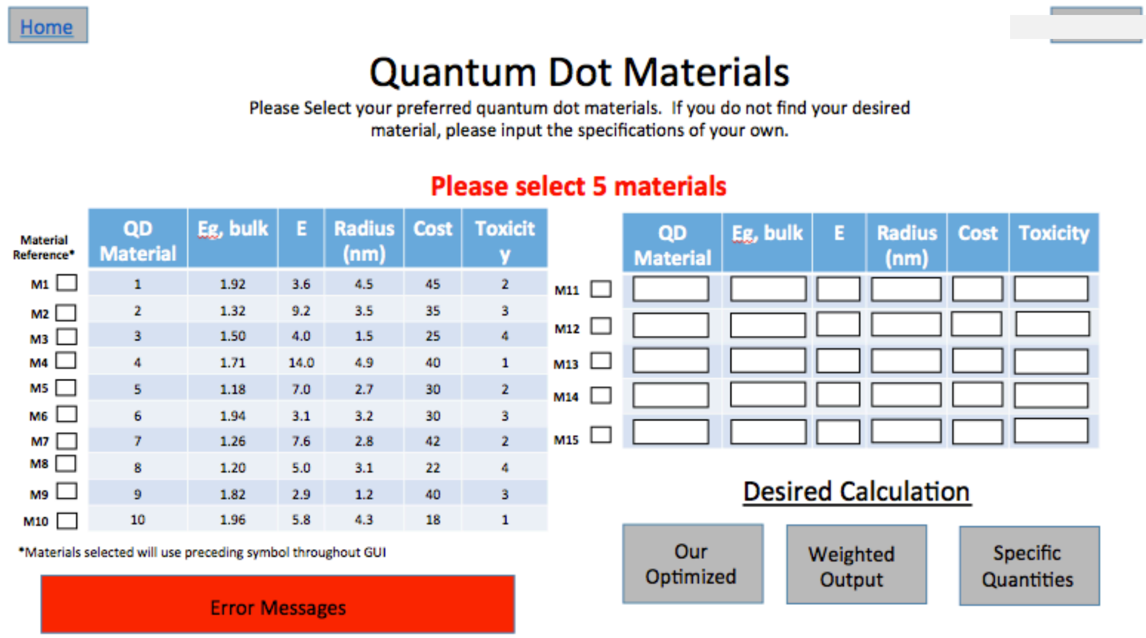

Figure 4.6. Team B's QDSC M4 Material Selection GUI

The proposed QDSC Model simulation (Figure 4.7) used the materials selected in the Material Selection GUI as an input. The GUI also required the user to input a target band gap energy. Numeric values for the total cost and toxicity based on their QDSC model to minimize both cost and toxicity were the outputs. The models to minimize cost only or toxicity only were not included, as proposed in Milestone 3. This GUI is an example of a black-box model because it does not have visualized outputs. The GUI contained a button "Graph Material Usage" that takes the user to their proposed Material Composition simulation. These two GUIs linked together meet the requirements of a simulation.

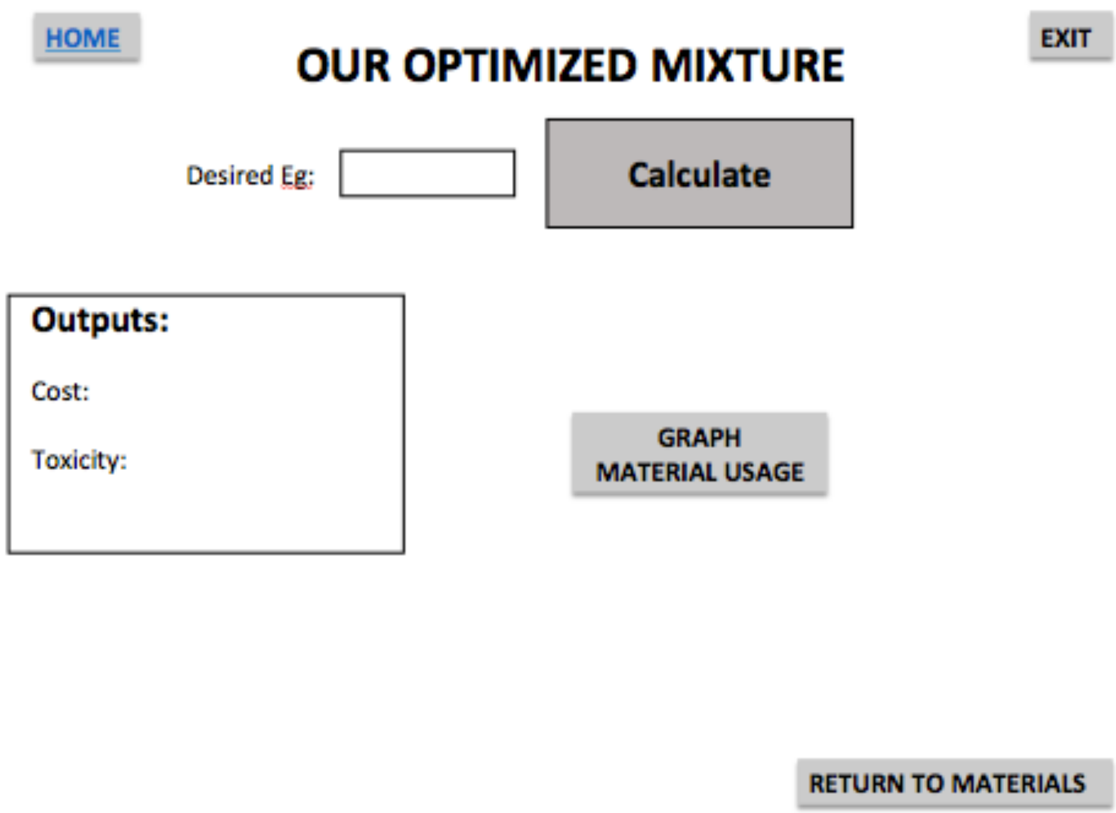

Figure 4.7. Team B's QDSC M4 Simulation Prototype – QDSC Model

The proposed QDSC Weighted Model simulation (Figure 4.8) also used the materials selected in the Material Selection GUI as an input. There was no supplemental text to further explain this proposed simulation. Based on interpretation of their provided figure, the user could input a target band gap energy and use the slide bar to select the weighted importance of cost to toxicity. The presented GUI is only a black-box model because it does not present visualization within the proposed simulation. Similar to the proposed QDSC Model simulation, this proposed simulation had a "Graph Material Usage" button (likely navigating to their proposed Material Composition simulation). This is another example of two GUIs that would make one complete simulation.

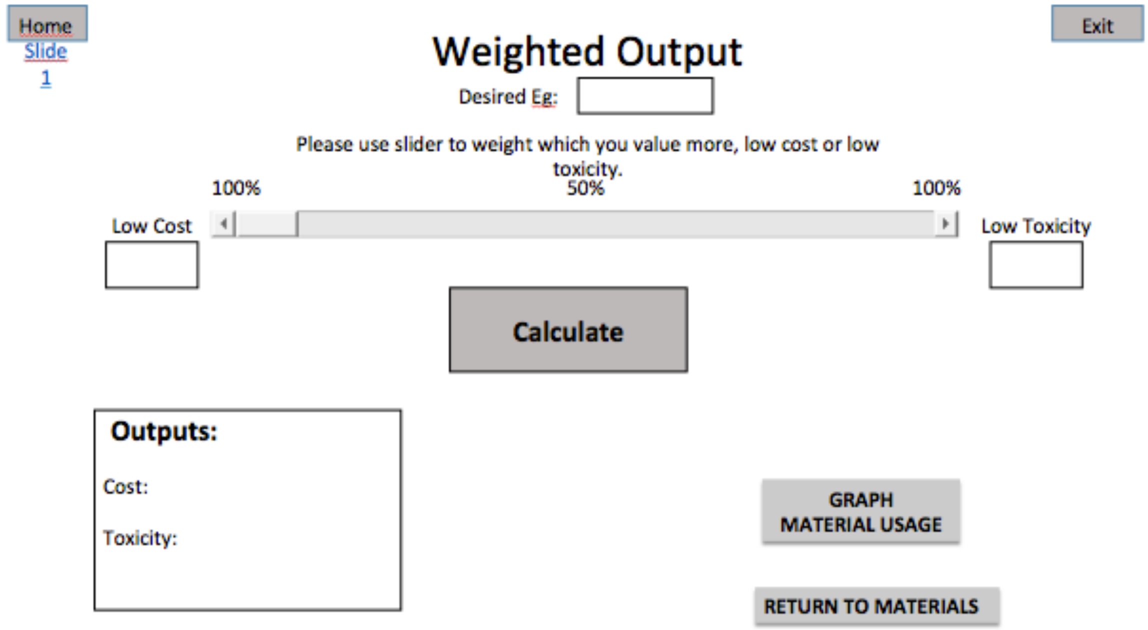

Figure 4.8. Team B's QDSC M4 Simulation Prototype – QDSC Weighted Model

The proposed Material Mixing simulation (Figure 4.9) required the user to input the percentages of the five previously selected materials (from the Material Selection GUI) for their solar panel. The underlying QDSC model would output the total cost, total toxicity, and effective band gap energy for their mixture. There is no discussion about material constraints for the input percentages of the material composition. This is another example of a black-box model because there is no visualization of the model. This proposed simulation also has a "Graph Material Usage" button, which would navigate the user to the proposed Material Composition simulation. This visual is not as meaningful for this proposed simulation; the visual would only display the inputs to the user, which is not informative to the underlying model.

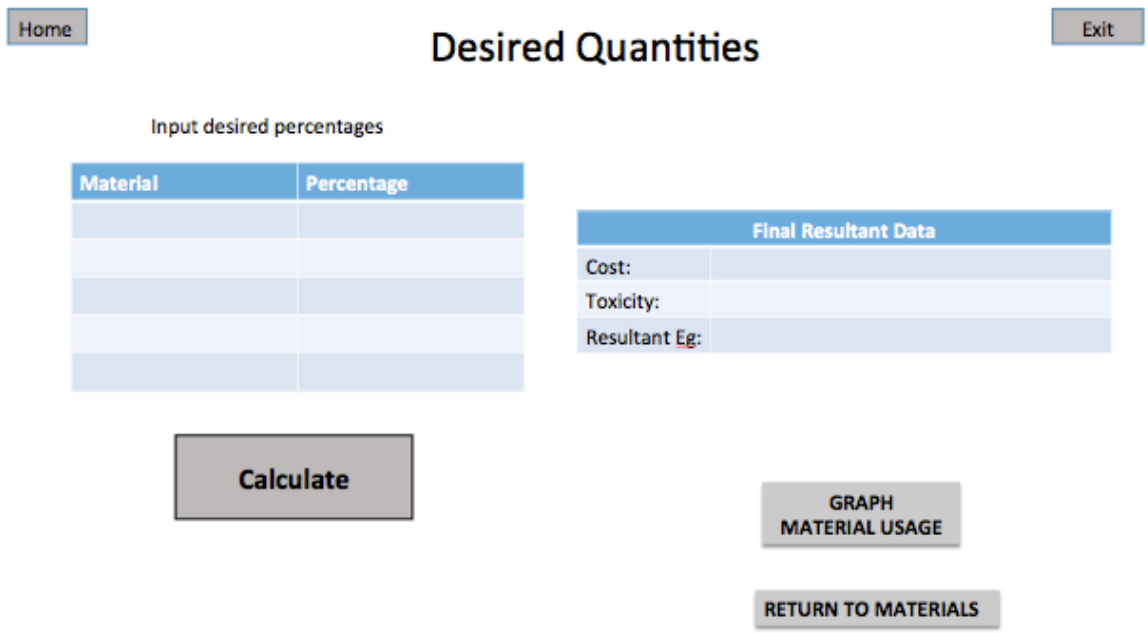

Figure 4.9. Team B's QDSC M4 Simulation Prototype – Material Mixing

The proposed Material Composition simulation (Figure 4.10) displayed content from the team's other three proposed simulations. The team seems to understand that this not a simulation because there is no discussed underlying model, but they still count this as a simulation for their requirement. The team described this GUI by stating; "The GUI is basically a plot based on the data calculated on previous slide to show user how much percentage will each material take. So there is no special mathematical models for this slide." The TA further verified this lack of a simulation stating, their "fourth simulation is not a kind of simulation" in feedback the team received on this milestone.

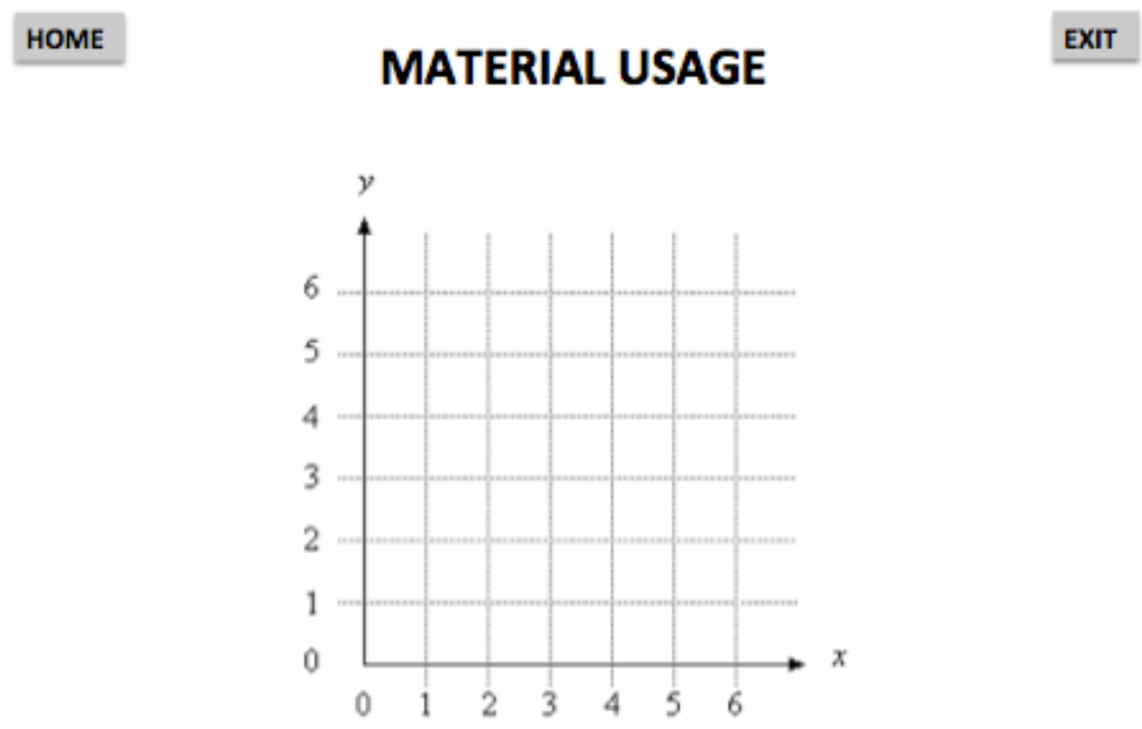

Figure 4.10. Team B's QDSC M4 Simulation Prototype – Material Composition

In Milestone 5, the team did not discuss addressing the feedback about their proposed Material Composition simulation, but appeared to address it by adding another simulation. The new proposed simulation presented a black-box model that calculated energy savings. This simulation was not based on the QDSC model and was not further analyzed. Although the team added a new simulation, their student assignments show one student only doing the Material Composition GUI – meaning they are most likely still counting this for one of their simulations. This continued to be treated as its own simulation, as the team designed it, throughout this analysis.

There were no changes to the proposed QDSC Model and Material Mixing simulations in this milestone submission. The proposed QDSC Weighted Model simulation added supplemental text that described the simulation in their own words – confirming how it was previously described. The proposed Material Composition simulation was slightly revised to include more displayed information; it displayed the same bar graph of material composition with additional textboxes of something not describe (Figure 4.11).

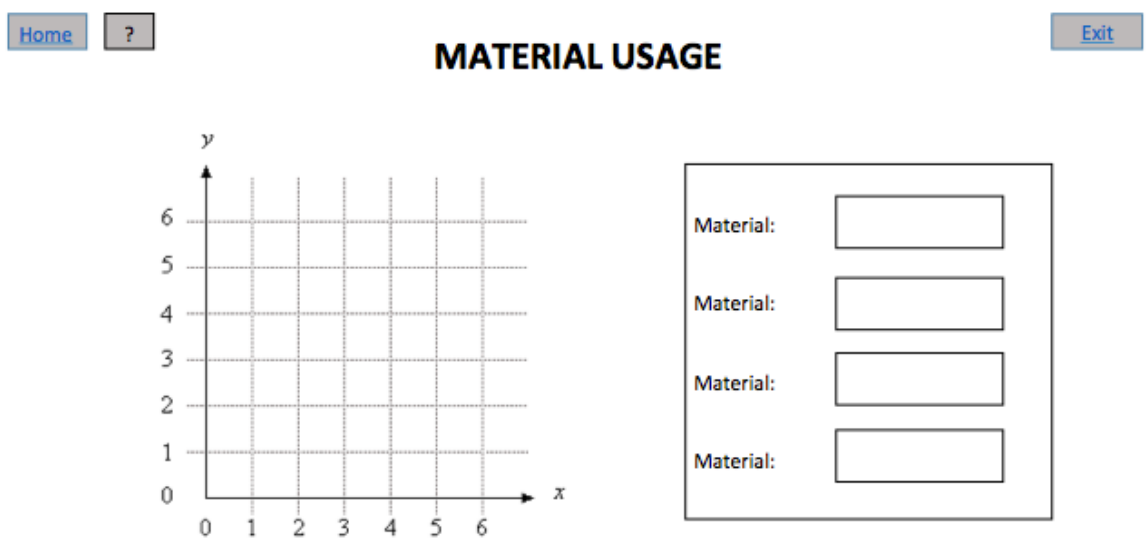

Figure 4.11. Team B's QDSC M5 Simulation Prototype – Material Composition

The team received feedback that their project did not have mathematical models, so the team stated they would show their mathematical models in their GUIs. Three of the proposed QDSC simulations did have underlying models and they were discussed in the supplemental text or the text at least pointed to their MEA for their QDSC model. This feedback did not seem valid for their submission. This feedback could have been potentially helpful if tailored to explain why their Material Composition simulation was really only the visualization component for three other models.

In Milestone 6, the team converted their proposed GUIs into actual GUIs. The QDSC Model simulation wrote the underlying model on the GUI, as the team stated they would in response to their received feedback. The other proposed GUIs were developed in MATLAB® exactly as proposed in their previous milestone. The coding did not include their mathematical models and the GUIs were not functioning at this stage, which was acceptable for this Milestone. The team did not receive any feedback and did not document any changes that they made to this submission.

The team added functionality to their GUIs in Milestone 7, as required for this submission. All four QDSC simulations had the same underlying concepts and similar layouts as proposed in previous milestones.

The Material Selection GUI (Figure 4.12) required the user to select five QDSC materials (out of 10 given materials and 5 materials that the user could input). The underlying model for this GUI calculated the band gap energy for any materials that the user inputs.

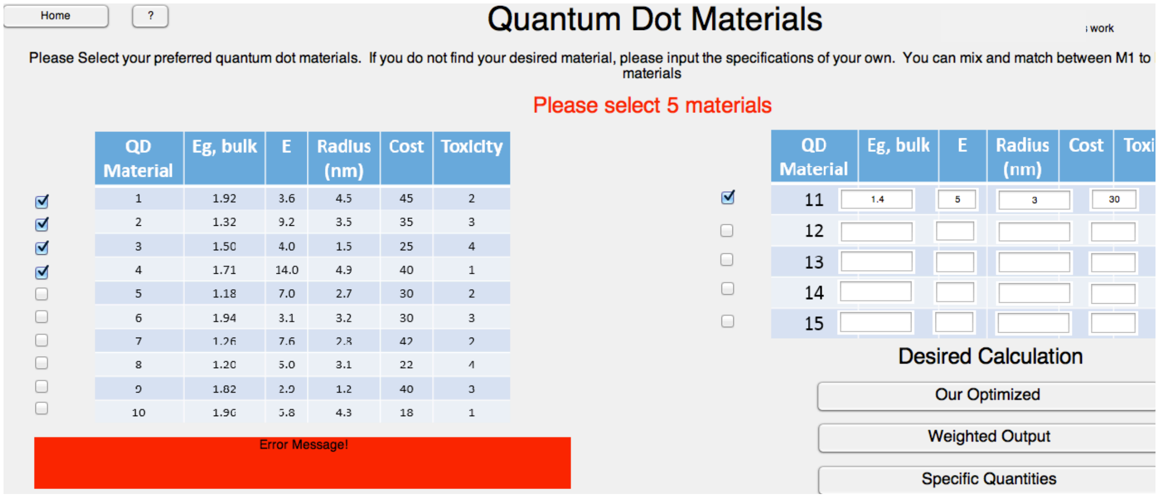

Figure 4.12. Team B's QDSC M7 GUI – Material Selection

The QDSC Model simulation (Figure 4.13) was developed as proposed in previous milestones. The underlying model uses the same model for minimizing both cost and toxicity that the team proposed in their MEA Final Response.

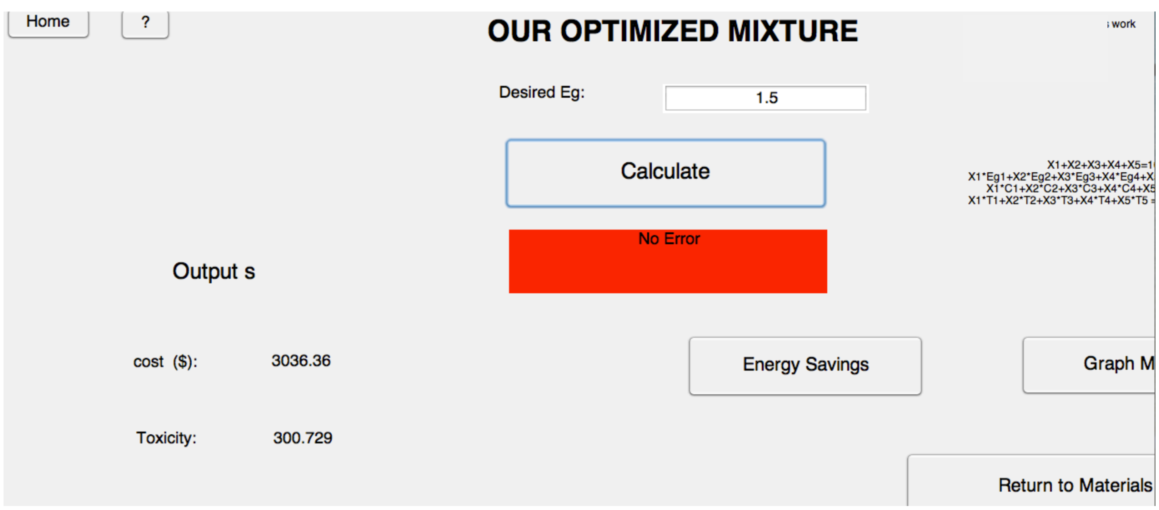

Figure 4.13. Team B's QDSC M7 Simulation – QDSC Model

The QDSC Weighted Model simulation (Figure 4.14) had the layout that was proposed in previous milestones, but the underlying model was not functioning as described. The model used was written on their GUI (shown on the right side in Figure 4.14). The underlying model only allowed the user to see the output for minimizing cost only or minimizing toxicity only. The model needed to be revised to enable the weighted importance input to function.

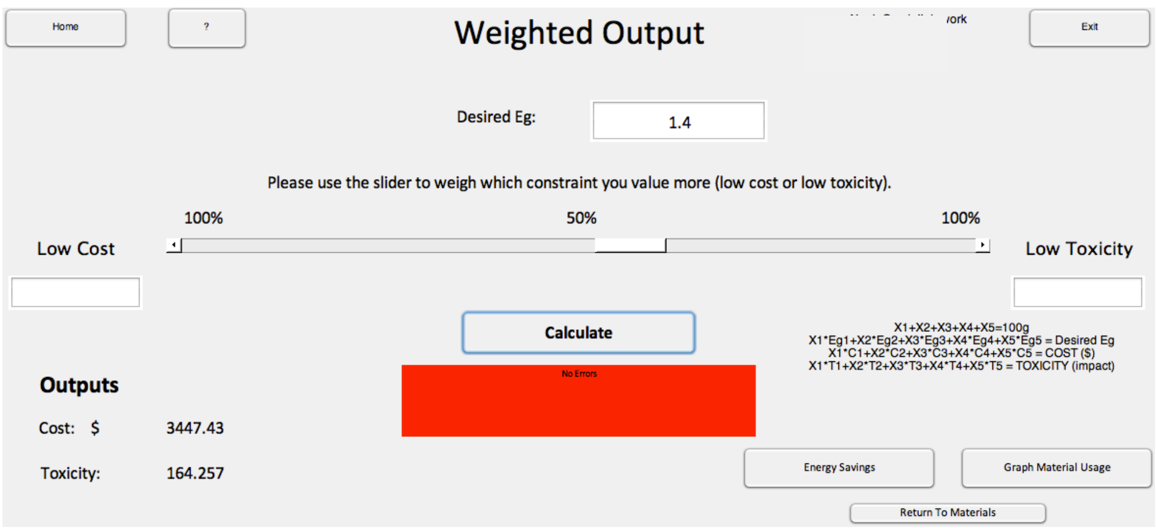

Figure 4.14. Team B's QDSC M7 Simulation – QDSC Weighted Model

The Material Mixing simulation (Figure 4.15) was developed as proposed in previous milestones. The simulation enabled the user to select any material composition of five materials with the material constraints of each material equaling at least one percent. The underlying models were written on the bottom right of the GUI.

