

WIP: Application of Enzyme Catalysis in Synthetic Environment as an Experiential Teaching Tool in Freshman Engineering Curriculum

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Abstract

This Work in Progress aims to address the need for practical analytical applications using basic programming skills for chemical and biomedical engineering students enrolled in a first-year engineering curriculum. First-year engineering curriculum typically focuses on the student knowledge developed through fundamental building block-based concepts from science, technology, engineering, and mathematics (STEM). While foundational coursework in engineering problem solving and design and basic programming using languages such as MATLAB are taught, the information is often provided to students in abstract terms with limited real-world connection. This has the potential to hinder students' perception of the importance of the topics, thus limiting their enthusiasm and participation in acquiring the necessary skills and eroding their developing engineering identity. To combat this, a chemical and biomedical engineering (CBE) specific section of an introduction to MATLAB course at an R1 institution was created and taught by a member of the CBE faculty with the goal of demonstrating more relevant applications of the discussed topics. This work provides a proposed project-based module about enzyme applications in the CBE industry. The study explores the use of fundamental MATLAB concepts such as matrix indexing, conditional statements, loops, and plotting into performing data filtering, transformation, and analysis of enzymatic chemical reactions as related to the listed applications. Future directions for module improvement were identified through usage of focused surveys to evaluate students' integration, knowledge development, as well as their overall engagement in the teams. An additional offering of the class in Spring 2026 will be used to help refine best practices for teaching real-world applications using programming language.

Introduction/Background

First-year engineering curriculum typically focuses on the student knowledge developed through fundamental building block-based concepts from science, technology, engineering, and mathematics (STEM). Specifically, at higher institutions across the United States, coursework for the freshman engineers generally includes mathematics courses, natural science courses, English courses, and fundamental engineering courses which typically covers topics focusing on the engineering design process and MATLAB programming respectively [1], [2], [3], [4]. The natural science and mathematics courses are typically being taught as self-distinguishing entities, with limited exploration of any interconnected relationships [5], [6], [7]. MathWorks MATLAB along with its toolboxes and Simulink, for instance, introduce students to the basics of programming in terms of coding logic and structure [8], [9], [10], as well as develops students' ability to translate engineering problems into pseudo-code problem [10], [11], [12] however often in abstract terms with limited real-world connections. At the fundamental level, freshman engineering MATLAB course generally involves matrices and arrays with indexing and manipulation, loops and logical functions, 2D plotting, and user defined input and outputs [13], [14], [15], [16], [17].

In addition, engineering coursework typically requires the gathering of known information for practical problem-solving experience with information to be evaluated and synthesized based on

data integration. Students recruited to engineering who do not comprehend how new information can be utilized to solve real-life problems could find their engineering experience challenging and thus could show limited enthusiasm and participation in acquiring new knowledge, thereby impairing their engineering identity [18], [19]. Therefore, project-based learning has been explored to help engineering students demonstrate problem solving skills while increasing their engineering identity. For instance, curricula have integrated the creation of game-based programming [20], development of window moving average filters [21] and integration with the discontinued LEGO Mindstorm NXT robotic units [22], [23] to expose students to practical concepts through the use of math programming language. However, while these fundamentals topics are necessary for the development of students' building blocks, real-life analysis problems (namely, Finite Element Analysis (FEA) [24], [25], Computational Fluid Dynamics (CFD) [26], [27], Digital Signal Processing (DSP) [28], [29], etc.) require the use of more advanced and complex numerical methods topics (i.e. root-finding via Newton-Raphson method [30], [31], [32], solving partial differential equations (PDEs) [31], [32], ordinary differential equations (ODEs) [31], [32], etc.) and have shown limited to no integration in the freshmen curriculum.

Herein, a synthetic module-based group project was developed to introduce practical concepts in an engaging way so that it helps freshmen students assimilate information about application of enzymes in a synthetic environment to support lifelong learning outcomes [33], [34]. For this, freshmen students enrolled in prerequisite to a chemical and biomedical engineering major at an R1 institution were introduced to the concepts of enzyme kinetics and how kinetics could be affected by inhibitors with specific application examples in beer brewing, wine-making process, laundry detergent production, chemotherapy drugs, alcohol dependency drugs, and biofuel production respectively. Such applications of enzymes were assessed through the student's ability to design a MATLAB analysis file that was capable of analyzing pertinent kinetic parameters with input from relevant literature references by (1) filtering data, (2) transforming filtered data into a linear regression to obtain slope and y-intercept, (3) calculating K_M and V_{max} , and (4) creating a "fitted" Michaelis-Menten curve for each of those data.