Figure 4.15. Team B's QDSC M7 Simulation – Material Mixing

The Material Composition simulation (Figure 4.16) presented the materials that were included in the composition on the right side of the GUI. The bar graph visually presented the material composition.

The team received feedback to complete commenting for each GUI, revise error messages to ensure they are all appropriate, and add limitation hints for the inputs. The team noted they would address all of this feedback. The team did not receive any feedback about their underlying models or lack of visualization.

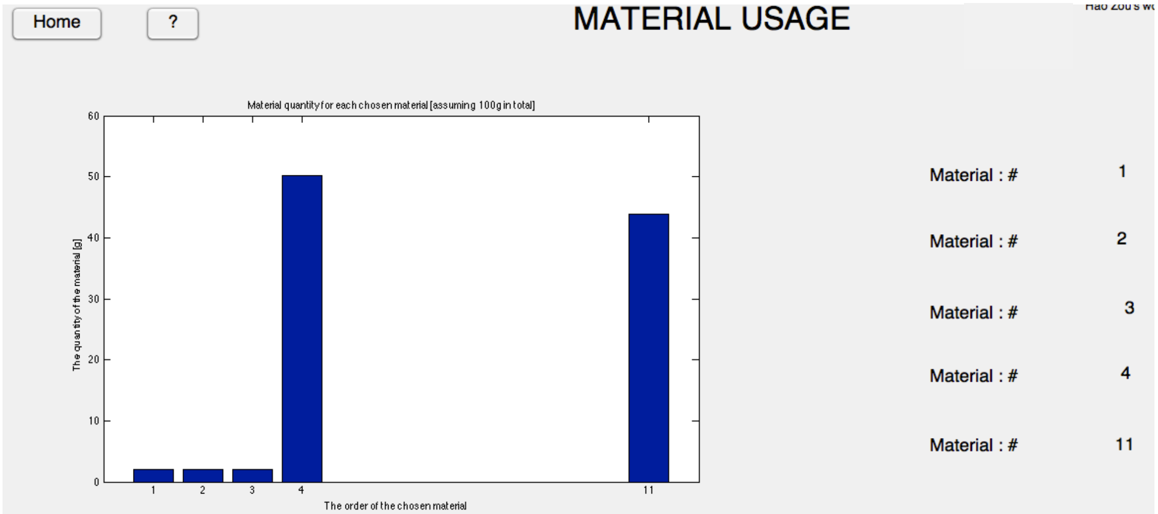

Figure 4.16. Team B's QDSC M7 Simulation – Material Composition

In Milestone 8, there were no significant changes to their project. The user-controlled weighting for their QDSC model still did not function properly. The team received two major piece of feedback about their project pertinent to the QDSC models. They were told that the Material Composition simulation was not a simulation. There was also feedback that there was an error in the coding for the QDSC Weighted Model; this error was unclear and may have been connected to the lack of functionality in the weighting.

In Milestone 9, the team added visualization to their QDSC Model and QDSC Weighted Model simulations. The Material Mixing simulation only had some minor formatting changes (e.g. layout, text color) and did not incorporate any visualization. The Material Composition simulation implemented an additional output.

The QDSC Model simulation (Figure 4.17) functioned the same as it did in the previous milestones. The team changed this black-box model into a simulation by adding its own visualization. It still provided a numeric output of the total cost and toxicity (not pictured to focus on new visual). The graph enabled the user to track how changing their band gap energy affects the total cost and toxicity of their output material compositions. The GUI still had a button to link to the Material Composition simulation (also not visible in this image). The GUI also implemented text that identified the range of possible target band gap energies based on the five selected materials and an underlying model to calculate this (red text below the "Desire Eg" input).

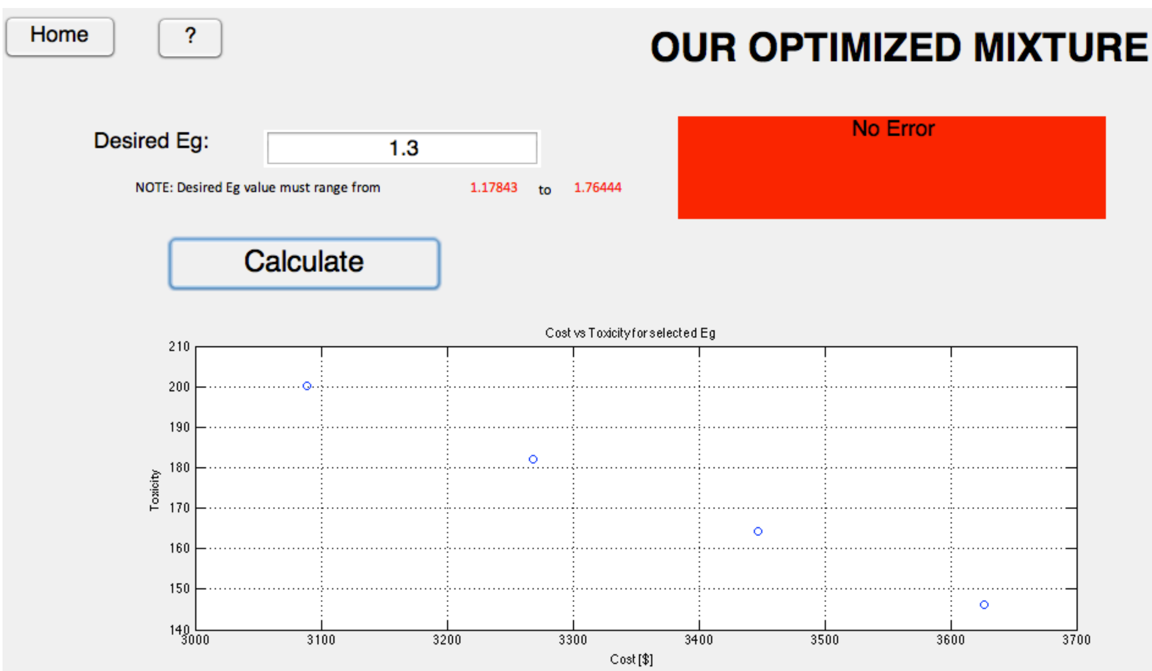

Figure 4.17. Team B's QDSC M9 Simulation – QDSC Model

The QDSC Weighted Model simulation (Figure 4.18) fully functioned, as originally proposed, in this version and incorporated in a visualization to allow the user to see the range of costs and toxicities for different weighted importance for the target band gap energy. The underlying model used an iterative solution changing all five materials to enable more variation in the cost-toxicity importance weighting. An example of a resulting material composition from this revised model is displayed in Figure 4.19.

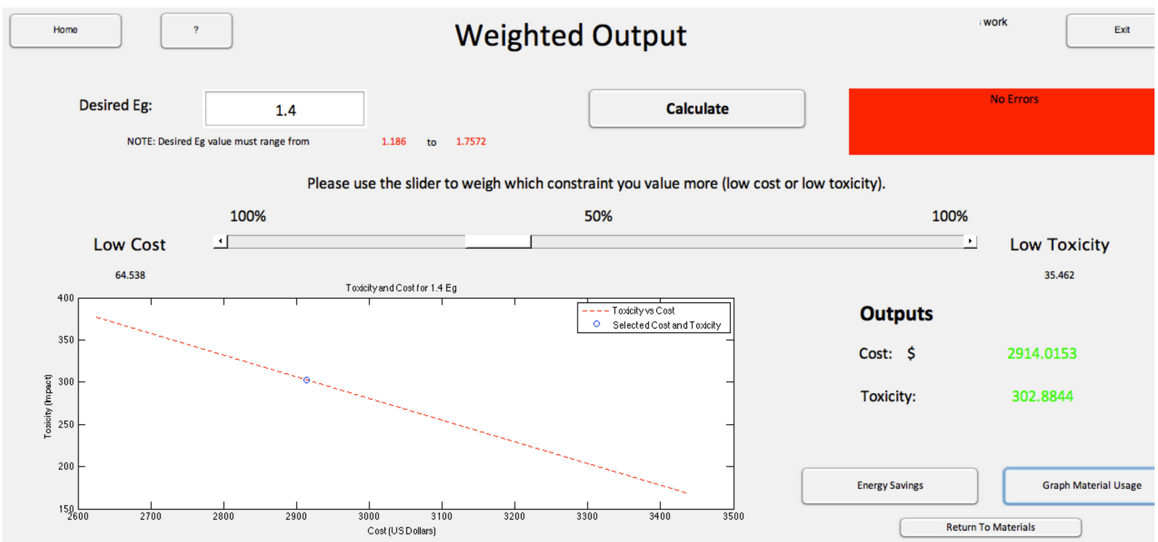

Figure 4.18. Team B's QDSC M9 Simulation – QDSC Weighted Model

The Material Composition simulation (Figure 4.19) was revised to include the output grams of each QDSC material in the material composition.

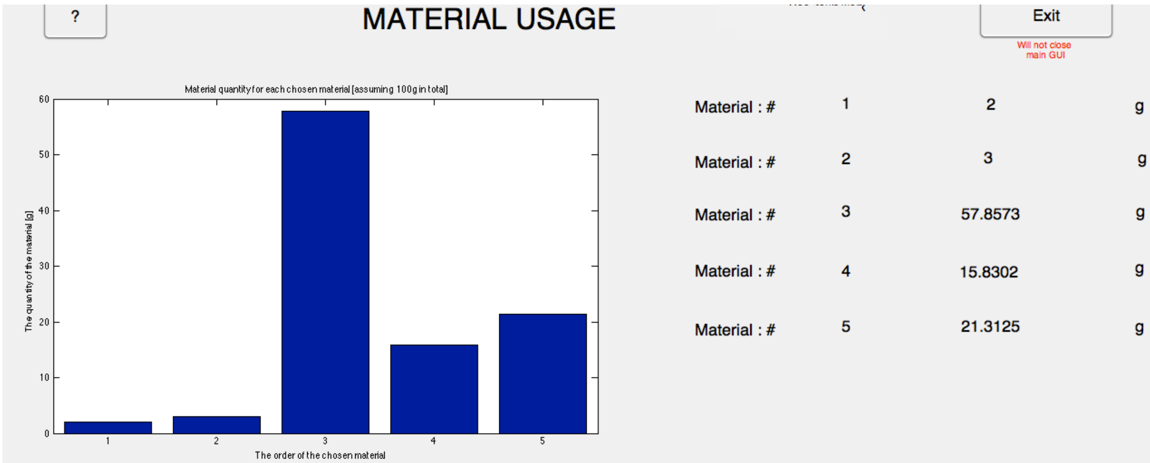

Figure 4.19. Team B's QDSC M9 Simulation – Material Composition

The input and output variables for their QDSC model within their MEA and four simulations are shown in Table 4.9, Table 4.10, Table 4.11, and Table 4.12. The inputs and outputs stayed constant through the MEA since this was a requirement, but the input options for the 5 QDSC Material input varied across the submissions (i.e. only 5 given materials in Draft 1, 10 given materials in Draft 2, and 12 possible materials in the Final Response). These are described at the beginning of all four tables.

Table 4.9 described the input and output variables of the QDSC Model simulation. The team removed the input option of selecting the type of mechanism (i.e. minimize cost only, toxicity only, or both). The simulation was preselected by the design of the simulation to use the model to minimize both cost and toxicity. This was set throughout all the milestones. The team modified the 5 QDSC materials input to allow the user to input any five materials from the original 10 preset materials and 5 options for user-input materials. This same input was used throughout all the milestones. The target band gap energy input was modified to allow the user to input any target band gap energy that was possible based on the five selected QDSC materials. This input was further clarified in Milestone 9 to enable the user to know the possible target band gap energies for their mixture. The original simulation only output the total cost and toxicity of the final mixture (one of the MEA QDSC model's outputs). In Milestone 9, the team incorporated a graph that enabled a different way to view the total costs and toxicities for mixtures with different target band gap energies.

Table 4.10 described the input and output variables of the QDSC Weighted Model simulation. The 5 QDSC materials and Target band gap energy inputs changed through the same way and submissions as the QDSC Model simulation. The team changed the Type of mechanism input to the Cost-toxicity importance weighting input. The proposed input in early milestones is not explained in detail and when first implemented in their simulation does not enable the proposed idea of changing the importance weighting of cost and toxicity. In their final version of this simulation, the proposed idea is functioning and allows the user to change the importance of cost and toxicity by increments of 0.2717%. This changed the nature of their QDSC model from only having three possible inputs (i.e. minimum cost, minimum toxicity, and some optimization of both) to hundreds of possible inputs on spectrum of minimizing cost only to minimizing toxicity only. They also provide an output graph in their final simulation that enables the user to explore the possible cost and toxicity totals for different band gap energies.

Table 4.11 described the input and output variables of the Material Mixing simulation. The 5 QDSC materials input changed through the same way and submissions as the QDSC Model simulation. The material composition was an output in the MEA version of the model, but this was an input throughout their simulation version of the model. This meant the type of model to use (i.e. minimize cost, toxicity, or both) was no longer a component of the model in the simulation. In relation to this, the effective band gap energy became an output throughout the simulation – it was no longer an input, as it was in the MEA. This transformed the function of the model from finding a material composition for a target band gap energy and based on criteria (i.e. minimize cost, toxicity, or both) to calculating the band gap energy for a given material composition. The model still output the total cost and toxicity throughout the simulation, like the MEA. Similar to the MEA, the material mixture had a minimum percentage requirement for each material, but it was one percent in the simulation instead of one.

Table 4.12 described the input and output variables of the Material Composition simulation. The simulation was dependent on the three previously described simulations. The only input for this model was the outputs of the QDSC Model or QDSC Weighted Model simulations or the inputs for the Material Mixing simulation. This was constant throughout its development. This simulation, similar to the MEA, displayed the QDSC material composition throughout. The information displayed for this output grew across the milestones – from only the percentages, to including an explicit list of the materials, and finally to including the grams of the material composition.

Table 4.9. Team B's Variables for QDSC Simulation – QDSC Model

Sub.	Input	Possible Inputs	Output
MEA FR	5 QDSC materials	12 possible (preset) materials	QDSC material mixture composition (%)
	Target band gap energy	1.33 ev or 1.65 ev	Total cost and toxicity
	Type of mechanism	Min. cost, toxicity, or both	
M4	5 QDSC materials	15 possible materials (10 preset materials)	Total cost and toxicity
	Target band gap energy	No range stated (possible range dependent on mixture)	
M5	Same as M4	Same as M4	Same as M4
M6	Same as M4	Same as M4	Same as M4
M7	5 QDSC materials	15 possible materials (10 preset materials)	Same as M4
	Target band gap energy	Possible range dependent on mixture	
M8	Same as M7	Same as M7	Same as M4
M9	5 QDSC materials	15 possible materials (10 preset materials)	Total cost and toxicity
	Target band gap energy	Possible range dependent on mixture (range clearly stated on GUI)	Graph of cost vs. toxicity for different selected target band gap energies

Table 4.10. Team B's Variables for QDSC Simulation – QDSC Weighted Model

Sub.	Input	Possible Inputs	Output
MEAFR	5 QDSC materials Target band gap energy Type of mechanism	12 possible (preset) materials 1.33 ev or 1.65 ev Min. cost, toxicity, or both	QDSC material mixture composition (%) Total cost and toxicity
M4	5 QDSC materials Target band gap energy Cost-toxicity importance weighting	15 possible materials (10 preset materials) No range stated (possible range dependent on mixture) 100% cost to 100% toxicity (increments between not stated)	Total cost and toxicity
M5	Same as M4	Same as M4	Same as M4
M6	Same as M4	Same as M4	Same as M4
M7	5 QDSC materials Target band gap energy Cost-toxicity importance weighting	15 possible materials (10 preset materials) Possible range dependent on mixture 100% cost or 100% toxicity (increments between did not function)	Same as M4
M8	Same as M7	Same as M7	Same as M4
M9	5 QDSC materials Target band gap energy Cost-toxicity importance weighting	15 possible materials (10 preset materials) Possible range dependent on mixture (range clearly stated on GUI) 100% cost to 100% toxicity (increments of 0.2717%)	Total cost and toxicity Line graph of cost vs. toxicity possible for target band gap energy

Table 4.11. Team B's Variables for QDSC Simulation – Material Mixing

Sub.	Input	Possible Inputs	Output
MEA FR	5 QDSC materials	12 possible (preset) materials	QDSC material mixture composition (%)
	Target band gap energy	1.33 ev or 1.65 ev	Total cost and toxicity
	Type of mechanism	Min. cost, toxicity, or both	
M4	5 QDSC materials	15 possible materials (10 preset materials)	Total cost and toxicity
	Mixture composition (%)	100% total, no minimum percent per material stated	Effective band gap energy
M5	Same as M4	Same as M4	Same as M4
M6	Same as M4	Same as M4	Same as M4
M7	5 QDSC materials	15 possible materials (10 preset materials)	Same as M4
	Mixture composition (%)	100% total, 1% minimum per material	
M8	Same as M7	Same as M7	Same as M4
M9	Same as M7	Same as M7	Same as M4

Table 4.12. Team B's Variables for QDSC Simulation – Material Composition

Sub.	Input	Possible Inputs	Output
MEA FR	5 QDSC materials Target band gap energy Type of mechanism	12 possible (preset) materials 1.33 ev or 1.65 ev Min. cost, toxicity, or both	QDSC material mixture composition (%) Total cost and toxicity
M4	Model to visualize material composition for	Output of QDSC Model, Output of QDSC Weighted Model, or Inputs of Material Mixing	QDSC material mixture composition (%)
M5	Same as M4	Same as M4	Same as M4
M6	Same as M4	Same as M4	Same as M4
M7	Same as M4	Same as M4	QDSC material mixture composition (%) List of QDSC materials used in mixture
M8	Same as M4	Same as M4	Same as M7
M9	Same as M4	Same as M4	QDSC material mixture composition (%) QDSC material mixture composition (grams) List of QDSC materials used in mixture

4.4.3 Team C

Team C's ability to meet the mathematical model requirements, as assessed by the QDSC *I-MAP*, for each pertinent submission is summarized in Table 4.13.

Table 4.13. MEA and Design Project Submissions for Team C

MEA or Design Project Submission	**Mathematical Model Analyzed: QDSC *I-MAP* (from** Table 3.6**)**									
	Material Constraints		**Given Equations Included**		**Given Equation Functions**	**Optimization Strategy**			**Search Space**	**Final Score (out of 18)**
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	
Draft 1	2	2	0	2	1	1	1	n/a	1	10
Draft 2	2	2	2	2	2	2	2	1	1	16
Final Response	2	2	2	2	2	2	2	1	1	16
Milestone 4	Y	Y	Y	Y	Y	Y	Y	Y	n/a	n/a
Milestone 5	Y	Y	Y	Y	Y	Y	Y	Y	n/a	n/a
Milestone 6	Y	Y	Y	Y	Y	Y	Y	Y	n/a	n/a
Milestone 7	2	2	2	2	2	2	2	1	1	16
Milestone 8	2	2	2	2	2	2	2	1	1	16
Milestone 9	2	2	2	2	2	2	2	1	1	16

Team C significantly improved their QDSC model from Draft 1 to Draft 2 based on the *I-MAP* rubric items. From Draft 2 to Milestone 9, no more changes can be seen in the team's QDSC model through the lens of the *I-MAP* as evidence by the final score of 16 for all submissions after Draft 1 (in Table 4.13). However, the team's model did change during the QDSC design project because the team changed their goals and purpose for implementing the QDSC model. Their model was still capable of all its originally designed optimization strategy goals and met the assessed constraints in at least one of their two simulations, but the team manipulated the model and incorporated visualization to enable new perspectives in their two simulations. These changes along with the process of their development are further described in this section. The formation of the QDSC model through the MEA is explained first; followed by an explanation of how their model was transformed to enable its use in two simulations.

4.4.3.1 Team C's QDSC MEA

Throughout MEA Draft 1, Draft 2, and Final Response, Team C's QDSC mathematical model fully addressed the material constraints of there being a minimum of two grams of each material (*I-MAP* Item 2 in Table 4.13) and a total of 100 grams in the mixture (*I-MAP* Item 1 in Table 4.13). In MEA Draft 1, they set the material with the lowest toxicity or cost (depending on the mechanism used) to 92% and the other four materials to two percent. Their model implicitly assumed one percent was equal to one gram. The percentages of two materials (including the one that started at 92%) were altered to obtain the target band gap energy, while maintaining the total mixture at 100 grams and 2 grams of each of the other three materials. It was unclear in their model how the second material was chosen and how the two materials' amounts were altered. During Draft 1 peer feedback, one peer indicated this problem by stating, "No explanation was given to how the mathematical model optimizes the materials mass percentage." In MEA Draft 2 and Final Response, the team continued to fully address both of these material constraints. In the Final Response, the results incorporated more examples based on the data they generated for an assignment prior to this submission (i.e. Data Generation in Table 3.1). For the Final Response submission they also included a data file that they programmed their MATLAB® code to read so the user could easily change the given material data for the problem. (A peer recommended this coding change in feedback that they received before Draft 2.) These changes did not affect their score on the *I-MAP* Items, but they are examples of how the team began to make their mathematical model better prepared for handling QDSC materials with different properties and easier for their direct user to use their MATLAB® program.

Team C included both given equations in their MEA Draft 2 and Final Response, but only included one of them in their first submission (*I-MAP* Items 3 and 4). In MEA Draft 1, the team did not include nor discuss the use of the equation to calculate the band gap energy of quantum dot materials (*I-MAP* Item 3 in Table 4.13). The team did include the equation needed to determine the effective band gap energy (*I-MAP* Item 4 in Table 4.13), but did not describe how to apply this equation in their model with enough detail for the direct user to use it (*I-MAP* Item 5 in Table 4.13). In MEA Draft 2 and Final Response, the team fully addressed the inclusion of given equations and functionality of given equation (*I-MAP* Items 3-5 Table 4.13). The revised procedure began with calculations of the bad gap energy for each quantum dot material provided to implement in this requirement (refer to score change from Draft 1 to Draft 2 for *I-MAP* Item 3 in Table 4.13). The team also explained their procedure to obtain the desired bad gap energy in greater detail through clear sample calculations and steps (refer to score change from Draft 1 to Draft 2 for *I-MAP* Item 5 in Table 4.13).

Team C used a MATLAB® solve function for their optimization strategy in their first submission, but then revised their MEA to use a described non-iterative solution in their

MEA Draft 2. In MEA Draft 1, the team somewhat addressed the two required mechanisms for their QDSC model – one for minimizing cost and the other toxicity (*I-MAP* Items 6 and 7 in Table 4.13). Their models required the direct user to select the material with the lowest cost or toxicity (depending on the desired mechanism) and then identify the material that would have the "greatest impact" to raise or lower the effective band gap energy, as needed to achieve the target band gap energy. This step required the user to determine what "greatest impact" meant for their procedure. Then the team used a "solve function" in MATLAB® to determine the amount of each of the two identified materials to reach the desired band gap. The team did not explain how the MATLAB® solve function worked. Within their MATLAB® code it did use systems of equations, but the lack of explanation in their memo did not meet the MEA requirements. The four students that gave this team feedback on their Draft 1 submission focused primarily on their MATLAB® file. One of these students kept focusing on elements of their MATLAB® code that made their solution lengthy and stated their model needed to be "simple and elegant". One student gave two pieces of feedback that prompted the team to provide more details on how the MATLAB® code and written model were connected; this and the previous feedback (from this same student) about the lack of explanation for their material optimization were the only feedback that focused on the team's model in their written memo and potentially resulted in the team's changes seen in Draft 2.

For MEA Draft 2, Team C was further challenged and required to add a mechanism to minimize both cost and toxicity. Their revised procedure accounted for all three goals – minimizing cost only, toxicity only, and both (*I-MAP* Items 6 – 8 in Table 4.13). The team fully addressed the criteria for their models to minimize cost or toxicity only (*I-MAP* Items 6 and 7 in Table 4.13). From MEA Draft 1 to Draft 2, the team replaced the MATLAB® "solve function" with a clear procedure to solve a system of equations (refer to score changes from MEA Draft 1 to Draft 2 for *I-MAP* Items 6, 7, and 9 in Table 4.13). The team also more clearly explained the process by which the direct user could identify the materials to change to attain the target band gap energy for the mixture depending on the desired mechanism – no longer requiring the direct user to interpret "greatest impact". The team somewhat addressed the search space criteria by providing a non-iterative solution, but they did not discuss the effects of limiting the search space through a non-iterative solution (*I-MAP* Item 9 in Table 4.13). The team only somewhat addressed the criteria for their model to minimize both cost and toxicity because they did not have an option for user-input to set the weighting for the importance of cost versus toxicity (Item 8 in Table 4.13). Their minimize cost and toxicity model used the same method as their other models, but the user selected the material with the lowest value for cost times toxicity (rather than cost or toxicity only). There were no changes to the team's mathematical model in their Final Response.

It is common for TAs to focus their feedback on the *I-MAP* dimensions or rubric items on which a team has low scores. As the team did not have low mathematical model scores for MEA Draft 2 and Final Response, the TA's feedback focused on other dimensions. On MEA Draft 2, the TA gave the team feedback prompting them to clarify some components (share-ability), give more details about the problem context (re-usability), revise assumptions (re-usability), and provide more rationales (modifiability). On the

Final Response, the TA gave the team a perfect score on all of the *I-MAP* dimension items and provided no constructive feedback with only generic praise (e.g., "All good.").

4.4.3.2 Team C's QDSC Design Project

Team C approached implementing their QDSC model in two different ways in their simulations. Each simulation had a different approach of changing their features within the *Material Constraints*, *Given Equations Included*, *Given Equation Functions*, *Optimization Strategy*, and *Search Space* categories.

The Material Mixing simulation presented new opportunities beyond the original material constraints (i.e. *I-MAP* Items 1 and 2) and another perspective for the effective band gap energy – efficiency (i.e. *I-MAP* Items 4 and 5). This simulation enabled the user to select how many materials they want to use (i.e. 1 to 5 materials) with varying percentages (i.e. no minimum material constraint), as shown through the inputs in Table 4.14. The team added a new element to the effective band gap energy equation in this simulation. The team incorporated an equation to calculate the efficiency based on the calculated effective band gap energy (output in Table 4.14) in the simulation. The team removed the models to minimize cost, toxicity, and both, so this simulation did not enable any new functionality to this aspect of the QDSC model.

The QD Optimization Chart simulation maintained the same material constraints (i.e. *I-MAP* Items 3 and 4), optimization strategy of developed mechanisms (i.e. *I-MAP* Items 6-

8), and search space (i.e. *I-MAP* Item 9). This simulation modified the way of approaching the target band gap energy (i.e. *I-MAP* Item 5). Instead of presenting the user with a single total for the cost and toxicity, they allowed the user to visualize how the band gap energy affected the cost and toxicity for the results of the selected mechanism through their line graph (output in Table 4.15).

In Milestone 1, the team communicated the given project deliverables, function, criteria for success, constraints, possible stakeholders, and potential direct users for their simulation suite. The team selected undergraduate students subscribed to nanoHUB.org seeking further education about alternative energy sources as their direct user. The team then assumed the user would have an "adequate baseline of context about solar cells". The team went on to write, "… the simulations will be able to focus on more theoretical or mathematical relationships rather than background information as to what a solar cell is". The team received full points on the deliverable, so they did not receive any feedback on their understanding of the project or their potential direct user. In response to this lack of feedback the team explained in their M2 documentation, "Because all the feedback we received was positive, we are moving forward with M2 by generating our concepts for our deliverable exactly based on our description of our direct user."

As part of the team's submission for Milestone 1, the team members had an individual assignment in which they had to evaluate prototypical student-completed GUIs. Three out of the four students on this team completed this assignment. All three students correctly identified the GUIs that were demonstrations of interactive only (i.e. was not a model or a simulation), a black-box model (i.e. was a model, but not a simulation), and a simulation (i.e. was a model and a simulation). No student correctly identified the animated simulation; they each thought this was not an example of a model or a simulation when it was an example of a simulation. These three students demonstrated an understanding of when a model and simulation was present in the majority of the GUIs. Each student received auto-generated feedback on this assignment based on their individual responses, but the team did not refer to this feedback in their documentation of changes response.

For Milestones 2 and 3, the team generated and described 20 concepts for potential simulations and then evaluated these ideas through voting and lists of pros/cons to select four ideas for their four simulations, respectively. Out of the 20 proposed simulations, five were based on the QDSC model. One proposed simulation focused on the analysis of the cost over a period of time for the QDSC solar panel compared to a traditional solar panel. The team selected this simulation in Milestone 3, because the simulation would provide a visual graph, a "global scope" (i.e. the context would have global relevance), and "simple inputs" (i.e. the user interface would be simple and easy for an inexperienced user to navigate). A second proposed simulation would compare cost and toxicity of different material compositions that met the target band gap energy, while increasing the amount of cost to see how this can lower the toxicity. This concept was selected because the simulation would provide a visual graph, be based on the QDSC model, and allow a user to visually explore solar cell fabrication. The third simulation proposed would prompt the user to input a region of the U.S. and five QDSC materials and output the solar panel's cost, toxicity, and energy generated in that location over a day. This idea was not selected nor further considered in Milestone 3, since the majority of the team voted against this idea. The fourth proposed simulation would calculate various costs of QDSC mixtures with different effective band gap energies based on their minimized cost model. The team evaluated this concept in their Milestone 3 and decided not to select it because they explained it would not provide a visual graph nor compare alternative energies. The last proposed simulation would compare the amount of energy produced over time for the QDSC solar panel compared to a conventional solar panel. The team evaluated this concept in their Milestone 3 and determined not to select it because it did not provide information about the fabrication of solar cells and the inputs for the model were unclear. The team did not receive any model development related feedback on their Milestones 2 or 3 submissions.

For this team's Milestone 4 prototype, this team submitted one presentation showing and describing their simulation suite GUIs. Their presentation contained the two pertinent QDSC simulations that the team proposed and selected in Milestones 2 and 3, respectively. These simulation are called Materials Mixing and QD Optimization Chart. The inputs and outputs for each of these simulations were identified in their presentation slides and corresponding text.

The proposed Material Mixing simulation (Figure 4.20) would enable the user to investigate the cost of energy options (i.e. QDSCs, traditional solar cells, oil, and gas); the oil and gas options were added in the text description of this milestone and were not discussed as part of this proposed simulation in their previous milestones. The user inputs would be the five QDSC materials (represented by the five drop down menu images on the top-left in Figure 4.20) and the percentage composition of these (represented by white boxes to the right of each material selection in Figure 4.20). One type of output would be numerically displayed values for the QDSC solar panel option (i.e. cost, toxicity, and band gap energy based on 100 grams) and the traditional solar panel option (i.e. cost, toxicity, and band gap energy), which was going to be a fixed amount (two gray boxes in the bottom left of Figure 4.20). The other type of output would be a graph displaying the differences in costs over time for the different energy sources (represented by the white box with an x across it in Figure 4.20).

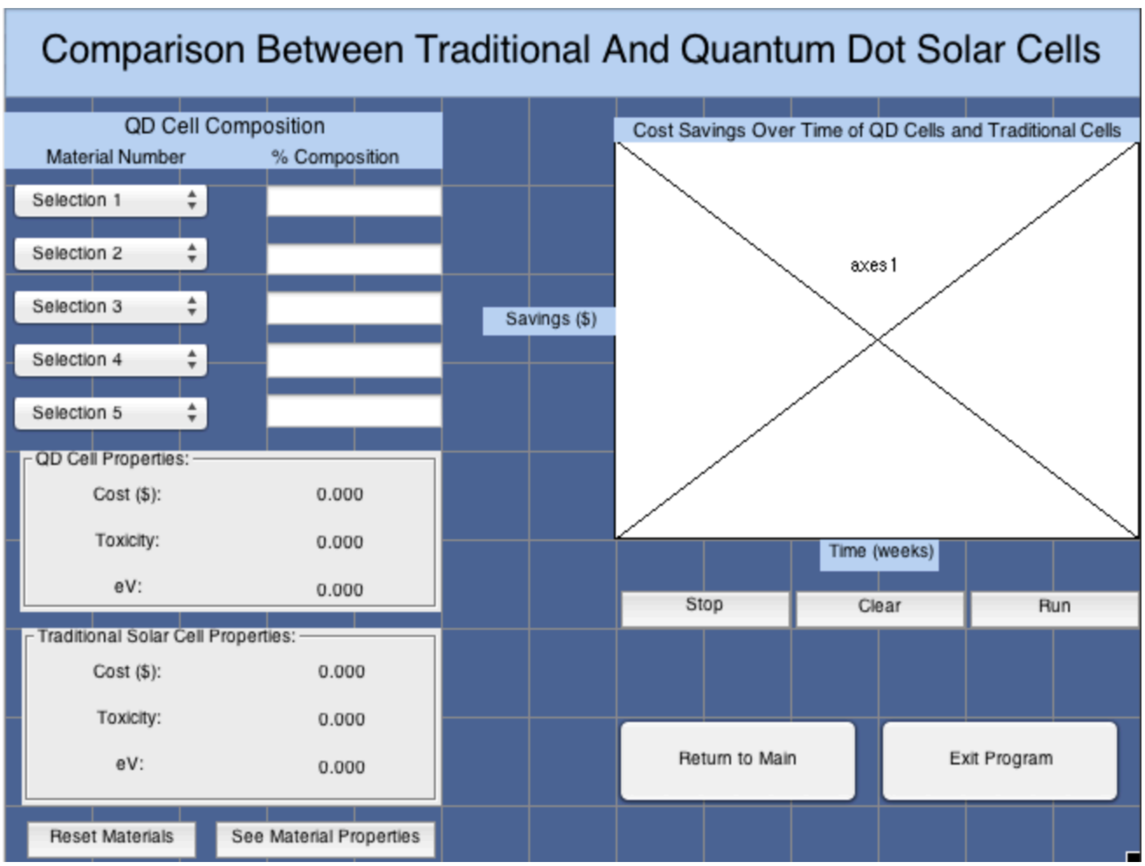

Figure 4.20. Team C's QDSC M4 Simulation Prototype – Material Mixing

The proposed QD Optimization Chart simulation (Figure 4.21) would enable the user to see the cost and toxicity of QDSC panels with different band gap energies. The inputs would require the user to select the five QDSC materials to mix (represented by the five drop down menu figures stating Material # on the top-right of Figure 4.21) and the type of model to use – either minimize cost, toxicity, or both (represented by the radio buttons in Figure 4.21). The output would show two X-Y plots that display cost and toxicity, respectively, for different target band gap energies (represented by the two potential graphs on the bottom of Figure 4.21).

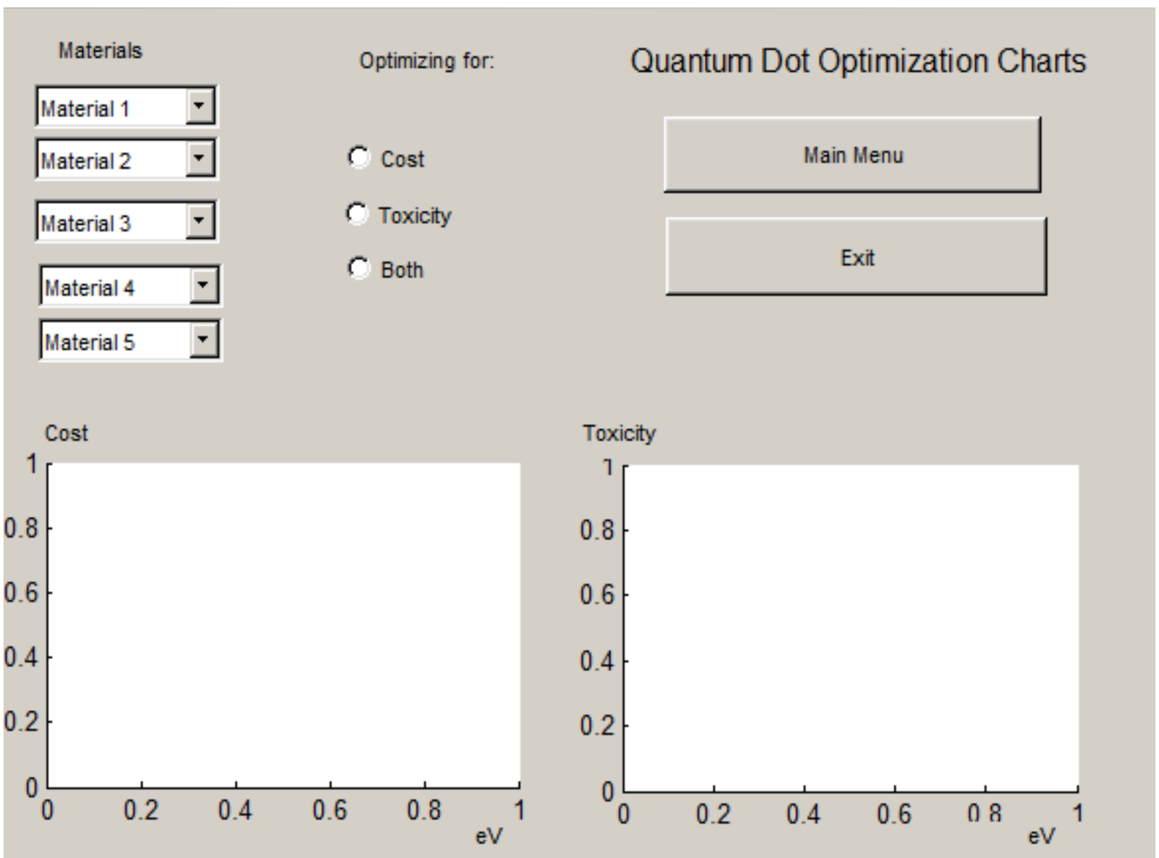

Figure 4.21. Team C's QDSC M4 Simulation Prototype – QD Optimization Chart

The team received feedback on their Milestone 4 that was mostly positive and summative. The only constructive feedback directly related to their simulations that they received was a suggestion to utilize slider bars instead of numeric inputs to increase ease of use.

In Milestone 5, both the Material Mixing and QD Optimization Chart simulations incorporated a slider bar in response to the received feedback. The context and output was also updated for the proposed Material Mixing simulation. For the proposed QD Optimization Chart simulation, only an updated image for the GUI was presented; there was no accompanying text to explain any of the GUI changes.

The proposed Material Mixing simulation (Figure 4.22) presented two context changes to (1) focus only on the comparison of traditional solar cells and QDSCs and (2) look at the cost of energy for a common household (represented by the two white boxes with an x across them in Figure 4.22).

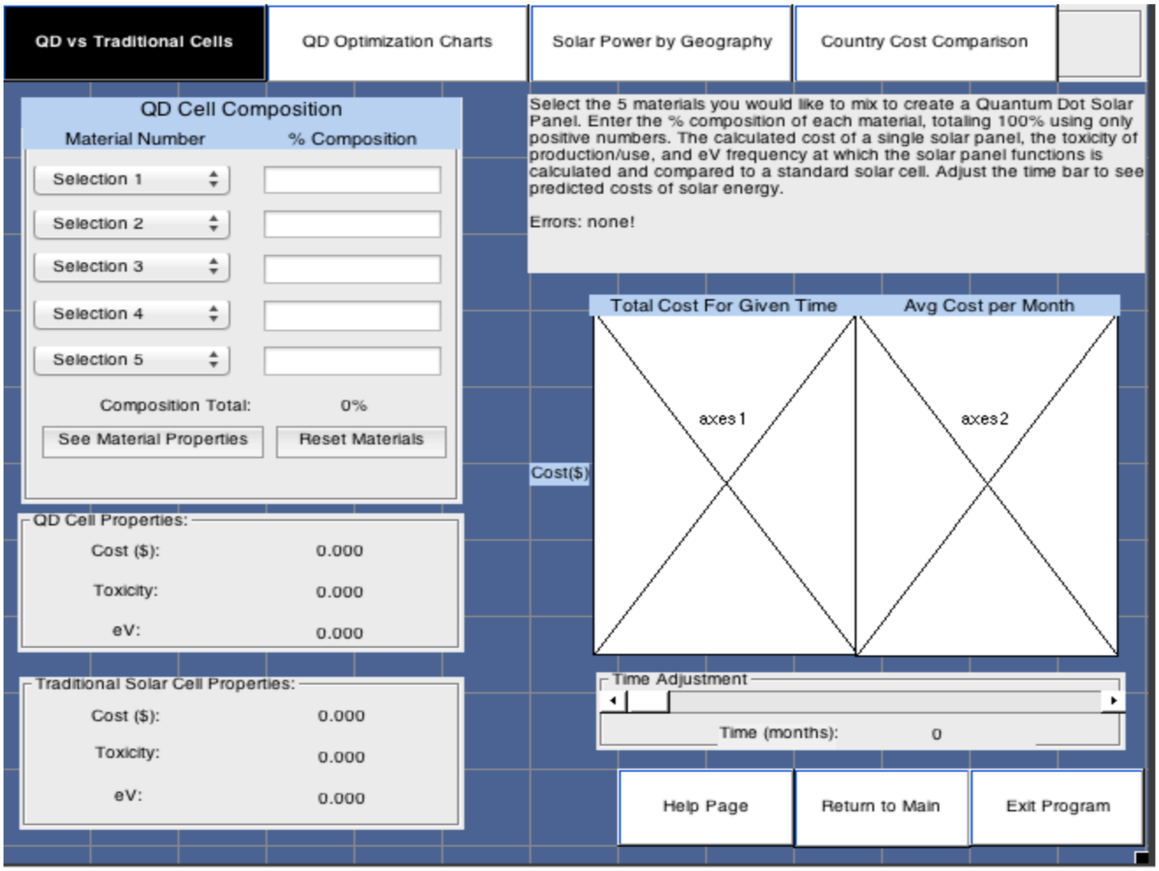

Figure 4.22. Team C's QDSC M5 Simulation Prototype - Material Mixing

The visual was changed from one graph to two graphs – one bar chart to compare costs for a user-input period of time and a second bar chart that compared the cost for one month of energy usage. The period of time was made into a new input that the user could control with a slide bar (see the slider bar at the bottom right of Figure 4.22). There was also some text added to the GUI prototype to better explain the simulation’s function and purpose (the gray box on the right of Figure 4.22).

The proposed Material Mixing simulation (Figure 4.23) incorporated a slide bar to change the band gap energy; the only text to help explain this was found on the prototype "help page" for this GUI. The slide bar was designed to change the target band gap energy and display a bar graph of the corresponding cost and toxicity. This GUI was identified as missing in the feedback from their TA – most likely because there was no additional text to explain the presented figures. The team noted that they would be more thorough in future submissions to ensure that all of their materials were submitted.

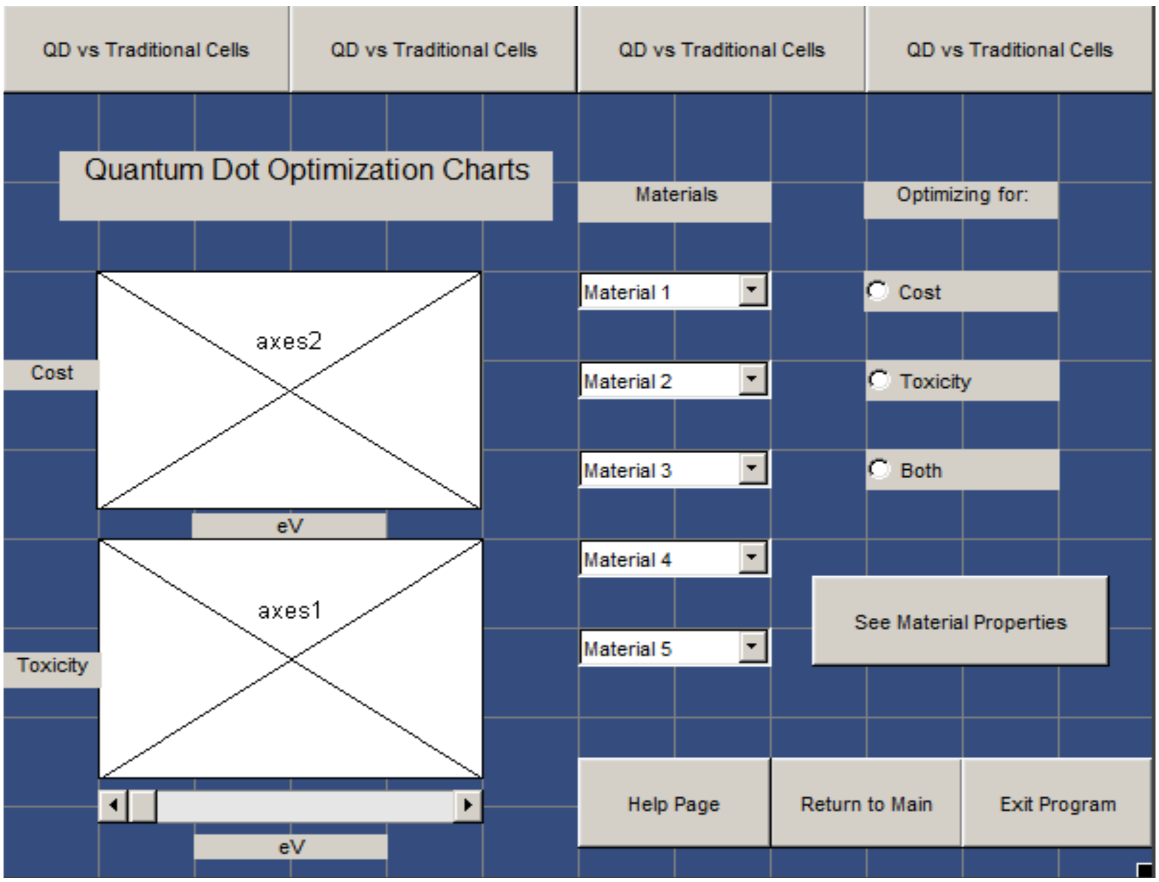

Figure 4.23. Team C's QDSC M5 Simulation Prototype - QD Optimization Chart

In Milestone 6, all the GUI layouts displayed in the previous presentation files as images were submitted as MATLAB® layouts. For this milestone, these GUIs were not required to and did not function. The Material Mixing simulation (Figure 4.24) was revised to no longer contain the traditional solar cell cost or property comparison. There was no indication that they had the necessary data or equations to code their previous ideas. There was also no discussion explaining this simulation change. There were no changes to the proposed QD Optimization Chart simulation.

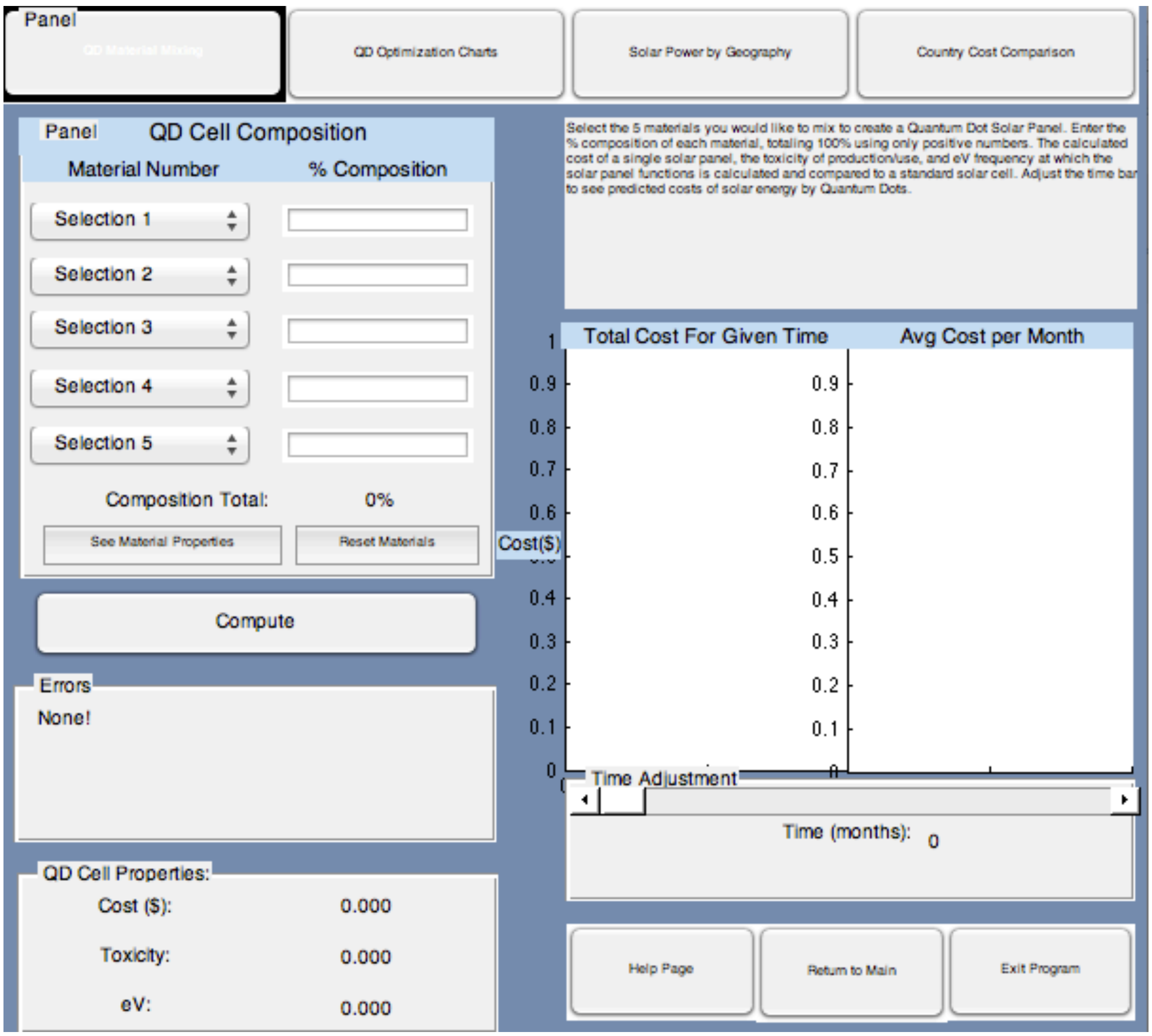

Figure 4.24. Team C's QDSC M6 Simulation Prototype - Material Mixing

In Milestone 7, the QDSC mathematical models to be run behind the GUIs were fully functioning, as required for this milestone. Between the two simulations all of the required equations were incorporated, the material constraints were still upheld, and the models in place were all coded.

The purpose of the Material Mixing simulation changed from investigating cost over time to displaying the material mixture composition, along with the efficiency of the manufactured QDSC panel (Eq. 2). The team did not explicitly state their source for this equation. In their comments they describe this equation as, “estimated parabola for the max efficiency based on eV”.

$$efficiency = 100\left(0.33 + \left(-.4 * \left(1.4 - (target\ band\ gap\ energy)\right)^2\right)\right) \quad (Eq. 2)$$

The simulation had the same inputs. The graphs no longer displayed cost relative to time; it presented a bar chart of the material composition (%) and the efficiency of the mixture (%) (in Figure 4.25). The numerical textbox outputs still displayed the cost, toxicity, and effective band gap energy of the mixture, as previously discussed.

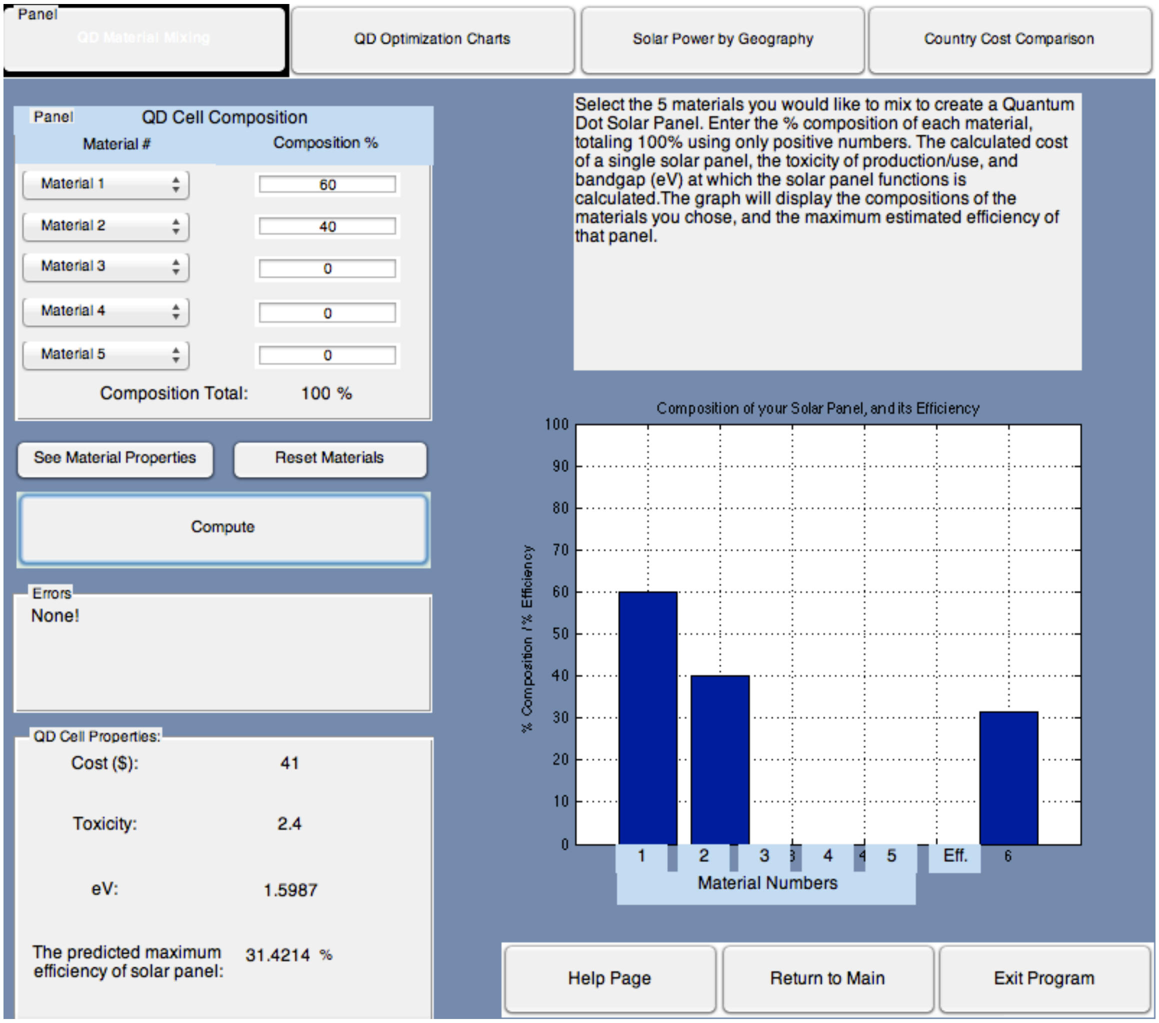

Figure 4.25. Team C's QDSC M7 Simulation – Material Mixing

The QD Optimization Chart simulation (Figure 4.26) was unchanged beyond the updated functionality required for this milestone.

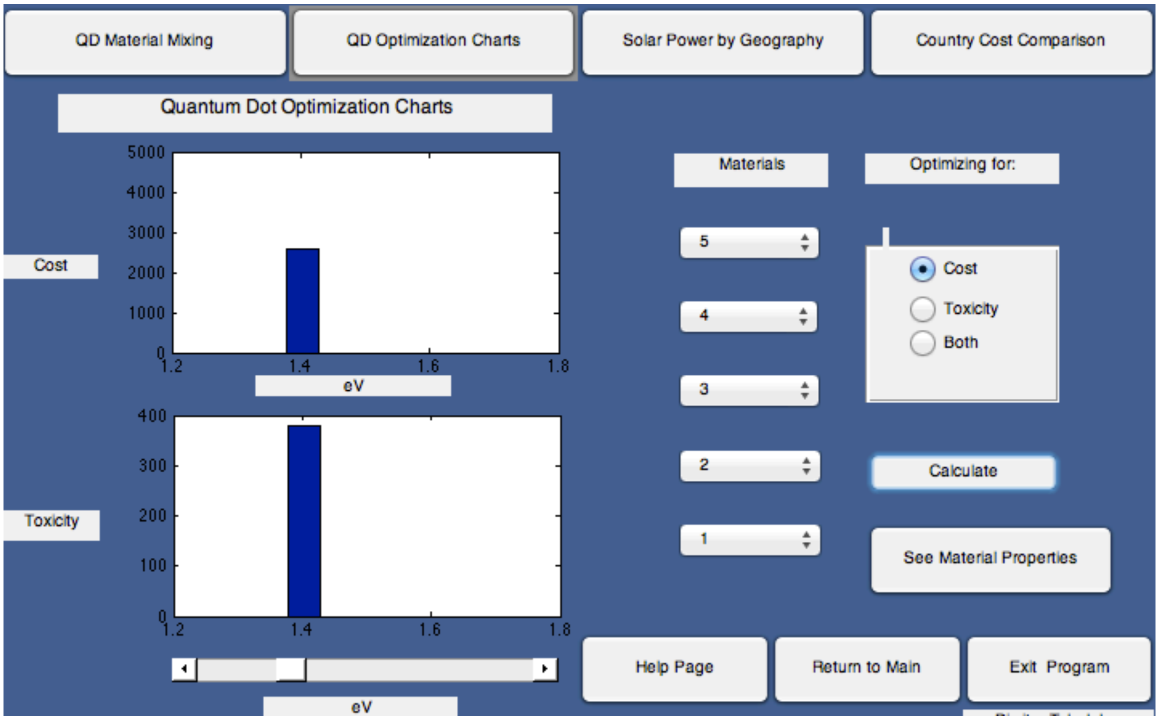

Figure 4.26. Team C's QDSC M7 Simulation – QD Optimization Chart

For Milestone 8, there were no major changes in the Material Mixing simulation and some changes to the inputs and outputs for the QD Optimization Chart simulation. For the Material Mixing simulation, the layout was slightly modified, but all of the content was the same. This simulation looked exactly like the one submitted for Milestone 9 (Figure 4.28) without the learning objective in the top right corner. The slide bar in the QD Optimization Chart simulation (Figure 4.27) was removed and instead the line graph was used to display the cost and toxicity for the optimized material composition for all possible effective band gap energies, as originally proposed in Milestone 4.

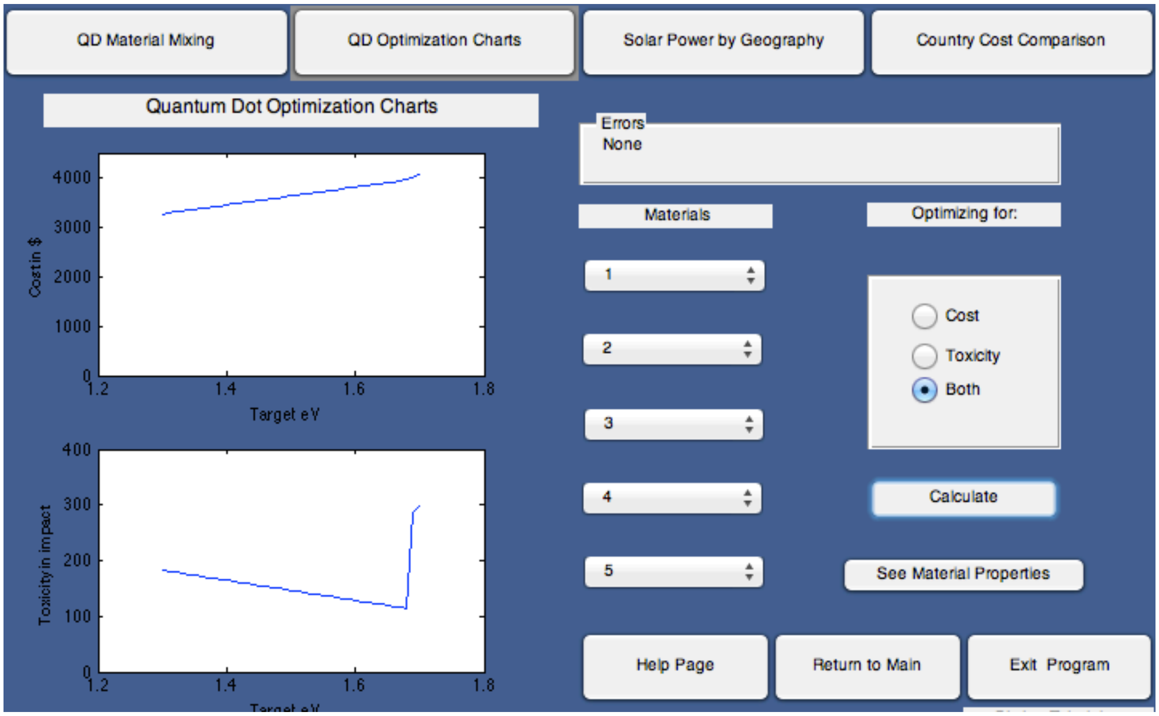

Figure 4.27. Team C's QDSC M8 Simulation – QD Optimization Charts

The team received feedback from a nanoHUB representative on Milestone 8 that prompted them to create a consistent, professional, and user-friendly format across the simulation suite. No feedback targeted the underlying models.

In Milestone 9, the team had the same underlying models for both QDSC simulations, as the previous milestone. The Material Mixing simulation (Figure 4.28) was slightly modified, incorporating the learning objective textbox seen in the top left corner.

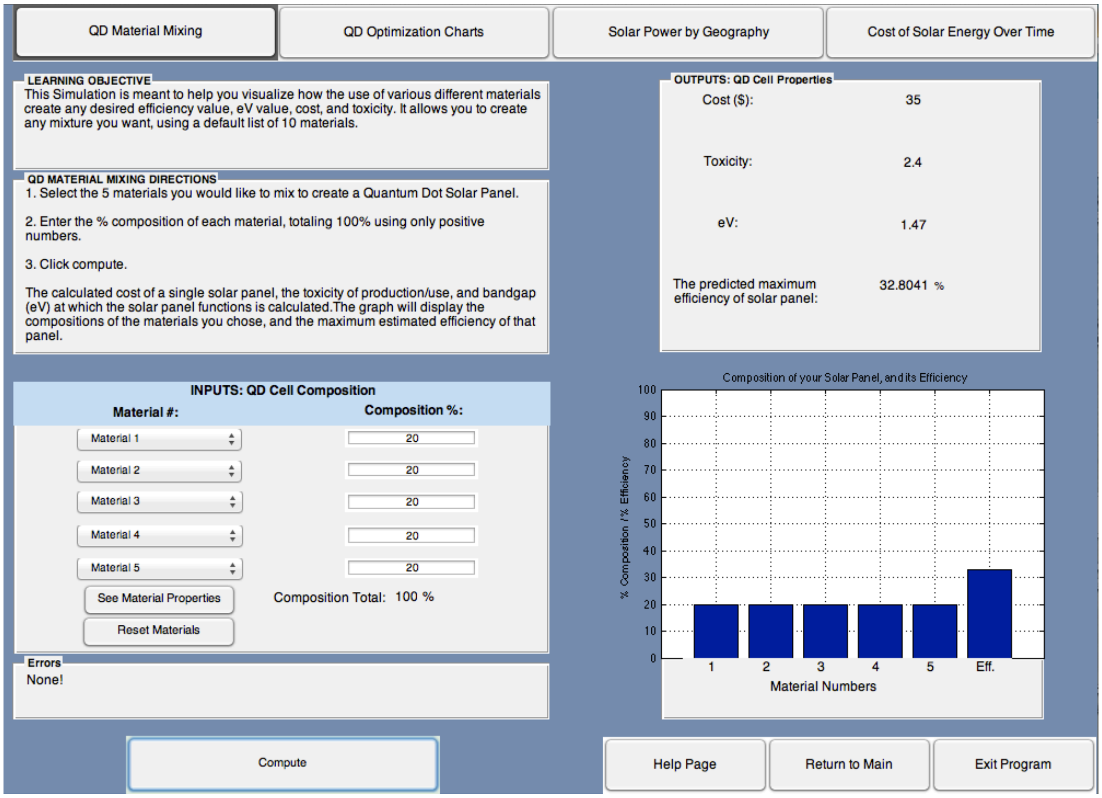

Figure 4.28. Team C's QDSC M9 Simulation – Material Mixing

The QD Optimization Chart simulation (Figure 4.29) had an updated layout to match the Material Mixing layout and format. The simulation contained a learning objective, directions, an updated color scheme, and repositioned content. The inputs, outputs, visualization, and underlying model were the same for Milestone 8.

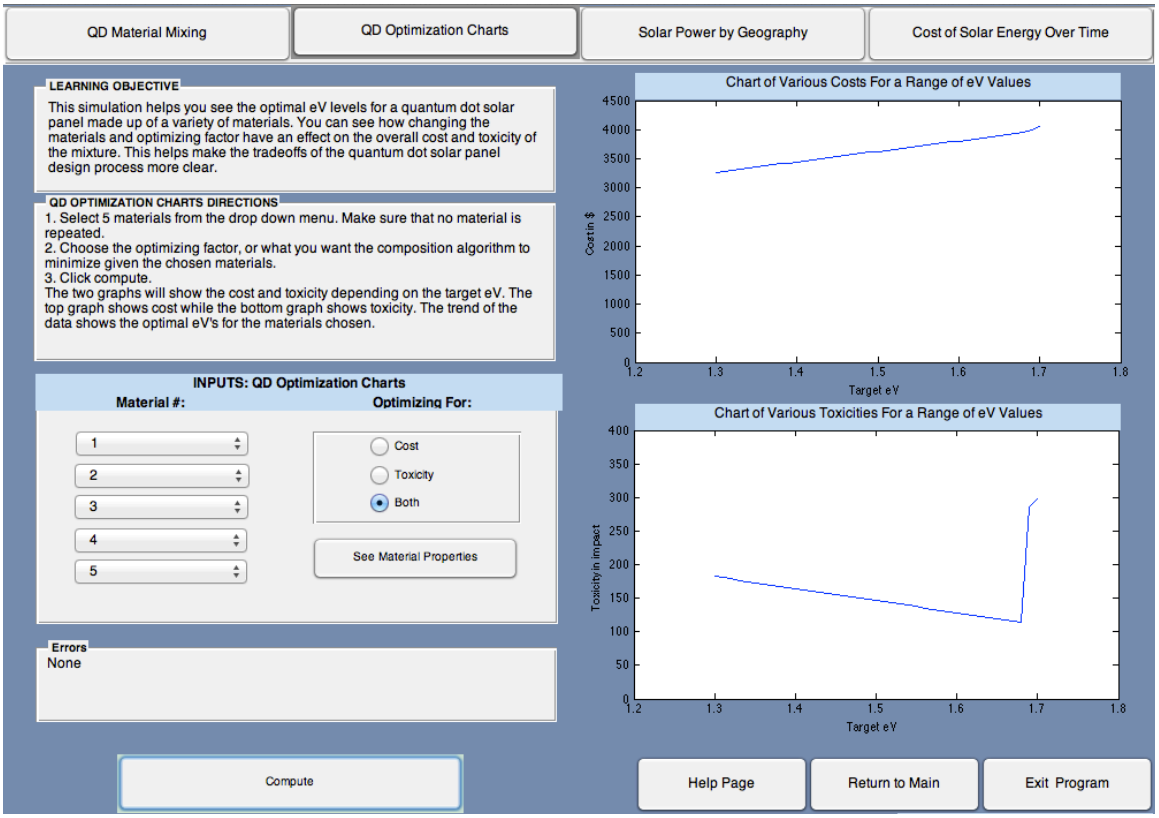

Figure 4.29. Team C's QDSC M9 Simulation – QD Optimization Chart

The input and output variables for their QDSC model within their MEA and two simulations are shown in Table 4.14 and Table 4.15. The inputs and outputs stayed constant through the MEA since this was a requirement, but the input options for the 5 QDSC Material input varied across the submissions (i.e. only 5 given materials in Draft 1, 10 given materials in Draft 2, and 12 possible materials in the Final Response). These are described at the beginning of all four tables.

Table 4.14 shows the input and output variables of the QDSC Material Mixing simulation. The material composition was an output in the MEA version of the model, but this was an input throughout their simulation version of the model. This meant the type of model to use (i.e. minimize cost, toxicity, or both) was no longer a component of the model in the simulation. In relation to this, the effective band gap energy became an output throughout the simulation – it was no longer an input, as it was in the MEA. The model still output the total cost and toxicity throughout the simulation, like the MEA. Unlike the MEA, the material mixture did not have a minimum percentage requirement for each material so the final material composition could consist of between 1 and 5 different QDSC materials. These pertinent inputs (i.e. 5 QDSC materials and Mixture composition) remained the same throughout all of the milestones. This transformed the function of the model from finding a material composition for a target band gap energy and based on criteria (i.e. minimize cost, toxicity, or both) to calculating the band gap energy for a given material composition.

The outputs of this simulation (other than the constant effective band gap energy, total cost, and total toxicity) changed across their milestones. These various outputs required the addition of another equation to the transformed QDSC model. The original output proposed in Milestone 4 would compare the cost of the QDSC solar panel to the cost of traditional solar panels, oil, and gas over time. This was changed to only compare the cost of the QDSC solar panel to the cost of traditional solar panels over time in Milestone 5. In Milestone 6, the output only presented the cost of the QDSC solar panel over time. For two milestones (i.e. Milestones 5 and 6) the Material Mixing simulation incorporated a time input (relevant to the alternative goal of the simulation), but this was discontinued in Milestone 7. In Milestone 7, the cost analysis over time was dropped completely and a new calculation was incorporated – efficiency. This was an output throughout the remainder of the milestones.

Table 4.15 tracks the input and output variables of the QDSC Optimization Chart simulation. Throughout all six milestones, this simulation had the same 5 QDSC Materials and Type of Mechanism inputs. These were two of the three inputs for the MEA version of the QDSC model. Milestones 4, 8, and 9 had the third input from the MEA (i.e. Target band gap energy) as an output (i.e. Effective band gap energy). The function of the model was changed from finding a mixture for a target band gap energy to finding every mixture and visually presenting the potential costs and toxicities for different band gap energies. In Milestones 5 through 7 the team reverted the QDSC model back to the same model developed in the MEA, where the target band gap energy was an input.

Table 4.14. Team C's Variables for QDSC Simulation – Material Mixing

Sub.	Input	Possible Inputs	Output
MEA FR	5 QDSC materials Target band gap energy Type of mechanism	12 possible (preset) materials 1.33 ev or 1.65 ev Min. cost, toxicity, or both	QDSC material mixture composition (%) Total cost and toxicity
M4	5 QDSC materials Mixture composition (%)	10 potential (preset) materials 0 – 100% per material, 100% total	Graph of savings vs. preset time (compare QDSC mixture, gas, oil, and traditional solar) Total cost and toxicity Effective band gap energy
M5	5 QDSC materials Mixture composition (%) Period of time	10 potential (preset) materials 0 – 100% per material, 100% total no range stated	Graph of savings vs. preset time (compare QDSC mixture and traditional solar) Graph of savings vs. user-input time (same) Total cost and toxicity Effective band gap energy
M6	Same as M5	Same as M5	Graph of savings vs. preset time Graph of savings vs. user-input time Total cost and toxicity Effective band gap energy
M7	5 QDSC materials Mixture composition (%)	10 potential (preset) materials 0 – 100% per material, 100% total	Total cost and toxicity Effective band gap energy Efficiency
M8	Same as M7	Same as M7	Same as M7
M9	Same as M7	Same as M7	Same as M7

Table 4.15. Team C's Variables for QDSC Simulation – QD Optimization Chart

Sub.	Input	Possible Inputs	Output
MEA FR	5 QDSC materials	12 possible (preset) materials	QDSC material mixture composition (%)
	Target band gap energy	1.33 ev or 1.65 ev	Total cost and toxicity
	Type of mechanism	min. cost, toxicity, or both	
M4	5 QDSC materials	10 potential (preset) materials	Line graph of effective band gap energy vs. cost
	Type of mechanism	min. cost, toxicity, or both	Line graph of effective band gap energy vs. toxicity
M5	5 QDSC materials	10 potential (preset) materials	Total cost and toxicity
	Type of mechanism	min. cost, toxicity, or both	
	Target band gap energy	no range stated (possible range dependent on mixture)	
M6	Same as M5	Same as M5	Same as M5
M7	Same as M5	12 potential (preset) materials	Same as M5
		min. cost, toxicity, or both	
		range dependent on mixture	
M8	5 QDSC materials	10 potential (preset) materials	Line graph of effective band gap energy vs. cost
	Type of mechanism	min. cost, toxicity, or both	Line graph of effective band gap energy vs. toxicity
M9	Same as M8	Same as M8	Same as M8

CHAPTER 5. DISCUSSION

The ability to understand, use, and build models and simulations are fundamental skills that underlie all of engineering (Carberry & McKenna, 2014; Zawojewski et al., 2008). Although the development and use of models and simulations are implemented in engineering curriculum, it is rarely explicitly taught (Carberry & McKenna, 2014). Some research within the M&MP and CADEX framework investigated students' abilities to develop modeling skills (Lesh & Doerr, 2003; McKenna, Linsenmeier, & Cole, 2011). This study used the M&MP as a theoretical framework to further investigate the development of mathematical modeling skills. This study considered the CADEX framework to begin to investigate students' development of simulations. There is a need to continue this research with emphasis on further exploring the development of students' understandings of models and simulations. This study focused primarily on students' development of mathematical models.

Research within the M&MP focused on the development of students' mathematical modeling skills through activities to develop (i.e. MEAs), apply (i.e. model-exploration activities), and repurpose (i.e. model-adaptation activities) mathematical models (Lesh & Doerr, 2003). These efforts began and are still continued in mathematics education research. The identified need to develop modeling skills in engineering and the opportunity this research in the M&MP presented for engineering was recognized. Research around model development, specifically MEAs, was transformed within engineering education research (Hamilton t al., 2008; Zawojewski et al., 2008).

There has been little research around the use of model-adaptation activities within mathematics education and even less within engineering education. In this study, the investigation into a type of model-adaptation activity began to address this need and the need to explicitly teach simulation development. How students' mathematical models changed through a challenge to create a simulation based on a model developed through a MEA was the focus of this study.

In the first research question, the nature of the teams' mathematical models upon completion of their MEA and their simulation design project was investigated. These findings focused on the 122 teams' MEAs and design projects (Section 5.1).

In the second research question, how students' mathematical models changed from the MEA through simulation development was explored. The findings from the analysis of the 122 teams' projects through the *I-MAP* are briefly discussed to highlight some changes (Section 5.2). The majority of changes discussed are related to the case study of the three teams (Section 5.2).

In the third research question, types of feedback that influenced changes in students' mathematical models was investigated. Through the case studies it was found that the teams received little feedback on their design projects related to their simulations or underlying models, so external factors (e.g., requirements for the project and submissions) and internal factors (e.g., self-assessment, teaming) that may have impacted teams' changes are discussed (Section 5.3).

Implications for practice (Section 5.4), implications for nanoHUB (Section 5.5), future research (Section 5.6), and limitations (Section 5.7) of this study are also discussed. There is more discussion about the differences across sections, the nature of simulations, the nature of the projects implemented, and methods used in this study in these sections.

5.1 Research Question 1 – Nature of Mathematical Models

The QDSC models were required to meet the *I-MAP* criteria throughout the MEA. The QDSC models within the design projects were only required to be present; this was assessed in some sections, but as presented in the findings and further discussed in the implications for practice (Section 5.4) many sections did not enforce this project requirement. The *I-MAP* criteria for a mathematical model that fully addresses the complexity of the problem was used to assess the QDSC model at the end of the MEA and design project to understand and then compare the nature of the mathematical models.

The student teams were required to meet two given material constraints in the MEA: (1) the mixture equaled 100 grams (*I-MAP Item 1*) and (2) each of the materials in the mixture contained at least two grams (*I-MAP Item 2*). Based on the QDSC *I-MAP* assessment, all 122 teams fully addressed the criteria for the *Material Constraints* category within their MEA. These findings showed that the students could easily embed these constraints in their models. Upholding clearly communicated constraints proved easy for students. Students typically struggle more with projects and specifically MEAs because of the embedded ambiguity (Diefes-Dux et al., 2008). This was one aspect of their model that had a single right answer and all of the student teams ensured their model contained these constraints.

The teams were required to utilize two given equations in the MEA: (1) the band gap energy for quantum dot materials equation (*I-MAP Item 3*) and (2) the target or effective band gap energy equation (*I-MAP Item 4*). Although this was also not very ambiguous, some teams struggled with this requirement. Both of the equations were fairly simple in terms of mathematics, but the quantum dot nanotechnology context was probably more complex than the students were familiar with. Many students and instructors may have not had previous experience with nanotechnology concepts prior this class. Based on the QDSC *I-MAP* assessment, the majority (70 teams) of the 122 teams fully addressed the criteria for the *Given Equations Included* category on the MEA. The majority of the teams that did not fully address the criteria used the equations, but did not sufficiently communicate them in their MEA. The underlying problem appeared to be a lack of written communication and not a lack of implementing the given equations in the teams' models. This challenge of communicating one's own thoughts is embedded in the MEA and it is important that the instructors give feedback to teams targeting this aspect of model development to help them improve their written document. The *model-*

externalization principle ensures students are challenged to communicate and reflect on their thought process in model development (Lesh et al., 2003; Lesh et al., 2000). Since some teams were unable to communicate this portion of their model, they did not had as much opportunity to reflect on their corresponding thought process. Instructors must understand that this written document enables teams to reflect on their thought process and must prompt students to improve their communication through constructive feedback.

In relation to the effective band gap energy equation, the teams were also assessed on their ability to implement this equation in their QDSC models (i.e. *I-MAP Given Equation Functions* category, *I-MAP Item 5*). The majority of the teams (83 teams) fully addressed the criteria for this category in their MEA. These teams demonstrated enough understanding to both use the equation and communicate how to use the equation. The teams that did not communicate how to use the equation may not have fully understood the equation and how they applied it or they may have just lacked the ability to effectively communicate to someone else how to use it in their MEA. The examples where teams provided supplemental files showing how they used the equation showed they were capable of implementing it, but again struggled with the *model-externalization principle* that required them to communicate their work. The one team that did not implement the equation in their QDSC model did not display an ability to understand the simple mathematics embedded in the problem. This particular team's struggle was an outlier and does not reflect that the MEA was too complex. The required mathematics were determined appropriate for the students through the creation of the QDSC MEA and application of the *simple prototype principle* (Rodgers et al., 2016; Lesh et al., 2000).

The greatest struggle for the teams was demonstrated in the assessment of teams' optimization strategies used to develop the three required mechanisms (i.e. *I-MAP Optimization Strategy* category). This part of the MEA had the greatest amount of ambiguity. The *Optimization Strategy* category presented an open-ended challenge with criteria that helped the teams judge the quality of their models, aligning with the *self-evaluation principle* (Rodgers et al., 2016; Lesh et al., 2003; Lesh et al., 2000). Minimizing the cost (*I-MAP Item 6*), toxicity (*I-MAP Item 7*), or both cost and toxicity (*I-MAP Item 8*) and limiting the search space (*I-MAP Search Space* category, *I-MAP Item 9*) were the primary criteria used to judge the models. The *Optimization Strategy* category composed the majority of the unique components of the teams' QDSC models.

There were two major categories of solution types: (1) non-iterative and (2) iterative. The non-iterative models identified two equations (i.e. the sum of the materials equaled 100 grams and the effective band gap energy equation equaled the target band gap energy), limited the changing materials to two to create only two unknown variables, and used the system of equations to find both unknown variables to calculate the final QDSC mixture. The iterative models used some system to test all possible combinations (most commonly looping structures in MATLAB®) by changing the percentages of different materials (most commonly only changing two materials) and then used some created criteria to select a final QDSC mixture.

The teams typically had two approaches for selecting the material composition with lowest cost or lowest toxicity (depending on the mechanism used): (1) first select two materials with the lowest cost or lowest toxicity (with one above and the other below the target band gap energy) to change and set the rest to two grams or (2) calculate the cost and toxicity for every possible combination and then select the one with the lowest cost or lowest toxicity.

The first approach of material selection was most common in teams' models. For non-iterative models, the teams that used the first approach used systems of equations to solve the two unknowns once the materials were identified. These solutions had the most limited search space possible (i.e. *I-MAP Search Space* category). For iterative models, the first approach required the user to calculate the band gap energy for every combination and then identify one with the target band gap energy.

For non-iterative models using the second material selection approach, the team would use their systems of equations approach to calculate the cost and toxicity for all possible material combinations (up to 10) and then select the ideal combinations. For iterative models using the second material selection approach, there were a variety of answers involving changing different numbers of materials at once and a variety of approaches to do this. These solutions were typically the poorest at addressing the need to limit the search space (i.e. *I-MAP Search Space* category).

The majority of QDSC models for minimizing both cost and toxicity looked the same as the teams' models for minimize only cost or only toxicity. The one major difference in their optimization strategy for this mechanism was that a few teams developed a user-input weighting that enabled the user to establish their own level of importance of cost compared to toxicity.

The greatest variation between the mechanism to minimize both cost and toxicity and the others (i.e. minimize cost only or toxicity only) was how to select the material or total values with the minimum cost and toxicity. Most teams created some type of cost-toxicity factor. The teams' MEA solutions presented a variety of different approaches for developing a cost-toxicity factor. One common factor involved adding cost and toxicity, which would require adding together two values with different units and ranges of values. Another common factor involved the multiplying cost and toxicity, which also does not acknowledge their different units. There were also a variety of factors that involved the teams developing a procedure to make cost and toxicity dimensionless to add or multiply these resulting values together, which better acknowledged that cost and toxicity have different units. Understanding units is an important component of mathematical model development (Lesh & Doerr, 2003) that these findings show many students struggle with. It is important that throughout engineering students' education instructors continue to emphasize the importance and meaning of units. Some teams created cost-toxicity factors that were also dependent on the materials' band gap energies to determine the potential impact of individual QD materials on the target band gap energy in the QDSC mixture.

When the teams adapted their QDSC models into simulations through the design project, the nature of the QDSC models had much more variation in solutions. Some teams maintained the same requirements and goals from the MEA in their design project. Some teams decided to no longer adhere to the MEA requirements and criteria to completely repurposed their model. Most teams had some middle of the road approach that still used the majority of the requirements and criteria of the MEA, but focused more on one component of the model that they selected (e.g., one mechanism, a given equation).

In their underlying QDSC model for their simulations, the majority of teams (88 teams) fully addressed the criteria for the *I-MAP Given Equation Functions* category (i.e. the ability to successfully implement the effective band gap energy equation in their QDSC model). Some teams implemented the effective band gap energy equation in the same way in their simulations as they did in their MEAs. Some teams changed the purpose for implementing the effective band gap energy equation. Some teams used the equation to calculate the effective band gap energy of various QDSC material composition input by the user; these teams removed the optimization strategy components from their original QDSC Model. These types of simulations only used given equations for their underlying models and no longer presented students with the opportunity to further explore development of their own model.

As previously explained with the freedom to repurpose their QDSC model, teams included any combination of none to all the three original mechanisms from the MEA (i.e. minimize cost only, toxicity only, or both). In their simulations, the majority of teams that implemented a model to enable a mechanism or models to enable mechanisms somewhat addressed the criteria for the corresponding *I-MAP Item* from the *I-MAP Optimization Strategy* category. This meant the majority of teams used an iterative solution that used for or while loops in their MATLAB® code. The types of QDSC models related to these mechanisms were the same types found in the teams' MEA solutions. The same types of teams' approaches also meant the same range of ways the teams addressed the search space. Many teams still were not seeing the importance of more efficient programming by decreasing the number of iteration in looping or using non-iterative solutions. This was evident in the amount of time it took some of the teams' programs to run. Team A's MEA Final Response presents an example of a team that did not limiting the search space in their model and it resulting in an inefficient code (Section 4.4.1.1).

5.2 Research Question 2 – How Mathematical Models Changed

With a better understanding of the types of models students submitted in their MEAs and design projects, the changes that happened in teams' models across the projects are further explored in this section. This discussion begins with a big-picture perspective based on the findings of the changes in the 122 teams' models and then a more in-depth viewpoint based on the changes found in the case study teams' models.

Although the findings showed that across the 122 teams the teams' average scores decreased across all *I-MAP* categories, further investigation showed that the majority of the decrease in the teams' scores was due to teams not continuing different components of their QDSC model from their MEA in their simulations. Upon further investigation, the teams' average scores even increased for some categories when only comparing teams that included the relevant *I-MAP Items*. These resulting scores were fairly similar from the MEA Final Response submission to the Milestone 9 design project submission.

The analysis of the 122 teams based on the *I-MAP* highlighted a few differences for the *Given Equation Functions*, *Optimization Strategy*, and *Search Space* categories.

Due to either the change in the mode of communicating their model or the need for the effective band gap energy equation to function in their simulation, seven more teams fully addressed the criteria for the *Given Equation Functions* category (*I-MAP Item 5*) in their simulation than their MEA. As discussed in the previous section (Section 5.1), teams struggle with written communication and the design project no longer required teams to communicate through written text how to implement the equation; the design project tested only students ability to make the implemented equation function. The design project changed how the *model-externalization principle* was addressed and enabled them to reflect on their thought process form a different perspective.

Based on the teams' developed models, there were the same variations in the types of optimization strategies used in the MEAs and the design projects. Team A in the case study presents an uncommon case where a team improved their optimization strategy for minimizing cost or toxicity only by going from an iterative solution in the MEA to a non-iterative solution in the design project. A few teams regressed the optimization strategy for minimizing cost or toxicity only in their models by programming an iterative solution in their simulation rather than the non-iterative solution that they presented in their MEA. The course material in ENGR 132 focuses on how to code for loops, while loops, and complex loops in MATLAB® for three weeks (see Appendix A) and the teams may have felt compelled to use this knowledge in their design projects. Teams may have also been more comfortable with coding loops and decided to change their model based on their knowledge of programming. Either way, this is an example of how some teams developed lower-quality models in the design project than the MEA. It was more common for teams to improve their optimization strategy for minimizing both cost and toxicity in their design project. There were more teams that developed and implemented the idea to allow the user to input their own importance of cost compared to toxicity for the model to minimize both in the design project than the MEA. Developing a simulation may have prompted the teams to think about user interaction more and possibly led more teams to think more creatively about how to engage their user. User interaction is a fundamental component of simulation development (Alessi, 2000).

Due to the changed requirements from the MEA to the design project, the teams were not required to document their model for the simulations. This meant that no teams discussed the need to limit their search space in their simulations, although only 19 teams did this in their MEA Final Response submissions. The other changes related to the *I-MAP Search Space* category were based on the changes to the teams' optimization strategies.

The changes in the mathematical models through their simulation development was made much more evident in the case studies. These changes present opportunities for teams to explore their mathematical models from different perspectives and develop higher-quality models. The major lenses used to describe the change of the mathematical models through the design projects were: (1) the *I-MAP* categories and (2) the changing input and output variables. The changes to input and output variables helped better identify what was happening in the underlying model through their simulation development. This discussion focuses on the changes made within different *I-MAP* categories and the opportunities they may present.

Pertinent to the *I-MAP Material Constraints* category, Teams B and C enabled new exploration of the model beyond the original constraints.

Team B enabled the user to input any QDSC material that they wanted. This made their model much more modifiable by allowing the user to evaluate any QDSC material they wanted. Team A presented a similar idea in their first prototype of their QDSC Model simulation, but did not continue this idea in their final simulation. This idea of developing mathematical models that can handle different data sets is important in MEAs, but many teams struggle with this (Diefes-Dux et al., 2010; Lesh & Doerr, 2003; Zawojewski et al., 2008). The MEA sequence involves giving students different sets of data throughout the submissions to ensure the teams develop models that can adapt to them. Team B went above and beyond on this aspect by creating a model that contained preset materials and allowed the user to put in up to five QDSC materials of their own. This simulation development may have presented this team with a platform where they could understand the need for addressing modifiability in their model. Continuation of model development through building a simulation may further promote the *model generalization principle* (Lesh et al., 2003; Lesh et al., 2000).

Team C enabled the user to select the number of QD materials (i.e. 1 to 5 materials) to include in their final QDSC mixtures with varying percentages (i.e. no minimum material constraint) in their Material Mixing simulation. This development enabled the team to explore their mathematical model with a different perspective, potentially giving the team a better understanding of their model and opportunities of further modification. This is another example of how the design project enabled a team to further address the *model generalization principle* (Lesh et al., 2003; Lesh et al., 2000). Team B also presented a variation to the original material constraints in their Material Mixing simulation, but did not add as much modifiability to their model. They changed the minimum material constraint of two grams per a QDSC material to one gram per a QDSC material.

Pertinent to the *I-MAP Given Equation Functions* category, Teams B and C enabled new exploration of the model beyond the original constraints.

Both Teams B and C repurposed the way they used the effective band gap energy equation in their Material Mixing simulations. They used the equation to calculate the effective band gap energy of a material composition instead of creating a material composition for a target band gap energy. This repurposing removed the need for the optimization strategy in their underlying models, but may have enabled the teams to better understand the given equation.

Team C also added an additional equation to their band gap energy equation in their Material Mixing simulation. The program added an equation to calculate the efficiency based on the calculated effective band gap energy. This demonstrated the team’s ability to see new applications and connections beyond the original equations and model.

In Team C's QD Optimization Chart simulation, they removed the original goal of finding a material composition for a target band gap energy. Instead they presented two line graphs – one that compared the different costs for different effective band gap energies and another that compared the different toxicities for different effective band gap energies. This enabled the team to visualize how the selection of different target band gap energies impacts the minimum costs and toxicities possible. These visuals and this exploration gave the team a new perspective of their QDSC model. This team's exploration of their model by changing a singular output to a linear output may have presented their model in a more meaningful and memorable manner. A goal of the *simple prototype principle* is to ensure the mathematics used are memorable to students (Lesh et al., 2003; Lesh et al., 2000).

Pertinent to the *I-MAP Optimization Strategy* category, Teams A and B both improved their ability to address the criteria through their simulation development. Pertinent to the *I-MAP Search Space* category, Team A minimized their search space and Team B developed a model that further disregarded the need to minimize their search space.

Team A improved the optimization strategy for their minimize cost only and toxicity only mechanisms in their QDSC Model simulation. The team changed their model from a solution that iterated through every possible material combination with two changing materials to a non-iterative solution using systems of equations. The time spent exploring their QDSC model through simulation development may have enabled the team to better understand their model and improve their optimization strategy. There is no clear explanation as to why this team improved this aspect of their model in their design project. The team did not do much exploration beyond the MEA challenge, but the team did develop a higher-quality model through their design project. MEAs are designed to ensure that all teams can succeed (Zawojewski et al., 2008) and this team's examples shows potential for this linked designed project to further this goal.

Team B presented an idea to improve the optimization strategy used in their model for minimizing both cost and toxicity in their QDSC Weighted Model simulation by enabling the user to select the importance of cost compared to toxicity on a spectrum of 100% importance for cost to 100% importance for toxicity. Some teams proposed this idea in their MEA submissions, but this team was not one of them. This improved optimization strategy cannot be attributed solely to the opportunities presented in the design project, but the simulation development process may have led this team to explore this idea. This team took until the last milestone to make their idea work, so the process of simulation development enabled this team to make this optimization strategy possible. This is another example of increased modifiability in a team's model through the design project.

5.3 Research Question 3 – Feedback

Since there was little feedback given to the teams on their mathematical models in the MEAs and almost no feedback in the design projects, this section also discusses some external factors that may have influenced changes and how self-assessment within the team may have played a big role in the teams improving their models. MEAs are developed in a way that ensures students are able to assess their own work to improve their models. The *self-evaluation principle* presents a need for criteria within a developed MEA to enable teams to assess their own models (Rodgers et al., 2016; Lesh et al., 2003; Lesh et al., 2000). The *model-externalization principle* also ensures models are communicated in a way that enables teams to reflect on their own though process (Lesh et al., 2003; Lesh et al., 2000).

Rodgers et al. (2015) found in a case study analyzing a team's development of three different MEAs that the team typically did not respond to peer feedback, even when it was constructive and potentially helpful, and the team responded to TA feedback, even when they did not understand it. These findings demonstrated a much better response to peer feedback to change their MEA solutions (for the better and worse). These findings showed a similar pattern for teams' responses to feedback from TAs that they made changes even when some of them did not make sense and probably was not what the TA was prompting them to do. Some of the feedback that led to changes in teams' mathematical models is discussed.

All three teams received a lot of feedback, especially from peers on their MEA Draft 1 submission, about different aspects of their model that needed to be further clarified. This feedback was typically more localized and direct, which is more commonly implemented and leads to specific changes (Nelson & Schuun, 2009; Matsumura et al., 2002; Shute, 2007). Most of this feedback led to models that were better communicated, which sometimes improved their scores assigned by the *I-MAP* assessment.

Both Teams B and C had relatively high scoring mathematical models (based on *I-MAP* assessment) in their MEA solutions throughout so they did not receive much constructive feedback on their models.

Team A has two telling examples of responding to feedback – one that led to a weaker model and another that potentially led to an improved model.

Team A received feedback from their peers on their Draft 1 MEA submission that prompted them to use MATLAB® for their calculations and better explain these calculations throughout. The team responded to this feedback by removing their original equations, doing all their calculations in MATLAB, and then only describing their MATLAB® file in their MEA. This meant the team no longer had the opportunity to interact with their communicated model to make it more visible for the purpose of self-reflection, therefore removing the goals of the *model-externalization principle* (Lesh et al., 2003; Lesh et al., 2000).

Team A was given constructive feedback on their Final Response MEA submission about their logic using iterations where it was not necessary and not limiting the search space. The team may have responded to this feedback in their design project because their optimization strategy was improved, as the TA prompted. This an example of feedback that potentially led to a significantly improved mathematical model.

There were very few pieces of feedback related to teams' models and simulations throughout the design project. There is an example of one piece of feedback that Team C received in their design project that led to a change in their model.

Team C received feedback from their TA on Milestone 4 to increase the ease of use by adding slide bars. This is another example of direct and localized feedback that was likely to lead to small changes (Nelson & Schuun, 2009; Matsumura et al., 2002). The team added slide bars into both of their QDSC simulations. When they added the slide bar to their QDSC Optimization Chart simulation, they removed the line graphs that enabled the user to explore how the effective band gap energy affects cost and toxicity. The team eventually went back to their initially proposed visuals, but this an example of a team responding to feedback and not realizing how it negatively affected their model.

The variation in instruction clearly impacted the students' QDSC models within the design project, as shown by the differences across sections. Based on the findings, Instructor F's sections were cases where the instructor forced the issue of mathematical models underlying simulations, but failed to really understand what constitutes a complete simulation. The teams from Instructor F's sections presented the most simulations that were actually black-box models because they were lacking visualized outputs (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). The sections with Instructors A, G, and H appeared to have a greater emphasis on GUI and simulation development rather than the QDSC model development because more teams from these sections did not maintain the QDSC model in their design projects. Instructor E's, Instructor C's, and Instructor D's sections seemed close to evenly split in the number of teams that included the QDSC model in their simulations, so it seemed the message to include the QDSC model in the simulation projects was maintained by them longer than Instructors A, G, and H, but not clearly delivered across all of the teams. Instructor B seemed to have the most success in ensuring the teams had both the QDSC model and complete simulations.

Throughout the case studies it is clear that the majority of the changes in the teams' models and simulations through the design project were influenced more by the challenges of the milestone than any feedback they received. All of three teams progressed in a similar manner across the milestones. They all first demonstrated awareness of the problem in Milestones 1 and 2, brainstorming ideas of how the were going to approach developing their simulation suite in Milestone 3, and then developing their actual ideas through prototyping and testing in Milestones 4 through 9. This is a demonstration of teams developing through the engineering design process.

Some changes do not appear to be connected to feedback that teams received or the challenges embedded in the projects themselves. These changes are most likely caused by the self-assessment that is happening within the team through their model development. Self-assessment is a principle that is designed within MEAs in the M&MP (Lesh et al., 2003; Lesh et al., 2000). The lack of evidence around these decisions is discussed within the limitations section (Section 5.7).

5.4 Implications for Practice

The challenge of having students continue model development (i.e. a MEA) with simulation development appears promising for developing understandings of both mathematical models and simulations. There are a few notes about project development, implementation, training, and feedback to prepare others for a similar endeavor.

It was crucial that the development of the QDSC MEA and QDSC Design Project was guided by previous research that described how to design the problems (i.e. the six design principles of the M&MP) and pointed to needs within engineering education (e.g., modeling skills, an ability to build simulations). Rodgers et al. (2016) discussed the development of the QDSC MEA in greater detail and presented an example of how to develop a MEA aligned to the course goals and a NSF grant goals. Although the linked QDSC MEA and QDSC Design Project appear to successfully enable students to explore model development, one variation of the design project is recommended to further investigate developing similar linked projects.

Based on the findings related to the QDSC Design Project, it may have been beneficial to have all of the students in a team either develop one simulation based on the QDSC model or each student in a team create their own simulation based on different ways of modifying the QDSC model. The QDSC Design Project implemented for this study required that each student develop one simulation and each team had at least one of their simulations based on the QDSC model. The team members that did not continue to develop the QDSC model in their simulation failed to engage in the opportunity to build a simulation based on their own mathematical model and potentially further explore it. These team members were required to find and familiarize themselves with other existing mathematical models on which to base their simulations. Requiring all of the students to build a simulation based on the QDSC model from the MEA ensures the students are familiar with the model. Some students created their own models based on prior knowledge and ideas for the solar energy context; most of these were simple models and did not have visualized outputs. For example, some students created a model that calculated the maximum area that could be used for a solar panel based on dimensions for a residential house roof or industrial lot. This is an example of a simple model that outputs a single result, an area. Such a calculation provided little opportunity to build modeling skills and visualize how inputs to the model impact outputs from the model. Requiring all of the students to build a simulation based on the QDSC model mitigates the problem of students using too simple of a model. To practice model development, students need a problem complex enough to challenge them to explore appropriate mathematics further and use the model refinement process (Lesh & Doerr, 2003).

Team B presents an example of a team that developed multiple simulations based on the QDSC model; almost their entire project stemmed from the original QDSC model. This team approached the QDSC Design Project in a way that enabled all of the students to build their own simulations, while starting from a more equal point of understanding of their underlying model. In all working with the QDSC model, this team also appeared to have a lot more opportunities for working as a team and assessing each other's work.

The instructor made a significant impact on students' experiences with the implemented projects, especially student participation in various project requirements. It is crucial that instructors have bought in to the reformed curriculum in their course and understand the purposes; otherwise students will not be guaranteed the same opportunities to gain the knowledge and experiences that were intended.

Two major goals of these projects were to engage students in a nanotechnology context and enable students to understand simulations are based on mathematical models. Many students that did not include the QDSC mathematical model, focused only on macroscale solar technologies. These students no longer benefited from the opportunity to engage in nanotechnology. The student teams that incorporated the QDSC mathematical model started with a model they were familiar with to build their simulation based on; the results showed this resulted in a higher percent of complete simulations (i.e. had user interactivity, mathematical models, and visualization) versus incomplete simulations (i.e. black-box models that were missing visualization or interactive GUIs that were not based on models). This purpose was based on previous research that showed students struggled to understand that simulations are based on mathematical models and incorporates visualization (Rodgers, Diefes-Dux, Kong, & Madhavan, 2015).

As far as performance, the two graduate student instructors had some of the teams with the highest scores on their models for the MEAs, but they also had teams with some of the lowest scores on their QDSC models for the design project. Having a formal TA training for the MEAs and not for the design projects may have had a significant impact on this finding. Most of the other instructors had more experience with training their TAs how to grade design projects. To mitigate this potential problem in the future, it may be beneficial to implement formalized training for TAs (or anyone grading projects) for all implemented projects (in this case, both the MEA and design project).

Rodgers et al. (2016) reported that after implementation of the QDSC MEA and design project and reflection on the differences across sections, they realized that some of the nanotechnology-specific content could have been difficult for some of the instructors to grasp. All of the instructors for the courses had access to the same nanotechnology materials to which the students had access, but there was no additional training for the instructors related to the new nanotechnology concepts incorporated into the specific projects. That is, there was a lack of appreciation with respect to the diversity of talents and training across the FYE instructor pool. The projects created for this FYE course were grounded in research, but there was not a rigorous process to prepare the instructors to implement the projects in their course.

Developing effective training for implementation of MEAs proved to be a crucial step in previous research around MEAs (Diefes-Dux & Imbrie, 2008; Verleger & Diefes-Dux, 2013). Effectively training instructors and TAs on how to grade students' work has been proven successful in improving the quality of students' work, especially for complex projects. The QDSC MEA presented a new challenge with the nanotechnology context appearing to be out of reach for some of the instructors (Rodgers et al., 2016). In implementing projects with a nanotechnology context there needs to be additional training that acknowledges instructors' backgrounds and prepares them to understand the relevant nanotechnology topics (e.g., quantum dot solar cells).

The findings showed TAs were more prepared to guide students through model development through the MEA process than the design project. There needs to be a formalized training for the design project. MEA training engages TAs in model development by challenging them to solve the MEA and teaches TAs how to assess students' solutions and provide effective feedback (Verleger & Diefes-Dux, 2013). In fashioning training for the design project on the MEA training, the training should have two major components: (1) challenge TAs to create their own simulations based on the model they developed in their MEA training and (2) show TAs how to assess prototypical student work and provide effective feedback targeting model development, visualized outputs, and user interaction.

Ideally improved trainings would improve the quantity and quality of feedback. There were examples of feedback that led to improvement (Section 5.3), but there was a huge lack of feedback throughout the case studies. It is important to understand how and why teams improve to harness their successes to help more teams improve in future simulation-building projects. Understanding the feedback that leads to improvement enables future instructors to give students more effective feedback regarding mathematical model and simulation development. It also presents crucial information for training and professional development programs that focus on giving effective feedback.

5.5 Implications for nanoHUB

This research was conducted in continuation of works completed within the Network for Computation Nanotechnology (NCN) education research team (e.g., Rodgers, Diefes-Dux, Madhavan, 2014; Rodgers, Diefes-Dux, Kong, & Madhavan, 2015; Diefes-Dux, Rodgers, & Madhavan, 2015). Since a lot of this research around simulation development is directly related to nanoHUB, this section discusses recommendations for nanoHUB to learn from and continue this research.

Based on the need for training about nanotechnology topics, there is an opportunity for nanoHUB to fulfill this need by creating online training materials targeting instructors. There is a need to further research various instructors' current exposure to, awareness of, and understandings of various nanotechnology topics. Throughout this investigation it would be beneficial to target instructors already interested in teaching and motivated to teach nanotechnology related topics, since teacher buy in is critical for successful implementation. This research would enable nanoHUB to develop videos and modules tailored to prepare instructors to teach nanotechnology related materials in their courses. It would also be beneficial to target instructors with a range of previous experience (e.g., no exposure to nanotechnology, some awareness of how nanotechnology impacts engineering, nanotechnology experts with no experience teaching nanotechnology through projects). There is also a need for training materials that explicitly guide instructors how to use nanoHUB and facilitate students' introduction to and exploration of the nanoHUB community.

This research begins to enable instructors to teach students how to build simulations, but nanoHUB has an opportunity to further this research by investigating the experts within their community. Since nanoHUB is an online community that enables experts to disseminate their simulations (Klimeck et al., 2008), nanoHUB should investigate their users' experiences with model and simulation development. Understanding the experiences of experts, can help educators better understand how to enable novice students to become more like experts (Bransford, Brown, & Cocking, 2000; Schwartz et al., 2005). Expert users' reflections on the model development and simulation building process, how building a simulation impacts their model refinement process, and how simulation distribution on nanoHUB to other users impacts their model refinement process should be collected and investigated. Beaulieu et al. (2013) presented their reflection on the impact of simulation development on their model development process. This is an example of research that can be continued with nanoHUB users.

5.6 Future Research

This study investigated how building a simulation on an existing model impacts teams' model development. The findings of this study point to four other major research categories around models and simulations that should be further investigated: (1) how this process impact students' understandings of mathematical models, (2) how building a simulation on an existing model impacts teams' simulation development and understandings of simulation, (3) how types of visualization enable different understandings and perspectives of underlying models, and (4) how changing the project requirements impacts students' models, simulations, and learning experiences.

Students' understandings of model, understandings of simulations, and transfer of knowledge from a MEA to a simulation-building design project should be further investigated through the CADEX framework. Schwartz et al. (2005) discuss adaptive expertise as a theory to describe transfer of knowledge. Adaptive experts are capable of repurposing, refining, and extending their skills to new problems with innovative thinking and an ability to try new methods of addressing a problem with their expert skill set (Schwartz et al., 2005). This theory is further elaborated on specifically to the context of developing computational and modeling skills in the CADEX framework (McKenna et al., 2008; Carberry et al., 2011). CADEX complements the type of learning experiences that the M&MP endorses (Lesh & Doerr, 2003). Continuing this research with the CADEX framework would complement the research conducted in this study.

This study identified how teams' models developed through the course of their simulation development and highlighted some potential growths in understanding, but there needs to be more research specifically investigating students' understandings of mathematical models through this process using both the M&MP and CADEX framework.

An improvement in the quantity of completed simulations (L4) in students' GUIs is something that was noted in these results, but was not the primary purpose of this study. Overall, this joined MEA and design project resulted in an improvement in the number of simulations incorporated in the projects compared to a previously implemented nanotechnology-based design projects that emphasized simulation building. Rodgers, Diefes-Dux, Kong, and Madhavan (2015) found that around one third of first-year engineering students developed complete simulations for a required design project, which was almost doubled in this project with a compared average of 64 percent overall and 75 percent of the QDSC simulations. Rodgers, Diefes-Dux, Kong, and Madhavan (2015) also found that all teams had at least one GUI that was not based on a model in the previously implemented project, which was only found in 14 students' GUIs (2%) for this project. This improvement was a benefit of considering research on previously implemented nanotechnology-based design projects.

There is a need for further investigation into the types of visualized outputs that students use in simulation development and how these visualizations impact their model development. Visualized outputs are a major component of simulations (Alessi, 2000; Rodgers, Diefes-Dux, Kong, & Madhavan, 2015). The case studies provided a couple examples of different types of visualization used in teams' simulations, but there were many more types seen across the 231 teams' simulations that were initially analyzed. For example, Team C selected a visualization that changed the outputs of the model and enabled them to explore the model through a different lens.

Based on the context of this study a few other research questions have arose about the impact of the problem context and project requirements on model and simulation development. The teams could select their own direct user for their design project and seemed to repurpose their models in different ways in their projects. This relationship should be further investigated. This project required teams to build multiple simulations with at least one based on the original model, as seen in Team C's project. In Team C's and Team B's projects they implemented the original model in more than one simulation. There should be more research around how changing this project requirement affects the types of simulations developed and modifications made to the original model for the different underlying models.

5.7 Limitations

There were four major limitations for this study: (1) the context of the design project, (2) instructor fidelity in implementing the design project, (3) the lack of feedback throughout the design project, and (4) the type of data selected for this study. The first three limitations were unplanned and arose throughout the data collection and data analysis. Implementing more rigorous training for the instructors and TAs could have mitigated or at least minimized these three limitations. The last limitation was designed in the study based on decisions about the type of data to collect for the established research questions.

The implementation of the QDSC MEA and QDSC Design Project resulted in instructors of varying backgrounds struggling with the content and adjusting project requirements to adapt to their struggles. It was apparent that the nanotechnology content was a difficult topic for some instructors to grasp and there needed to be more training in place to address this need. It was also apparent that instructors did not have a sufficient structure in place to seek guidance for project implementation throughout the course. Training would have helped instructors be more prepared for project implementation, may have helped them understand the goals related to each project requirement, and may have made it more clear how to seek assistance throughout project implementation, if needed.

There was little feedback presented throughout the three case studies (Section 4.4); this was addressed in the discussion by presenting other external factors that influenced project development (Section 5.3). It was apparent throughout the findings that the instructors and TAs had little guidance on the type of feedback to give teams on their design projects and the content to focus on throughout the feedback process. The teams typically received no feedback or only direct feedback that prompted small changes (e.g., adding/improving text on the GUI to better communicate its functions to the user, GUI layout). Throughout the QDSC Design Project, the TAs and instructors gave feedback that reflected the quality of a novice's feedback. Marbouti et al. (2015) found that experts typically give more indirect feedback to prompt higher-level changes, including major design decisions. The TAs gave feedback on the MEAs that was more focused on teams' mathematical models and consisted of both direct and indirect feedback. The TAs also received more directions and guidance on how to give feedback to teams on their MEA solutions than the design project milestone submissions. To mitigate this limitation in the future, there needs to be a rigorous training in place for the design project similar to the MEA training, as discussed in Section 5.4.

The qualitative nature of this data was acceptable for the deductive and inductive analyses used throughout this study, but it was not sufficient for an interpretive analysis (Hatch, 2002). The deductive analysis was selected to investigate how teams' models changed across all of the first-year engineering sections. The deductive analysis ensured meaningful selection of cases for the case study analysis and enabled the findings to be more generalizable. The inductive analysis was selected to gain a more in-depth understanding of how a few teams' models changed through the course of the semester and what affected these changes. These analyses were informative for addressing the research questions about model development, but an interpretive analysis would present another mode to further investigate how these linked projects impact students' understandings of mathematical models.

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APPENDICES

Appendix A Class Schedule from Syllabus – Spring 2015

*Please note that this schedule is subject to change. Your instructor will provide additional details about the topics and content for each class session.

Week	Dates	Class	Topics	Notes
1	1/12-1/16	A	Course Overview	*A classes meet on Mon, Tue, or Wed*
		B	MATLAB: Relational Operators & Logical Operators	*B classes meet on Wed, Thu, or Fri*
2	1/19-1/23	A	**Martin Luther King Day**	**All 2A classes canceled**
		B	Teaming, MEA Review & MEA Draft 1	
3	1/26-1/30	A	Flowcharting, Rationales	
		B	If/else/elseif/end Structures	
4	2/2-2/6	A	While Loops	
		B	For Loops	
5	2/9-2/13	A	Complex Loops	
		B	Exam Review	
6	2/16-2/20	A	Project Introducion; Project Partner Visit; Direct-User Profiles; Evaluation GUIs; Storyboards	Exam 1:Wednesday, Feb. 18, 6:30-7:30 pm, Elliott Hall of Music
		B	User-Defined Functions I	
7	2/23-2/27	A	User-Defined Functions II; Test Cases	
		B	User-Defined Functions III	
8	3/2-3/6	A	User-Defined Functions - Review	
		B	Graphical User Interface I	
9	3/9-3/13	A	Graphical User Interface II	
		B	Graphical User Interface III	
10	3/16-3/20	A	**Spring Break**	**No classes**
		B		
11	3/23-3/27	A	CDF I; Exam Review	Exam 2: Monday, Mar. 23, 6:30-7:30 pm, Elliott Hall of Music
		B	CDF II; Exam Review	
12	3/30-4/3	A	Regression	
		B	Regression	
13	4/6-4/10	A	Function Discovery	
		B	Function Discovery	
14	4/13-4/17	A	Project Work Time	
		B	Project Work Time; Exam Review	
15	4/20-4/23	A	Project Work Time; Exam Review	Exam 3: Tuesday, Apr. 21, 6:30-7:30 pm, Elliott Hall of Music
		B	Project Demo (practice); Project Work Time	
16	4/27-5/1	A	Project Demo	
		B	Project Presentation	
17	5/4-5/8		**Finals Week**	**No classes**

Appendix B Quantum Dot Solar Cell Exploration Activity

Quantum Dot Solar Cells

In this problem, you will read about Quantum Dot Solar Cells and then solve some related problems. This will prepare you for the upcoming Model-Eliciting Activity (MEA).

Step 1	Read the description of Quantum Dot Solar Cells below.
Step 2	Perform the following in MATLAB. You will need to pay close attention to units, particularly equivalent units for the joule.

a. Calculate the energy (in units of eV) associated with:
   i. a photon that has a frequency of 650 THz
   ii. a photon that has a wavelength of 600 nm

b. Figure 2 shows 6 solutions of quantum dot nanoparticles. Assuming that the energy of the colors emitted for each of the solutions is the same as the band gap energy of the materials, estimate the band gap energies (in units of eV) of the 6 solutions shown from left to right. (*Hint*: Locate and cite in your code necessary information on the wave lengths (in nm) for the visible light spectrum).

c. Predict the band gap energy of bulk silicon (in units of eV) if the observed band gap energy of silicon quantum dots (ε = 11.68) with a 2.5 nm diameter is found to be 1.5 eV. Compare this predicted value to the known band gap for silicon (*Hint*: Locate and cite a source for a known band gap value for silicon). If there is a discrepancy, discuss one potential cause.

Design and Operation of Quantum Dot Photovoltaic (QD-PV) Devices

Photovoltaic devices (*i.e.*, solar cells) offer the security of an environmentally-friendly energy source that is implantable across the globe, including locales that do not have widespread electrical grid infrastructures. The semiconducting material in photovoltaic devices absorbs energy in the form of light (*i.e.*, photons) and converts this energy to electricity (*i.e.*, in the form of electrons). The energy of a photon (*E*, in J) can be characterized by the following equation.

$$E = h\nu = \frac{hc}{\lambda} \qquad \text{(Equation 1)}$$

Here, h is Planck's constant (6.626×10^{-34} J·s), ν is the frequency of the photon (in Hz), c is the speed of light (3.0×10^{8} m s^{-1}, assuming that space is close to vacuum), and λ is the wavelength of the photon (in m). E is often presented in eV units, where 1 eV is equal to 1.602×10^{-19} J.

If this light-to-electricity conversion process is to be successful, the energy of the incoming photons must be large enough to promote the electrons from a trapped state (*i.e.*, tightly bound to the protons in the nucleus of the associated atom) to one where they can move in a free manner (*i.e.*, like electrons in a metal). Electrons in the bound state are said to be in the valence band (with energy E_v) of the material, and free electrons are said to be in the conduction band (with energy E_c) of the material. The difference in energy between these two states is the band gap energy (E_g). Therefore, the energy of the incoming photon must be larger than the band gap energy, if an electron is to be promoted to the conduction band. Only electrons in the conduction band can leave the solar cell and contribute to the electrical current; however, if the energy of the photon is much bigger than the band gap energy then a large amount of energy is wasted as the electron will quickly relax to the energy of the conduction band (Figure 1).

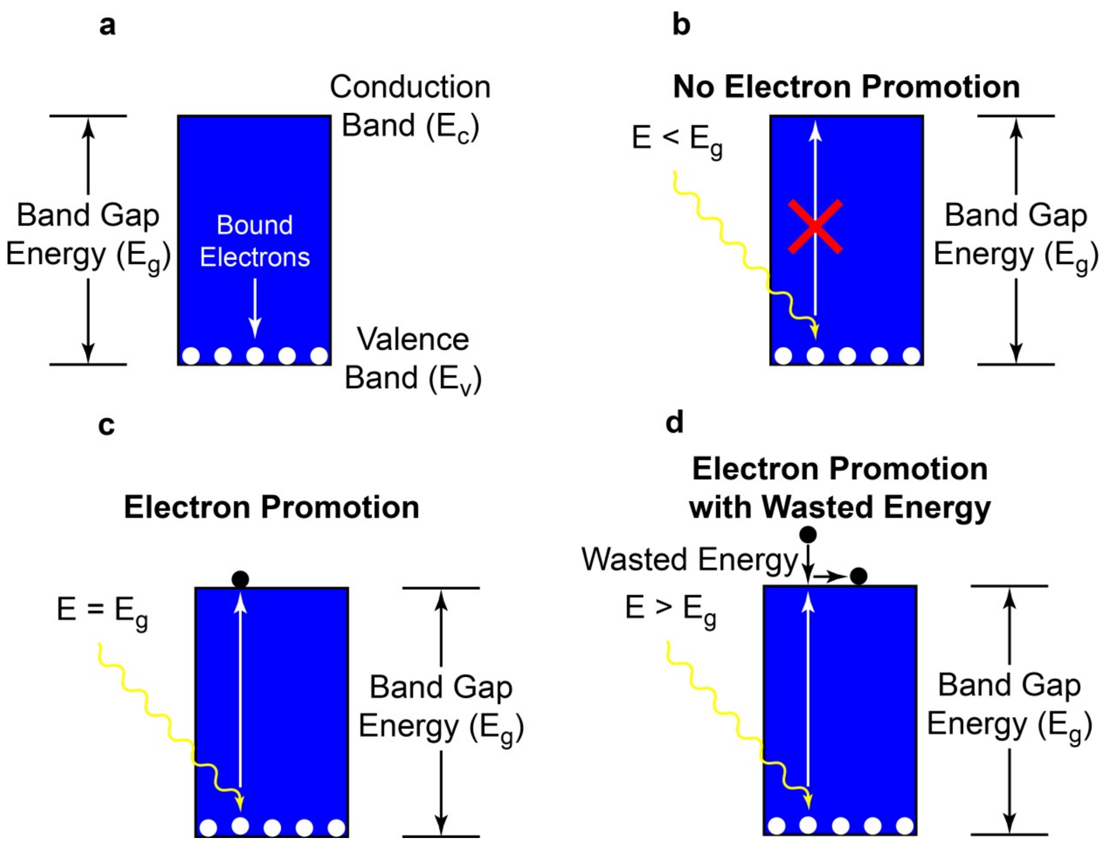

Figure 1. (a) Schematic showing the valence band containing bound electrons, the conduction band, and the band gap energy - the difference in energy between these two bands. (b) If the energy of the incoming photon is less than the band gap energy, the electron will not be promoted, and the electron will not be able to contribute an electric current. (c) If the energy of the photon matches the band gap energy, the electron can be promoted and contribute to the current. (d) The electron will be promoted if the energy of the photon is greater than the band gap energy; however, the electron will quickly lose any extra energy and relax to the conduction band energy level. The extra energy will be lost and will not contribute to the solar cell efficiency.

As such, it is important to design materials with band gap energies that are tuned to the light incoming to the solar cell. In this way, the engineer can make sure that the energy of the photons are large enough to promote the bound electrons to the conduction band without wasting energy that is greater than the band gap energy. Previously, the only ability engineers had to alter the band gap of solar cell semiconductors was by changing the chemical composition of the materials (*e.g.*, moving from a silicon (Si) semiconductor to a gallium arsenide (GaAs) semiconductor). Thanks to the arrival of nanotechnology, engineers now have the ability to fine-tune the band gap energy of a single material by making spherical nanoparticles of different diameters (ranging from 1 to 10 nm). Because of effects associated with quantum chemistry, these nanoparticle-based materials are called quantum dots, and photovoltaic devices made from these materials are called quantum dot solar cells (QD-SCs). As shown in Figure 2, the wavelength of light (and the energy of light, according to Equation 1) absorbed and emitted by quantum dots can be tuned across the electromagnetic spectrum. All of the differently-colored solutions shown in Figure 2 are composed of the same semiconducting material, but with nanoparticle diameters that range from 2.3 nm to 5.5 nm.

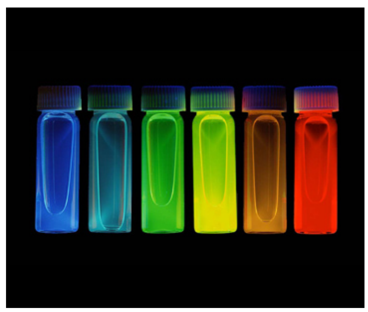

Figure 2. Six solutions of semiconducting quantum dots with different band gap energies that range across the visible spectrum of electromagnetic radiation. While each solution contains the same semiconducting material, the diameters of the semiconducting nanoparticles range from 2.3 nm to 5.5 nm. The image is reproduced from original work performed at Drexel University.

In fact, the band gap energy of the semiconducting quantum dot nanoparticles [E_g (quantum dot), in eV] can be predicted from the following relationship.

$$E_g\ (quantum\ dot) = E_g\ (bulk) + \frac{h^2}{4m_e r^2} - \frac{1.8e^2}{4\pi\varepsilon\varepsilon_0 r} \qquad \text{(Equation 2)}$$

Here, E_g (bulk) is the band gap energy of the semiconducting material in the bulk (i.e., without nanoconfinement effects) (in eV), r is the radii of the nanoparticles (in m), m_e is the mass of an electron (9.11×10^{-31} kg), e is the charge on an electron (1.602×10^{-19} C), ε is the material's dielectric constant (dimensionless), and ε_0 is the permittivity of free space (8.854×10^{-12} F m^{-1}, where F is the unit farad = coulomb/volt). Note that as the radii of the quantum dot nanoparticles gets increasingly large (*i.e.*, $r \rightarrow \infty$) that the band gap energy of the quantum dots goes to the band gap energy of the bulk material, as expected.

Appendix C QDSC MEA Problem Context Individual Questions

Modeling Activity Task 1: Understanding the Problem

This is an individual assignment.

Instructions:

Step 1

Watch Modeling Activity Online Modules 1-3. These modules will orient you to mathematical modeling in ENGR 132.

Read the mathematical modeling problem:

1. Read the company profile and the memo from Teresa Wall (**Error! Reference source not found.**).

2. When you read the memo from Teresa Wall, you will see a link for two videos that are available on the nanoHUB.org website.

Step 2

Learn about the context of the problem:

Nanoscience and **nanotechnology** are affecting every field of engineering. Use and document (with proper citations) at least ***two*** external and ***trustworthy*** resources to learn ***three*** things about how nanotechnology is affecting your intended field of study in engineering.

Step 3

Learn more about the problem: Answer the following five questions.

Problem Formulation – take a big-picture view of the problem

a. List as many stakeholders as you can think of who may be impacted by the deliverable your team has been asked to create. For each stakeholder, explain the relationship between the stakeholder, the problem, and the deliverable.
b. Your solution will be implemented in the context described here and potentially in other contexts. Describe issues (minimum five) that might arise for stakeholders when your generalizable solution is implemented.

Problem Identification – take a task-picture view of the problem c. Consider your list of stakeholders. Who is the direct user of the deliverable your team is being asked to create?

c. Consider your list of stakeholders. Who is the direct user of the deliverable your team is being asked to create?
d. In a few sentences and in your own words, what does the direct user need? (Remember to describe the deliverable, its function, the criteria for success, and the constraints.)
e. Consider the immediate problem as described and the sample data provided. Describe at least two ideas you have for why this problem might be complex to solve.

Step 4

Watch Modeling Activity Online Module 4. This module will prepare you for solving the modeling activity.

Appendix D QDSC MEA Memo for Draft 1

Quantum Dot Solar Cells Company Profile – Power-by-Nano Technologies

Power-by-Nano Technologies is an emerging quantum dot solar cell company founded in 2001 to develop next-generation quantum dot – photovoltaic (QD-PV) devices from nanomaterials. The solar cells of the Power-by-Nano Technologies team will be easily integrated as the power generation component for a wide variety of applications. Because they can be dissolved in solution (*see Figure 1*), the nanomaterials developed by our company can be coated over a sheet of plastic using printing and coating machines that perform roll-to-roll manufacturing in a manner similar to how newspaper is printed on large rolls of paper. Initial cost estimates suggest that by using our nanomaterials and printing technologies, the scale-up of our production line could lead to a 10-fold cost reduction of our solar modules, relative to the state-of-the-art. In one of our most recent developments, new quantum dots have been synthesized by our team, and the initial device performance -results appear promising. Because we must design new materials, generate large amounts of these materials, print them onto flexible substrates, and engineer functional electronic devices from them, Power-by-Nano Technologies hires a wide swath of technical expertise. In particular, our product development teams include materials engineers, electrical engineers, chemical engineers, and mechanical engineers. These groups interface with chemists and computational modelers to develop novel quantum dot solar cell nanomaterials in as rapid of a manner as possible. By connecting the molecular scale with the nanoscale and macroscopic devices, Power-by-Nano Technologies is able to deliver on our mission of providing new energy solutions to people and communities from all across the globe. This affords us the ability to be at the cutting edge of engineering development for the PV industry.

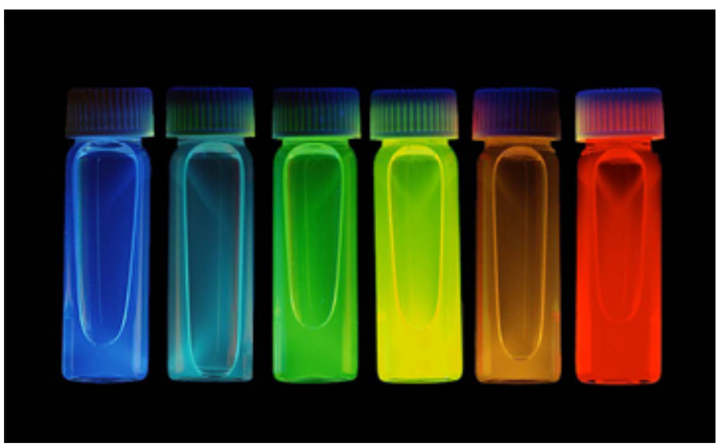

Figure 1. Six solutions of semiconducting quantum dots with different band gap energies that range across the visible spectrum of electromagnetic radiation. While each solution contains the same semiconducting material, the diameters of the semiconducting nanoparticles range from 2.3 nm to 5.5 nm. The image is reproduced from original work performed at Drexel University.

Interoffice Memo: Power-by-Nano Technologies

To: Quantum Dot Photovoltaic (QD-PV) Characterization Team

From: Teresa Wall, Vice President of Research

RE: Optimizing a Mixture of Quantum Dots for a PV Customer

The development of new materials is at the heart of our technological edge in the QD-PV device market. Recently, Power-by- Nano Technologies' nanoparticle chemists have generated novel materials that have been predicted to produce devices with never-before-seen device efficiencies, according to computational models from our simulation engineers. Our Purdue University collaborator Dr. Bryan Boudouris has created a video titled *Introduction to Quantum Dots and Solar Energy Conversion Devices* that explains the basics of quantum dot technologies. Further, we have automated our process such that it occurs in a manner similar to that shown in a video from the Lawrence Berkeley National Laboratory (LBNL). Both videos are available at: https://nanohub.org/groups/qdsc_fyedesignproject.

We would like to expand our capabilities and market base with the help of your team. In particular, representatives from a potential customer have asked that we develop a strategy for providing low-cost, limited-toxicity solar cell materials from QD materials with varying optical properties. They have agreed that we will be able to mix the QD materials to achieve optimal absorption, and our computational chemists, who are part of the QD Synthesis Team, have determined that combining mixtures of quantum dots yields averaged band gap energies. That is, an estimation for the effective band gap $(E_{g,quantum\ dot})_{eff}$ of a mixture of QD materials is a weighted average of the individual QD materials as follows.

$$\left(\mathrm{E}_{\mathrm{g,quantum\ dot}}\right)_{\mathrm{eff}} = \sum_{i=1}^{5} x_i \left(E_{g,quantum\ dot}\right)_i$$

Here, x_i is the mass fraction of a specific QD material and $(E_{g,quantum\ dot})_i$ is the band gap of that particular QD material. In addition to matching the required band gap specified by the customer, the customer also has asked that both the cost and toxicity of the resultant QD mixture be minimized. Because we anticipate this being a common request from future customers, we are requesting that you develop an algorithm to quickly screen materials to optimize the band gap energy of the mixture while taking into account the potential cost and toxicity constraints associated with next-generation nanoparticles. The QD-PV Fabrication Team will subsequently use your algorithm when working with our customers. To accomplish this goal, we ask that you create optimization algorithms for the following scenarios.

Scenario 1: Minimum cost with no concern for toxicity

Scenario 2: Minimum toxicity with no concern for cost

At a future date, I will need your team to also create an optimization algorithm to minimize both cost and toxicity. Apply your algorithms to the QD materials listed in Table 1 using the demonstration specifications below. Assume that you are mixing 100 g of total QD material; the minimum contribution of each material must be 2% by mass.

Table 1. Properties of QD Materials

QD Material	$E_{g,bulk}$ (eV)	ε	Radius (nm)	Cost ($ g^{-1})	Toxicity (Impact g^{-1})
1	1.92	3.6	4.5	45	2
2	1.32	9.2	3.5	35	3
3	1.50	4.0	1.5	25	4
4	1.71	14.0	4.9	40	1
5	1.18	7.0	2.7	30	2

Demonstration A: Mix **all** materials 1 to 5 to achieve an $(E_{g,quantum\ dot})_{eff}$ of 1.33 eV

Demonstration B: Mix **all** materials 1 to 5 to achieve an $(E_{g.quantum\ dot})_{eff}$ of 1.65 eV

In a maximum 2-page technical brief, write a detailed description of your team's algorithms and the final results of the demonstrations. For the demonstrations, report the make-up, cost, and toxicity of the optimized mixtures for each combination of demonstration (A & B) and scenario (1 & 2). Please be sure to include your team's rationale for each key step in your optimization algorithms. Thank you for your efforts in this endeavor, I appreciate your prompt attention to this assignment.

Appendix E QDSC MEA Memo for Draft 2

Interoffice Memo: Power-by-Nano Technologies

To: Quantum Dot Photovoltaic (QD-PV) Characterization Team

From: Teresa Wall, Vice President of Research

RE: Optimizing a Mixture of Quantum Dots for a PV Customer

I have reviewed your team's optimization algorithms. It appears that your team is making progress. At this time, I would like your team to revise your procedure by considering additional QD material data.

Table 1. Properties of QD Materials

QD Material	$E_{g,bulk}$ (eV)	ε	Radius (nm)	Cost (\$ g^{-1})	Toxicity (Impact g^{-1})
1	1.92	3.6	4.5	45	2
2	1.32	9.2	3.5	35	3
3	1.50	4.0	1.5	25	4
4	1.71	14.0	4.9	40	1
5	1.18	7.0	2.7	30	2
6	1.94	3.1	3.2	30	3
7	1.26	7.6	2.8	41	2
8	1.20	5.0	3.1	22	4
9	1.82	2.9	1.2	40	3
10	1.96	5.8	4.3	18	1

Continue your development of algorithms for the following scenarios:

Scenario 1: Minimum cost with no concern for toxicity

Scenario 2: Minimum toxicity with no concern for cost

Scenario 3: Minimum cost and toxicity

Again, **all** ten different QD materials must be mixed to achieve a desired $(E_{g,quantum\ dot})_{eff}$, but no material can be present in the mix by less than 2% by mass.

In addition to Demonstrations A and B, apply your algorithms to the QD materials using the specifications for Demonstrations C to F below. Assume that you are mixing 100 g of total QD material.

Demonstration A: Mix materials 1 to 5 to achieve an $(E_{g,quantum\ dot})_{eff}$ of 1.33 eV

Demonstration B: Mix materials 1 to 5 to achieve an $(E_{g,quantum\ dot})_{eff}$ of 1.65 eV

Demonstration C: Mix materials 6 to 10 to achieve an $(E_{g,quantum\ dot})_{eff}$ of 1.33 eV

Demonstration D: Mix materials 6 to 10 to achieve an $(E_{g,\ quantum\ dot})_{eff}$ of 1.65 eV

Demonstration E: Mix materials 2, 3, 4, 7, and 9 to achieve an $(E_{g.quantum\ dot})_{eff}$ of 1.33 eV

Demonstration F: Mix materials 2, 3, 4, 7, and 9 to achieve an $(E_{g,quantum\ dot})_{eff}$ of 1.65 eV

In a 2-page technical brief, write a detailed description of your team's algorithms and the final results of the demonstrations (*Note*: results may be presented starting on page 3). For the demonstrations, report the make- up, cost, and toxicity of the optimized mixtures for each combination of demonstration (A-F) and scenario (1-3). If an iterative method is employed, report the number of iterations required to optimize the nanoparticle mixture in each case. Please be sure to include your team's rationale for each key step in your team's optimization algorithms.

Thank you for your team's continued efforts in this endeavor.

Appendix F QDSC MEA Memo for Final Response

Interoffice Memo: Power-by-Nano Technologies

To: Quantum Dot Photovoltaic (QD-PV) Characterization Team

From: Teresa Wall, Vice President of Research

RE: Optimizing a Mixture of Quantum Dots for a PV Customer – Final

I have again reviewed your team's optimization algorithms. It appears that your team is making progress. Now, I would like your team to finalize your solution.

I understand that your team has been developing additional test cases for testing the robustness of your solution. I'd like to see the results of some of these demonstrations. So, in addition to the 10 QD materials used in the A-F Demonstrations I requested last time, I would like your team to add two QD materials used in two demonstrations to your results. ***Make sure you provide the properties of the two new QD materials and two new demonstrations in your technical brief and describe how these new materials and demonstrations are useful for testing your model.***

As before, you must have algorithms for the following scenarios:

Scenario 1: Minimum cost with no concern for toxicity

Scenario 2: Minimum toxicity with no concern for cost

Scenario 3: Minimum cost and toxicity

Remember, the set of QD materials specified for each demonstration must be mixed to achieve a desired $(E_{g,quantum\ dot})_{eff}$, and no material can be present in the mix by less than 2% by mass. Assume that you are mixing 100 g of total QD material.

In a 2-page maximum (not including results) technical brief, write a detailed description of your team's algorithms and the final results of the demonstrations. Results may be presented on page 3. Results must be complete, concise, and easy to interpret; a table of results is recommended. For the demonstrations, report the make-up, cost, and toxicity of the optimized mixtures for each combination of demonstration (***A-F, plus your two new test cases, call them G and H***) and scenario (1-3). If an iterative method is employed, report the number of iterations required to optimize the nanoparticle mixture in each case. Please be sure to include your team's rationale for each key step in your team's optimization algorithms.

Thank you for your team's final push to achieve robust algorithms.

Appendix G QDSC MEA *I-MAP*

Purpose of Instructor Feedback on Team Solutions:

Overall

- Narrow the gap between actual performance and reference level performance (indicated below). That is, encourage improvement across each dimension (below) from drafts to final response. Note that the reference level never changes from start to finish.
- Enable better performance in subsequent problem solving activities (e.g. MEAs, design projects…)

Mathematical Model

- Guide students towards identifying the complexity in the problem
- Guide students to develop models that are simple and elegant but addresses the complexity of the problem
- Guide students to thinking with data in three dimensions
- Mitigate the misconception that statistical analysis on aggregated data will always be meaningful

Share-ability

- Guide students towards writing a procedure that others can successfully implement
- Guide students towards presenting meaningful results that demonstrate that their model works
- Guide students towards finding a balance between providing detail and being concise

Re-usability

- Guide students to describe the task-level view of the problem and overview their solution so that others can understand when the model can be applied

Modifiability

- Guide students to engage in rational capture – articulation of decisions made to create the model
- Guide students to write evidence or context based rationales

High-Quality Feedback for Team Solutions:

- Focused on the specifics of the task, rather than on the students themselves
- Related to the students' current response (response-specific)
- Clear and simple, but elaborate enough to guide students to closing the performance gap
- Praise is NOT effective, particularly when it is mixed with the identification of problems and recommendations for improvements

Mathematical Model

A mathematical model may be in the form of a procedure or explanation that accomplishes a task, makes a decision, or fills a need for a direct user. A high quality model fully addresses the complexity of the problem and contains no mathematical errors.

Specific to the Quantum Dot Solar Cells MEA

Complexity

In a high quality model:

- $E_{g,quantum\ dot}$ for each material is correctly computed
- $(E_{g,quantum\ dot})_{eff}$ is correctly computed
- Material quantities sum to 100 g.
- The minimum material quantity is 2% (2 g).
- There is a mechanism for achieving the desired $(E_{g,quantum\ dot})_{eff}$
- There are mechanism for minimizing cost, toxicity, and both cost and toxicity
- The solution space is searched with some attention to minimizing the number of iterations.

As student teams will address the seven main issues to varying degrees, the following rubric is used to determine the level of achievement of the mathematical model.

Mathematical Model Elements			
	Fully Addressed (2 pt)	**Somewhat Addressed (1 pt)**	**Missing or Inadequately Addressed (0 pt)**
$E_{g,quantum\ dot}$ for each material is correctly computed			
$(E_{g,quantum\ dot})_{eff}$ is correctly computed			
Material quantities sum to 100 g			
The minimum material quantity is 2% (2 g)			
There is a mechanism for achieving the desired $(E_{g,quantum\ dot})_{eff}$			
There are mechanism for minimizing cost			
There are mechanism for minimizing toxicity			
There are mechanism for minimizing cost and toxicity			
The solution space is searched with some attention to minimizing the number of iterations.			

[LEVEL assignments on next page]

LEVEL 4 – Rubric score of 15+

- Mathematical detail must be clear from start to finish.
- Mathematical errors must be eliminated.

LEVEL 3 – Rubric score of 12-14
LEVEL 2 – Rubric score of 9-11
LEVEL 1 – Rubric score of 6-8
LEVEL 0 – The model is not mathematical in nature or has serious faults.

An automatic Level drop will be applied in instances where statistical measures are not defined or applied correctly.

<u>*Accounting for Data Types*</u>
It must be determined whether the mathematical model *takes into account all types of data provided* to generate results. If any data type is not used in the mathematical model, an <u>*evidence based*</u> justification must be provided.

LEVEL 4 - All data types are used OR <u>*evidence based*</u> justifications are provided.

Justification similar to "we decided not to use …" or "it is not useful…" are not sufficient. Further, procedures that use data types in highly inappropriate ways (and seems designed to just use the data types for the sake of using data types) is not LEVEL 4 work.

<u>***Generalizability***</u>

Generally, one would not produce a mathematical model to solve a problem for a single situation. A mathematical model is produced when a situation will arise repeatedly, with different data sets. Therefore, the model needs to be able to work for the data set provided and a variety of other data sets. That is, a useful mathematical model is adaptable to similar, but slightly different, situations. For example, a novel data set may emerge that wasn't accounted for in the original model, and thus the user would need to revise the model to accommodate the new situation.

A mathematical model that is generalizable is share-able, re-usable, and modifiable. Thus, one should strive for clarity, efficiency and simplicity in mathematical models; as such models are the ones that are more readily modified for new situations. Although the student team has been "hired" as the consultant team to construct a mathematical model, direct user needs and wants to understand what the model accomplishes, what trade-offs were involved in creating the model, and how the model works.

<u>Re-Usability</u>

Re-usability means that the procedure can be used by the direct user in new but similar situations.
A *re-usable* procedure:

- Identifies who the direct user is and what the direct user needs in terms of the deliverable, its function, criteria for success, and constraints
- Provides an overarching description of the procedure
- Clarifies assumptions and limitations concerning the use of procedure. These include assumptions about the situation and the types of data to which the procedure can be applied. ***Even if there are no limitations, there must be a statement to this effect.***

Student teams should state that the procedure is designed to be used on QD material property values (bulk band gap energy, dielectric constant, and radius), cost, and toxicity. Students should also indicate limitations of their procedure (like it only works for 5 materials at a time or for 2% minimum quantities). Limitations may arise if the team hard-codes values in their procedure.

Re-Usability Item	**QDSC MEA**	**Yes (2 pts)**	**Sort Of (1 pt)**	**No (0 pt)**
Identification of direct user	QD-PV Fabrication Team			
Deliverable	Algorithms or procedures			
Function	To Optimize QD material mixture for a particular band gap energy		missing $E_{g, QD}$	
Criteria for success	Minimize cost and/or toxicity			
Constraints	Given QD material properties (bulk band gap energy, dielectric constant, and radius), cost and toxicity. Number of materials. Minimum % contribution of each material.		missing one of	No or just mention QD material data
Overarching Description	Should provide an overview of how algorithms work			
Assumptions and limitations concerning the *use* of procedure	Number of materials or minimum % contribution of materials to mixture			

LEVEL 4: rubric score of >= 12
LEVEL 3: rubric score of 8-11
LEVEL 2: rubric score <= 7

Modifiability

Modifiability means that the procedure can be modified easily by the direct user for use in different situations.
A modifiable procedure:

- Contains acceptable rationales for critical steps in the procedure and
- Clearly states assumptions associated with individual procedural steps.

Given this type of information, the direct user will be able to modify (change) the model for new situations.

Critical steps that need justification / rationale:

- Computations
- Iteration method
- Hardcoded values (e.g. bounds on the searchable space) imbedded in procedural steps require explicit explanation of where the values come from.

Rationales are tied to the mathematical model. So students need to be reminded that when their model changes, they need to revise, delete, and add rationales to make them appropriate for their model.

Share-ability

Share-ability means that the direct user can apply the procedure and replicate results. If the mathematical model is not developed in enough detail to clearly demonstrate that it works on the data provided, it cannot be considered shareable.

Results

LEVEL 4 achievement requires that the mathematical model be applied to the data provided to generate results in the form requested. Quantitative results are to be provided.

Results of applying the procedure MUST be included in the memo.
LEVEL 1 – No quantitative results or results do not seem to be those for the data set indicated. Ensure that the student teams are presenting results for the specified data sets. Multiple data sets may have been made available to the students and the analysis of only the latest may have been requested in the current memo.
LEVEL 2 – Partial or quantitative results. Units may be missing or contain errors. Significant figures or units are not appropriate.
LEVEL 4 – The teams must present quantitative results. Significant figures and units must be appropriate for the model presented.
Draft 1: Demonstration A and B results including mixture specifications, cost, and toxicity for Scenarios 1, 2, and 3. So, a total of 6 results must be presented.
Draft 2: Demonstration A to F results including mixture specifications, cost, and toxicity for Scenarios 1, 2, and 3. So, a total of 18 results must be presented.
Final Response: Demonstration A to F and G to H (using individually created data sets)

results including mixture specifications, cost, and toxicity for Scenarios 1, 2, and 3. So, a total of 24 results must be presented.

Apply and Replicate Results

A high quality product (i.e., model communicated to the direct user) will clearly, efficiently and completely articulate the steps of the procedure. A high quality product may also illustrate how the model is used on a given set of data. The description will be clear and easy to follow; it must enable the results of the test case to be reproduced. At a minimum, the results from applying the procedure to the data provided must be presented in the form requested.

The direct user requires a relatively easy-to-read-and-use procedure. If this has not been delivered, the solution is not LEVEL 3 work.
If you, as a representative of the direct user, cannot replicate or generate results, the solution is not LEVEL 3 work.

Results of applying the procedure that have unit problems or orders of magnitude issues do not get credit as being complete.

Extraneous Information

The mathematical model should be free of distracting and unnecessary text. This might include (1) outline formatting, (2) indications of software tools (e.g. MATLAB® or Microsoft® Excel or, more generally, spreadsheets) necessary to carry out computations, (3) explicit instructions to carry out common computations, (4) discussions of issues outside the scope of the problem, and (5) general rambling.

LEVEL 3 – If any of the following are present:

- *Discussions of QD materials or devices that are not expressly relevant to the algorithms or their uses.*
- *Discussions about clients and customers*
- *Outline formatting.*
- *Mentions of computer tools*
- *Descriptions of how to compute common values*

Appendix H QDSC Design Project – *Project Rubric*

Criterion 1: Targets a well-defined direct user and presents clear goals around planning PV solar panel fabrication
0-points: No attempt. **5-points:** • The direct user is clearly identified somewhere early in the simulation suite. Should answer the question – For whom is this simulation suite intended? • The goal for the direct user is clearly communicated somewhere early in the GUI package. Should answer questions like: - Why would the direct user want to use this simulation suite? - What would the direct user gain from using this simulation suite?
Criterion 2: Contains at least one mathematical model per student team member on which a simulation is based.
0-points: > 50% of models do not support goal or are too simple or are not math models **5-points:** 50% (e.g. 2 of 4) of models do not support goal or are too simple or are not math models **8-points:** 25% (e.g. 1 of 4) of models do not support goal or are too simple or are not math models **10-points:** • Use model to determine mix of QD materials to achieve a particular effective QD band gap energy while minimizing cost and toxicity to support goal • Other math models (one per students 2-4) support goal • Key equations/formulas for the models are clearly communicated (no black boxes)
Criterion 3: Each mathematical model should be made into a simulation that enables the target audience (direct user) to explore and visualize the relationship(s) between the inputs and outputs of the mathematical model.
0-points: No attempt. **10-points:** • Simulations provide effective means for using the mathematical models to answer what-if questions • It is clear how the mathematical model can be manipulated. o Inputs to the mathematical model are clear o Outputs from the mathematical model are clear o Key values needed to run the mathematical model that are not available to the user to manipulate are clear • Units on inputs and outputs are clear, including those on plot axes • Visualizations are graphical were possible

Criterion 4: Is highly interactive.
0-points: No attempt. **5-points:** • 2-way communication is meaningful (e.g. comparisons of outputs based on various inputs can be made; decisions can be made based on outputs) • User choice is meaningful (e.g. ways to navigate through suite; inputs to manipulate) • Keeps user memory load to a minimum (e.g. inputs and outputs are on the same GUI) • Interfaces are interesting and hold attention • Overall visually attractive (colors appropriate and not jarring, adequate white-space)
Criterion 5: Is easy to use and operate.

0-points: No attempt.
5-points:
• Organization is clear throughout o Users will know where they are in the suite at all times and navigation reflects map o Flow on a given GUI is clear (e.g. inputs on left to outputs on right; inputs on top to outputs on bottom)
• Conventions are consistent throughout
  o Navigation buttons are in the same place on ALL GUIs
  o Navigation buttons are in typical locations (e.g. not in the four corners)
  o Headings and groupings of content are similar throughout
  o Components (e.g. button) that perform functions similar to those in other programs operate in a familiar way
• Screens contain only relevant information (uncluttered)
• Language is appropriate for user throughout
• User errors are prevented throughout
• Help is provided to move forward and correct errors

Appendix I QDSC Design Project – Milestone 0 Learning Objectives

Learning objective	**To demonstrate full achievement, you must:**
Articulate appropriate clarifying questions to a project partner.	All three questions are: • Specific and informed by the project description (see partner memo) • Targeted to the project partner (as opposed to the instructional team) • Professional, meaning they promote a professional interaction between you and the project partner

Appendix J QDSC Design Project – Milestone 1 Learning Objectives

Learning objective	To demonstrate full achievement, you must:
Identify the needs of a project partner	• Review Online Module MEA 3: Understanding the Problem
Identify stakeholders and their relationships to a given problem and its solution (deliverable)	• Review Online Module MEA 3: Understanding the Problem from ENGR 13100. Even though this is a design problem, the techniques for understanding a problem are the same.
Select a direct user	• Clearly describe the direct user • Clearly state the team's interest in this direct user
Gather information about a direct user that will inform the development of an appropriate solution	• Provide 20 insightful and high quality pieces of information about the selected direct user insightful = clear how the information about the direct user will inform the design of simulation suite high quality = information comes from trustworthy sources
Provide proper citations for information gathered	• Provide a *minimum* of 12 different APA citations for information gathered on peers' knowledge; 6 for Part C.2 and 6 for Part C.3 • In-text citations are used to link the information gathered to the citation list.
Evaluate a GUI for the presence of a mathematical model(s) and simulation(s)	• For each of 4 GUIs, identify whether or not model(s) and simulation(s) are present. Explanations must be specific.
Define and relate mathematical models and simulations	• Clearly define the terms mathematical model and simulation • Describe the relationship between of mathematical model(s) and simulation(s)

Appendix K QDSC Design Project – Milestone 2 Learning Objectives

Learning objective	To demonstrate full achievement, you must:
Document changes based on feedback	Summarize feedback in own words Clearly articulate changes made based on feedback.
Generate multiple concepts to meet stated project partner criteria	Provide 20+ high quality ideas for models and simulations that enable the direct user to explore aspects of planning PV solar panel fabrication high quality = clearly stated how the idea relates to addressing criteria 1-3
Document concept generation tools used	For each idea, one or more concept generation tools is identified and evidence of the use of each tool is clear.
Provide proper citations for concept generation	All citations are in APA format All citations are in alphabetical order All citations appear as in-text citations in the idea generation list

Appendix L QDSC Design Project – Milestone 3 (A and B) Learning Objectives

Learning objective	To demonstrate full achievement, you must:
Document changes based on feedback	Summarize feedback in own words Clearly articulate changes made based on feedback
Reduce ideas through a voting process	Reduce the 20+ high quality ideas for models and simulations that enable your direct user to explore aspects of planning PV solar panel fabrication down to 10 using a voting process. The final vote is recorded and the ideas as listed in numerical order.
Perform an evaluation of ideas through a pros and cons analysis	For each of the 10 ideas, perform a pros and cons analysis. • Specific pros and cons must be related to the project partners' criteria, direct users' knowledge and interest, and potential for grouping with other ideas into a cohesive solution. • Each pro and con must be weighted and totals computed
Provide evidence-based rationales for pros and cons analysis weightings	For each of the 10 pros and cons analyses: • Rationales, based on evidence, must be provided for the weightings. Evidence may be based on your direct users' needs, research, prior art, expert opinion, and so on, but NOT on your team's opinions. • An APA citation list (in alpha-order) and in-text citations should be included as appropriate.
Select ideas based on pros and cons analysis and provide evidence-based rationales for selection	A list of 4 ideas selected using results of the pros and cons analysis is accompanied by a thoughtful discussion of how the selected ideas will meet project partners' criteria and how the ideas can be brought together into one cohesive solution. • Rationales must be based on evidence. Evidence may be based on your direct user needs, research, prior art, expert opinion, and so on, but NOT on your team's opinions. • An APA citation list (in alpha-order) and in-text citations should be included as appropriate.

Appendix M QDSC Design Project – Milestones 4 and 5 Learning Objectives

Learning objective	**To demonstrate full achievement:**
Document changes based on feedback	• Summarize feedback in own words • Clearly articulate changes made based on feedback.
Create a detailed navigation map	• All GUIs that are needed must be represented • For each GUI, an appropriate description (including developer, function, and user interaction) is provided • Opening GUI must be present and complete • Citation GUI must be present • Flow between GUIs must be clear and represented with arrow
Develop a professional looking rapid prototype	• All GUIs that are needed must be included • GUIs must be complete (detailed with intended features) • Layouts must be consistent and adhere to principles for user interface design • Opening GUI must be present and complete • Citation GUI must be present • Navigation options must be consistent with the navigation map and enable partial functionality
Include complete and detailed design notes with a rapid prototype	Design notes for each GUI must detail (with letter): a. describe how the direct user will interact with the interface. o What inputs will they enter? o What outputs will they see? o What other actions can they take? b. describe how each GUI works. For a GUI that is a simulation backed by a mathematical model, you must provide a concise but complete ***description of the mathematical model(s) that will be employed including equations*** (use PowerPoint's equation editor)***, user-inputs, and the visualizations that will result***. c. describe what error checking will be done as the direct user interacts with the interface, d. describe what help will be provided to assist the direct user in understanding the GUI and in overcoming errors, and e. state who on the team will be responsible for developing the GUI.
Meet project partner criteria	There must be evidence that all project partner criteria are fully being met in one cohesive solution that: 1. Targets a well-defined direct user (e.g., residential or industrial customer) and presents clear goals around planning PV solar panel fabrication. 2. Contains at least one ***mathematical model*** per student team member on which a simulation is based. 3. Each mathematical model should be made into a ***simulation*** that enables the direct user to explore and ***visualize*** the relationship(s) between the inputs and outputs of the mathematical model. 4. Is highly interactive. (e.g., the user is allowed to manipulate input variables and output displays) 5. Is easy to use and operate.
Provide proper citations for a rapid prototype	• Citations must be in APA format • Citations must appear as in-text citations in the concept generation list; format should be (Author or short title, year)

Appendix N QDSC Design Project – Milestone 6 Learning Objectives

Learning objective	To demonstrate full achievement:
Document changes based on feedback	• Summarize feedback in own words • Clearly articulate changes made based on feedback
Create a detailed file, tag, and variable inventory	For each GUI, • Appropriate filename is provided • All user-interactive and code-manipulated components are assigned Tags using the standard tag naming conventions • Variables that must be shared within and between GUIs are listed
Create a complete set of professional looking GUI layouts	• Layouts for all GUIs are complete and consistent with Navigation Map and Rapid Prototypes • Use of components is appropriate for tasks • Layout is organized and text is clear and concise
Develop a complete set of detailed flowcharts in preparation for GUI coding	• All GUIs (or groups of similar GUIs) have a detailed flowchart • GUI filename(s) is(are) indicated on each flowchart • Coder is indicated on each flowchart • Each flowchart identifies all possible functional paths in detail (including error checking) • Flowchart symbols are used appropriately
Code GUI navigation and exit options	• Navigation options on all GUIs are consistent with the Navigation Map and operate as intended • Exit/Close options are included in appropriate locations and are operate as intended

Appendix O QDSC Design Project – Milestone 7 Learning Objectives

Learning objective	To demonstrate full achievement:
Document changes based on feedback	• Summarize feedback in own words • Clearly articulate changes made based on feedback
Code GUIs for proper functionality	All GUIs are fully functional.
Code GUI navigation and exit options	• Navigation options on all GUIs are consistent with the Navigation Map and operate as intended • Exit/Close options are included in appropriate locations and are operate as intended
Document authorship	• Contributing team member's name is listed on each GUI layout • Contributing team member's name is listed within the code in the template provided

Apply coding standards to GUIs	• All GUI files are named appropriately
	  o **nanohubGUI_sec###_team##**
	  o **citationGUI_sec###_team##** or if multiple GUIs, **citationGUIx_sec###_team##**
	  o All others filename suffixes should be either **_authorlogin** or **_sec###_team##** to indicate coding authorship
	• Code is properly commented throughout

Provide proper citations on GUIs	• Citation list is complete • All citations are in APA format • All citations appear as in-text citations on GUIs (as needed)

Appendix P QDSC Design Project – Milestone 9 Learning Objectives

Learning objective	**To demonstrate full achievement:**
GUI Layouts & Coding	
Meet project partner criteria	There must be evidence that all project partner criteria are fully being met in one cohesive solution that: 1. Targets a well-defined direct user and presents clear goals around planning PV solar panel fabrication. 2. Contains at least one mathematical model per student team member on which a simulation is based. 3. Each mathematical model should be made into a simulation that enables the direct user to explore and visualize the relationship(s) between the inputs and outputs of the mathematical model. 4. Is highly interactive. 5. Is easy to use and operate.
Code opening, citation, and other non-simulation GUIs for proper functionality	• All GUIs have full functionality with no operational errors
Code simulation 1 and associated GUIs for proper functionality	• All simulation 1 GUIs have full functionality with no operational errors
Code simulation 2 and associated GUIs for proper functionality	• All simulation 2 GUIs have full functionality with no operational errors
Code simulation 3 and associated GUIs for proper functionality	• All simulation 3 GUIs have full functionality with no operational errors
Code simulation 4 and associated GUIs for proper functionality	• All simulation 4 GUIs have full functionality with no operational errors
Code GUI navigation and exit options	• Navigation options on all GUIs are consistent with the Navigation Map and operate as intended • Exit/Close options are included in appropriate locations and are operate as intended
Document authorship	• Contributing team member's name is listed on each GUI layout
	• Contributing team member's name is listed within the code in the template provided

Apply coding standards to GUIs	• All GUI files are named appropriately
	  o **nanohubGUI_sec###_team##**
	  o **citationGUI_sec###_team##** or if multiple GUIs, **citationGUIx_sec###_team##**
	  o All others filename suffixes should be either **_authorlogin** or **_sec###_team##** to indicate coding authorship
	• Code is properly commented throughout

Provide proper citations on GUIs	• Citation list is complete • All citations are in APA format • All citations appear as in-text citations on GUIs (as needed)

VITA

VITA

EDUCATION

Doctor of Philosophy in Engineering Education (Ph.D.)
Expected Graduation: August 2016
Purdue University, *West Lafayette, Indiana*

- Dissertation Title: Development of First-Year Engineering Teams' Mathematical Models through Linked Modeling and Simulation Projects
- Advisory Committee: Dr. Diefes-Dux, Dr. Madhavan, and Dr. Cardella (Engineering Education), Dr. Klimeck (Electrical and Computer Engineering), Dr. Boudouris (Chemical Engineering)

Bachelor of Science in Engineering (B.S.E.) Graduated: May 2011
Arizona State University (ASU) Polytechnic, *Mesa, Arizona*

- Primary Focus: Mechanical Engineering
- Secondary Focus: Materials Engineering

AWARDS

ENE Outstanding Research Award, Engineering Education, *Purdue University*
Spring 2015

- One award given by the School of Engineering Education to acknowledge outstanding research conducted.

2011 WISE Success Story Award, Women in Science and Engineering, *ASU*
May 2011

- Award received "in recognition of valuable contributions to Arizona State University Polytechnic"

ENGINEERING EDUCATION RESEARCH

Research Assistant, *Purdue University* August 2012 – Present
Network for Computational Nanotechnology (NCN) Cyber Platform (nanoHUB.org) (NSF EEC 1227110), PI: Dr. Gerhard, Co-PI: Dr. Madhavan, Supervisor: Dr. Diefes-Dux

- Conducted educational research as member of NCN education team focused on mathematical model and simulation development.

- Helped develop and implement a simulation design project subsequent to a modeling activity to teach first-year engineering students about models and simulations.
- Presented research to an external review panel at two annual NSF Site Reviews.
- Disseminated findings through conferences, workshops, and well-developed groups on nanoHUB.org (e.g. nanohub.org/groups/edresearch) (my contributions: nanohub.org/members/68942/usage).

Researcher, *Purdue University* August 2012 – August 2013
Purdue Graduate Student Government (PGSG) Discovery Engagement and Learning (DEAL) Grant, Peer Researchers: Farshid Marbouti (Engr. Ed.), Hyunyi Jung (Math Ed.), Alena Moon (Chem. Ed.)

- Studied the perspectives of first-year engineering undergraduate and graduate teaching assistants to help further improve Purdue's First-Year Engineering Program.
- Completed the necessary documentation to receive IRB approval.
- Conducted 8 structured interviews, created a survey tool based on interview results, distributed survey to 89 participants, analyzed survey responses from 44 participants, and disseminated findings.

Research Assistant, *Purdue University* August 2011 – August 2012
Formative Feedback Impacting the Quality of First-Year Engineering Student Work on Modeling Activities (NSF EEC 0835873), PI: Dr. Diefes-Dux, Co-PI: Dr. Cardella

- Collaborated on a diverse research team to create pedagogical approaches to develop instructors' ability to provide effective feedback and students' abilities to write, interpret, and utilize feedback.
- Qualitatively analyzed feedback from first-year engineering students to their peers and from teaching assistants to student teams on Model-Eliciting Activities (MEAs) to characterize the nature of their feedback.

Research Assistant, *ASU Polytechnic* Summer 2011
Teaching Engineering Design to Middle and High School Student using Rube Goldbergineering (funded by College of Technology and Innovation, ASU), Co-PIs: Dr. Jordan and Dr. Dalrymple

- Helped set up and put on summer camps for 6^{th} – 12^{th} grade students.
- Encouraged a positive learning environment by asking students questions that promoted critical thinking and nurturing teaming behaviors to ensure that all students were engaged in their Rube Goldberg projects.
- Participated in the data collection process by ensuring collection of consent forms from students and parents, organizing student work, and capturing additional data through well-strategized observation notes, computer screen capturing, pictures, and video recordings.

Research Lab Assistant, *ASU Polytechnic* Spring 2011
Cultivating Students' Adaptive Expertise Using Disassemble/Analyze/Assemble (DAA) Activities (funded by College of Technology and Innovation, ASU), PI: Dr. Dalrymple

- Structured a control group, experimental group, and combination group to prepare the necessary environments and materials for conducting research using the experimental method to analyze the effectiveness of Disassemble, Analyze, Assemble (DAA) pedagogy for teaching LabVIEW compared to a traditional lecture method.
- Developed DAA activities to encourage student learning on specific programming topics through challenging students to analyze and improve expert created LabVIEW programs in an ill-structured learning environment.

GRANT WRITING EXPERIENCE

Purdue College of Engineering Graduate Student Organization Grant, Engineering Education Graduate Student Association (ENEGSA), *Purdue University*
Fall 2014

- Awarded $2,200 from the College of Engineering to fund ENEGSA for a year – $1,200 for organization expenses and $1,000 for our proposal to increase undergraduate students' awareness and understanding of graduate school.

Research in Engineering Education Grant, *National Science Foundation (NSF)*
Fall 2013

- Participated in writing awarded NSF Research in Engineering Education (REE) Grant to further investigate feedback (Title: Expert-Novice Framework to Support Student and Instructor Feedback on Design, Award Number: 1329304, Awarded Amount: $300,00, PI: Dr. Cardella, Co-PI: Dr. Diefes-Dux).

Discovery, Engagement, and Learning (DEAL) Grant,
Purdue University – Purdue Graduate Student Government (PGSG) Fall 2012

- Awarded $1,980 to complete a mixed-methods study within an interdisciplinary team of STEM graduate students.

TEACHING EXPERIENCE

Presenter, Honors First-Year Engineering Teaching Assistant Training, *Purdue University*
Fall 2014

- Provided TAs with sample solution to practice giving feedback on, analyzed their written feedback, created a tailored presentation with samples of their feedback to teach effective feedback skills, and presented materials.

Expert Reviewer, First-Year Engineering, *Purdue University – nanoHUB.org*
Spring 2013, 2014, 2015

- Reviewed 5 to 15 student teams' design projects 1 to 2 times per semester to give them constructive feedback to help them improve their projects and scaffold their understandings of nanotechnology, models, and simulations.

Presenter, Honors First-Year Engineering Teaching Assistant Training, *Purdue University*
Fall 2014

- Provided TAs with sample solution to practice giving feedback on, analyzed their written feedback, created a tailored presentation with samples of their feedback to teach effective feedback skills, and presented materials.

Presenter, Training: Introduction to NanoRoughness MEA, *Arizona State University*
Summer 2013

- Collaborated with colleagues to host a 2.5 day interactive workshop to train faculty and graduate students how to implement and assess a model-eliciting activity (MEA) in an electrical engineering class.

Guest Lecturer, First-Year Engineering, *Purdue University* Fall 2012, Spring 2013

- Developed an activity and associated lecture material for a one-hour lesson to teach effective feedback skills.
- Taught the activity in a required FYE course (2 sections - up to 120 students/section).
- Revised the activity before instructors of all 14 sections of the required FYE course implemented in their class.

ENGINEERING EXPERIENCE

Project Manager, Capstone Project – Honeywell, *ASU Polytechnic*
August 2010 – May 2011

- Led a multidisciplinary team of two technology and three engineering students through design and manufacture of an innovative touchscreen-testing machine to meet customer's constraints and criteria with a $20,000 budget.

Engineering Intern, Refrac Systems, *Chandler, Arizona* April 2009 – February 2011

- Inspected aeronautical and medical parts after diffusion bonding and brazing processes to ensure proper bonding/filleting, hardness, strain, and other quality requirements per customer requests.
- Monitored deflection (strain), temperature, pressure applied, and vacuum readings of the furnace chamber and pump lines during the diffusion bonding and brazing processes to obtain optimal results in final inspection.
- Evaluated the tolerance of the in-house inspection tools quarterly to ensure tools met the ISO 9000 standards, including calipers, micrometers, height indicators, and dial indicators.

JOURNAL PUBLICATIONS

1. Kong, Y., Douglas, K. A., **Rodgers, K. J.**, Diefes-Dux, H. A., & Madhavan, K. (in review). Size and scale framework and assessment for first year engineering students. *Journal of Engineering Education*.

2. Verleger, M., Diefes-Dux, H. A., & **Rodgers, K. J.** (in press). Selecting effective samples to train students for artifact peer review. *Journal of Engineering Education*.
3. **Rodgers, K. J.**, Horvath, A. K., Jung, H., Fry, A. S., Diefes-Dux, H. A., & Cardella, M. E. (2015). Case study: Solution changes based on feedback in problem-based learning. *Interdisciplinary Journal of Problem-Based Learning*, 9(2).
4. Jung, H., Horvath, A. K., Diefes-Dux, H. A., **Rodgers, K. J.**, & Cardella, M. E. (2015). Characteristics of feedback that influence student confidence and performance during mathematical modeling. *International Journal of Engineering Education, 31(1), pp. 42–57*.

JOURNAL PUBLICATIONS in PREPARATION

1. **Rodgers, K. J.**, Diefes-Dux, H. A., Zielinski, M., & Madhavan, K. (in progress). Students' definitional knowledge of mathematical models. *Journal of Engineering Education.*
2. **Rodgers, K. J.**, Diefes-Dux, H. A., Zielinski, M., & Madhavan, K. (in progress). Investigating students' definitional knowledge of simulations. *IEEE Transactions on Education.*
3. Rynearson, A. M., **Rogers, K. J.**, & Diefes-Dux, H. A. (in progress) A revisit of the occupational and aspirational items of the Engineering Identity Development Scale. *Journal of Pre-College Engineering Education Research [J-PEER]*.

PEER-REVIEWED CONFERENCES with PROCEEDINGS

1. **Rodgers, K. J.**, Boudouris, B., Diefes-Dux, H. A., & Harris, M. (2016). Integrating exposure to nanotechnology through projectwork in a large first-year engineering course. *Proceedings of the 123rd ASEE Annual Conference and Exposition.* New Orleans, LA. June 26-29.
2. **Rodgers, K. J.**, Diefes-Dux, H. A., & Madhavan, K. (2015). Impact of simulation development on mathematical model development. *Proceedings of the Research in Engineering Education Symposium (REES),* Dublin, Ireland, July 13-15.
3. Diefes-Dux, H. A., **Rodgers, K. J.**, & Madhavan, K. (2015). Students' understanding of mathematical models, simulations, and their relationship. *Proceedings of the Research in Engineering Education Symposium (REES),* Dublin, Ireland, July 13-15.
4. **Rodgers, K. J.**, Kong, Y., Diefes-Dux, H. A., & Madhavan, K. (2015). Framework of basic interactions to computer simulations: analysis of student developed interactive computer tools. *Proceedings of the 122nd ASEE Annual Conference and Exposition.* Seattle, WA. June 14-17.
5. **Rodgers, K. J.,** Diefes-Dux, H. A., Madhavan, K., & Kong, Y. (2014). Mini Workshop – Developing engineers for a changing world through modeling and simulation-based pedagogy. *Proceedings of the 44th ASEE/IEEE Frontiers in Education Conference,* Madrid, Spain, October 22-25.

6. **Rodgers, K. J.**, Marbouti, F., Shafaat, A., Jung, H., & Diefes-Dux, H. A. (2014). Influence of teaching assistants' motivation on student learning. *Proceedings of the 44th ASEE/IEEE Frontiers in Education Conference,* Madrid, Spain, Oct. 22-25.
7. **Rodgers, K. J.**, Tafur, M., Marbouti, F., & Siepel, J. (2014). Physical response to feedback in game-based learning. *Proceedings of the 44th ASEE/IEEE Frontiers in Education Conference,* Madrid, Spain, October 22-25.
8. Shafaat, A., Marbouti, F., & **Rodgers, K. J.,** (2014). Utilizing MOOCs for blended learning in higher education. *Proceedings of the 44th ASEE/IEEE Frontiers in Education Conference,* Madrid, Spain,
9. Kong, Y., Diefes-Dux, H., **Rodgers, K. J.**, Douglas, K. A., & Madhavan, K. (2014). Work in progress: Development and validation of a Nano Size and Scale Instrument (NSSI). *Proceedings of the 44th ASEE/IEEE Frontiers in Education Conference,* Madrid, Spain, October 22-25.
10. Hanoglu, O., **Rodgers, K. J.**, Kong, Y., Madhavan, K., & Diefes-Dux, H. (2014). Work in progress: First-year engineering students¹ knowledge of nanotechnology. *Proceedings of the 44th ASEE/IEEE Frontiers in Education Conference,* Madrid, Spain, October 22-25.
11. **Rodgers, K.J.**, Diefes-Dux, H. A., & Madhavan, K. (2014). Investigating first-year engineering students understanding of computer simulations and interactivity. *Proceedings of the 41st SEFI (European Society for Engineering Education) Annual Conference,* Birmingham, England.
12. **Rodgers, K. J.**, Kong, Y., Diefes-Dux, H. A., & Madhavan, K. (2014). First-year engineering students' communication of nanotechnology size and scale in a design challenge. *Proceedings of the 121st ASEE Annual Conference and Exposition.* Indianapolis, IN. June 15 – 18.
13. Jung, H., Moon, A., **Rodgers, K. J.**, & Marbouti, F. (2013). Mathematical modeling problems: What affects teaching assistants' ability to provide feedback? *Psychology of Mathematics Education*. Chicago, IL. November 14 – 17.
14. **Rodgers, K. J.**, Diefes-Dux, H. A., & Madhavan, K. (2013). Case studies: First-year engineering nanotechnology-based design projects. *Proceedings of the 43rd ASEE/IEEE Annual Frontiers in Education Conference,* Oklahoma City, OK. October 23-26.
15. Moon, A., Jung, H., Marbouti, F., **Rodgers, K. J.**, & Diefes-Dux, H. (2013). Undergraduate and graduate teaching assistants' perceptions of their responsibilities – factors that help or hinder. *Proceedings of the 43rd ASEE/IEEE Annual Frontiers in Education Conference,* Oklahoma City, OK. October 23 – 26.
16. **Rodgers, K. J.**, Diefes-Dux, H.A., & Madhavan, K. (2013). First-year engineering students explore nanotechnology in engineering. *Proceedings of the 40th SEFI (European Society for Engineering Education) Annual Conference.* Leuven, Belgium. September 16 – 20.
17. **Rodgers, K. J.**, Diefes-Dux, H.A., Madhavan, K., & Oakes, B. (2013). First-year engineering students' learning of nanotechnology through an open-ended project. *Proceedings of the 120th ASEE Annual Conference and Exposition.* Atlanta, GA. June 23 – 26.

18. Marbouti, F., **Rodgers, K.J.**, Jung, H., Moon, A., & Diefes-Dux, H. (2013). Factors that help and hinder teaching assistants' ability to execute their responsibilities. *Proceedings of the 120th ASEE Annual Conference and Exposition.* Atlanta, GA. June 23 – 26.
19. **Rodgers, K. J.**, Fry, A. S., Diefes-Dux, H. A., & Cardella, M. E. (2012). First-year engineering students' peer feedback on open-ended mathematical modeling problems. *Proceedings of the 42nd ASEE/IEEE Annual Frontiers in Education Conference,* Seattle, WA. October 3 – 6.
20. **Rodgers, K. J.**, Diefes-Dux, H. A., & Cardella, M. E. (2012). The nature of peer feedback from first-year engineering students on open-ended mathematical modeling problems. *Proceedings of the 119th ASEE Annual Conference and Exposition,* San Antonio, TX. June 10 – 13.
21. Mathis, P. D., **Rodgers, K. J.**, Huffman, T. J., Purzer, S., & Gong, Y. (2012). Comparing the process of modeling for local and global problems completed by first-year engineering students. *Proceedings of the American Society of Engineering Education (ASEE) Illinois-Indiana Section*. Valparaiso, IN.

OTHER CONFERENCES and PRESENTATIONS

1. **Rodgers, K. J.**, Kong, Y., Diefes-Dux, H. A., & Madhavan, K. (2015). Development of a guided-instructional tool for evaluating simulations. *Poster presented at Engineering Education (ENE) Industrial Advisory Council semester review meeting*, West Lafayette, IN. April 14.
2. **Rodgers, K. J.**, Kong, Y., Diefes-Dux, H. A., & Madhavan, K. (2014). Development of a guided-instructional tool for evaluating simulations. *Poster presented at Engineering Education (ENE) Industrial Advisory Council semester review meeting*, West Lafayette, IN. November 7.
3. **Rodgers, K. J.**, Kong, Y., & Madhavan, K., Diefes-Dux, H. A. (2014). Development of a guided-instructional tool for evaluating simulations. *Poster presented at first nanoHUB user conference*, Phoenix, AZ. April 9 – 11.
4. Kong, Y., Diefes-Dux, H. A., & **Rodgers, K. J.** (2014). Nano size and scale instrument (NSSI). *Poster presented at first nanoHUB user conference,* Phoenix, AZ. April 9 – 11.
5. **Rodgers, K. J.**, Diefes-Dux, H. A., Jung, H., & Cardella, M. E. (2013). A comparative analysis of feedback from undergraduate and graduate teaching assistants on open-ended problems. *Paper presented at the annual meeting of the 2013 American Educational Research Association.* San Francisco, CA. April 26 – May 1.
6. Jung, H., Diefes-Dux, H.A., **Rodgers, K. J.**, Cardella, M. E., & Horvath, A.K. (2013). Characteristics of feedback that influence student confidence and performance during mathematical modeling. *Paper presented at the annual meeting of the 2013 American Educational Research Association.* San Francisco, CA. April 26 – May 1.

7. **Rodgers, K. J.**, Diefes-Dux, H. A., & Cardella, M. E. (2012) Preparing first-year engineering students to give effective peer feedback on open-ended mathematical modeling problems. *Poster presented at the Annual Graduate Student Educational Research Symposium*. West Lafayette, IN.
8. **Rodgers, K. J.**, Diefes-Dux, H. A., & Cardella, M. E. (2012) Learning to engage in peer review: a foundational aspect of stem practice. *Poster presented at the 2012 Sigma Xi Graduate Student Research Awards Competition Poster Session*. West Lafayette, IN.
9. **Rodgers, K. J.** (2011) Formative feedback: Impacting the quality of first-year engineering student work on model-eliciting activities. *Poster presented at the New Directions in Engineering Education Symposium*. West Lafayette, IN.

WORKSHOPS

1. Diefes-Dux, H., Marbouti, F., **Rodgers, K. J.**, & Shafaat, A. (2015). Feedback for systems engineers. *Workshop presented at International Council of Systems Engineers (INCOSE) Regional Conference. Cleveland, OH.* Oct. 25.
   - Conducted a professional development workshop for system engineers to improve their peer feedback skills.

2. **Rodgers, K. J.**, Hart, M., Budnik, M., Shuba, T., & Kong, Y. (2014). Nanotechnology as the content for stem learning & teaching. *K-12 Workshop presented at the 121st ASEE Annual Conference and Exposition. Indianapolis, IN.* June 14.
   - Organized a team and necessary materials to present to middle and high school teachers on how to introduce nanotechnology, focusing on size and scale, within curricula in a 2.5-hour session using interactive activities.

3. **Rodgers, K. J.**, Diefes-Dux, H. A., & Madhavan, K. (2013). NanoRoughness Model-Eliciting Activity (MEA). *Workshop presented at National Academy of Minority Engineering Program Association* (*NAMEPA), Purdue University: West Lafayette, IN*. Feb. 6 – 9.
   - Engaged 20-30 university administrators in a model-eliciting activity and discussed benefits of utilizing this pedagogy with emphasis on inclusion of underrepresented students.

ENGINEERING EDUCATION OUTREACH

Panel Speaker, Honors First-Year Engineering, *Purdue University*

Spring 2015

- Organized three panels of five engineering graduate students from various disciplines to increase first-year engineering students' awareness and understanding of graduate school; participated on one panel.

Volunteer, Women in Engineering Program (WiEP), *Purdue University*

Spring 2013, 2014, 2015

- Facilitated activities to engage high school girls in various discipline of engineering through problem-based learning. (*Purdue University, Introducing Girls to Engineering Day – IGED, Spring 2013, 2014, 2015*)
- Taught engineering through problem-based learning. (*Woodland Elementary, 3rd grade, Spring 2013*)

Volunteer, Birck Nanotechnology Center – NanoDays, *Purdue University*

April 2013, 2014, 2015

- Introduced middle school kids to nanotechnology through building physical models, interacting with computational models, and engaging conversations about how nanotechnology can impact their lives.

Volunteer, Engineering Projects in Community Service (EPICS), *Purdue University*

Fall 2013, Spring 2014

- Reviewed teams' projects and gave them constructive feedback at various phases of the design cycle.

Panel Speaker, American Society of Engineering Education (ASEE) Student Chapter, *The Ohio State University*

Fall 2014

- Participated on a panel to speak to undergraduate engineering students about engineering education research and my experiences in graduate school at Purdue University.

GRADUATE STUDIES COURSEWORK

- Selection of Completed Methods Courses:
  Qualitative Methods I & II; Models & Modeling Perspective; Applied Regression Analysis; Factor Analysis; Statistical Methods; Assessment Methods in Engineering Education

- Selection of Completed Engineering Education Courses:
  Content, Assessment, & Pedagogy; Theory Development & Engineering Thinking; Leadership, Policy, & Change in STEM Education; TA Perspectives I & II

- Completed Mechanical Engineering Courses:
  Micro/Nano Physical Processes; Bio-Inspired Robotics; Fundamentals of Wind Energy

SERVICE POSITIONS and MEMBERSHIPS

Student Member, Engineering Education Graduate Student Association (ENEGSA), *Purdue University* — Fall 2011 – Present

- **President** (Summer 2014 – Spring 2015): Led a team of graduate students through a year of community building (e.g., seminar with Dr. Hmelo-Silver, multiculturalism lunches).
- **Professional Development Committee Chair** (Summer 2013 – Spring 2014): Strategically planned Dr. Fortenberry's visit to present at the engineering education seminar and meet with graduate students.

Student Member, American Society for Engineering Education (ASEE)
January 2011 – Present

Graduate Student Member, ENE Faculty Search Committee, *Purdue University*
Fall 2014 – Spring 2015

- Served and voted on the committee to select faculty candidates for interviews, host candidates while at Purdue University, and advise department head on candidates to move forward.

Student Member, American Educational Research Association (AERA)
January 2012 – 2013

Founding Member, Women in Science and Engineering (W.I.S.E.), *ASU Polytechnic*
Spring 2009 – 2011

- Collaborated with a team of women to spearhead an encouraging environment for STEM women through mentoring.

SERVICE – REVIEWER

Interdisciplinary Journal of Problem-Based Learning (IJPBL) Nov. 2015

American Society for Engineering Education (ASEE) Annual Conference 2014, 2015, 2016

International Conference of the Learning Sciences (ICLS) Bi-annual Conference 2014, 2016

IEEE Frontiers in Education (FIE) Annual Conference 2012, 2013, 2014, 2015

Research in Engineering Education Symposium (REES) 2015

International Conference on Computer Supported Collaborated Learning (CSCL) Bi-annual Conference 2015

American Society for Engineering Education (ASEE) International Forum 2014