Project Approach

Proposed project topic

Enzymes were chosen based on their overall prevalence in nature and industrial processing as natural biological catalysts [35], [36], responsible for metabolic reactions with significantly rapid rates from pico- to micro-seconds [36], [37]. Biomedical scientists, engineers, and pharmacists leverage enzyme's specificity nature to develop disease diagnostic tools [38], markers [39], and novel drugs [40], [41] that are capable of targeting specific locations for drug release or treatment. In chemical engineering, enzymes serve as natural catalysts in industrial processes [42] from chemical plants, to food processing facilities [43], [44], [45], and water treatment plants [46], [47], [48], all utilizing enzymes to enhance production efficiency and optimize the performance of chemical reactions, by improving overall yield and sustainability respectively [42]-[48]. Michaelis-Menten model for enzymatic kinetic was the topic of the study since they are known traditionally to be simulated and researched with sets of ODEs in many high-level language coding programs such as C, Python, and MATLAB [49], [50]; the practical application of data analysis

was done via basic data filtering via conditional statements and logical indexing ($>$, $<$, $=$, $\sim=$, etc.) with the practical application of linear regression ($y = mx + b$) respectively.

The study population was composed of students enrolled in one introductory engineering course titled *Introduction to Chemical and Biomedical Engineering (CHE102)*, which is a prerequisite course for the advanced courses in the chemical and biomedical engineering department at an R1 institution. The course is primarily focused on teaching introductory MATLAB skills. A total of 20 students participated in this study design first offering. Teams were formed by pairing students based on their expressed interests in the given topic area, specifically beer brewing, wine-making process, laundry detergent production, chemotherapy drugs, alcohol dependency drugs, and biofuel production.

Course structure, project progression and deliverables

Students admitted to the engineering college at this institution must complete a common fundamentals of engineering curriculum, which includes a general introduction course to problem solving in MATLAB (ENGR 102). CHE 102 was first offered in Spring 2024 as an alternative to the general engineering version of the course. Because students are not required to declare a specific engineering major upon entry to the Fundamentals of Engineering Program, it is not required that students interested in chemical or biomedical engineering take the CHE version of the course, though it is recommended. All topics covered in the courses are identical, but the approach in CHE 102 involves direct application to chemical and biomedical engineering problems rather than spanning all engineering disciplines. Typical enrollment has been between 20 and 25 students, though the course could feasibly accommodate up to 55 students.

The project module was designed to accommodate 5 weeks with two classes per week. Prior to the project being released in Week 8, prerequisite MATLAB topics were covered from the beginning of the course up to conditional statements, as outlined in **Table A1**. Other preliminary topics included project management documentations (i.e., project charter, team charter, work breakdown structure, Gantt chart), structure of a technical report, and mechanisms of a PowerPoint presentation; however, these topics belonged to a prerequisite course that students must obtain a C- or higher to enroll in the CHE102 course.

In week 8 class 1, the instructor presented the project topic and its importance, then students were matched into groups based on their topic of interest. Once groups were formed, by the end of class, eight .csv files and the project description were made available to students to start performing their project. By the end of week 8, students were asked to submit their team charter and Gantt chart. Week 9 was dedicated to students conducting background research on the specific enzymatic reaction as a group, as well as researching the types of enzymatic inhibition in the specified applications.

Simultaneously, from week 9 to week 11, the students were asked to design a MATLAB file capable of analyzing the data files (in .csv format) by (1) filtering data from unwanted or outlier data, (2) transforming filtered data into a linear regression to obtain slope and y-intercept, (3) calculating K_M and V_{max} and (4) creating a “fitted” Michaelis-Menten curve for each of the data. Based on the calculated K_M and V_{max} values, students were then asked to categorize the inhibition types and justify their decisions. The students were asked to design and submit their MATLAB

file individually, whilst working with their group, in order to ensure collaborative discussion amongst the students to obtain the final solution together.

Weeks 12 and 13 were dedicated to project assessment based on the students' efficiency of the MATLAB analysis, the technical report evaluation, and their project presentation, with both assessment of content and quality produced and delivered by the team.

Data generated by the instructor

To ensure independent teamwork, each team received (1) one topic of enzyme application presented above, (2) eight .csv files and a MATLAB .m pre-written linear regression function file with a finite number of data points per file for each group, and (3) predefined number of competitive, uncompetitive, and noncompetitive inhibitions sets to compare against a standard amongst the 8 files. The data generator was developed in MATLAB via reverse engineering, meaning that the instructor established the K_M and V_{max} values beforehand for MATLAB to output the file based on the user's request. Briefly, the file asked for (1) the number of data points, (2) the intended value of V_{max} , (3) the intended value of K_M , (4) noise level, and (5) maximum substrate concentration respectively. The MATLAB code for this data generator can be found in the Appendix below.

Results and Discussion

Example of Student's Project Deliverables

Students were asked to perform and submit the following files: (1) team charter, (2) Gantt chart, (3) Background Research Summary, (4) MATLAB .m file, (5) technical report in a .doc or .docx format, and (6) presentation file in the .pptx format. The team charter and Gantt chart were submitted by the end of week 8. Briefly, the team charter comprised the team members' agreement of details such as meeting locations and times, responsibilities and contributions of each member towards the project, and the consequences of failure to meet established deadlines. Gantt chart reflected the breakdown of the projects' tasks with specific deadlines, and which team member was responsible for each task.

Students received:

- 8 files of 300-1500 data points
- 1 Standard + 7 “unknowns”

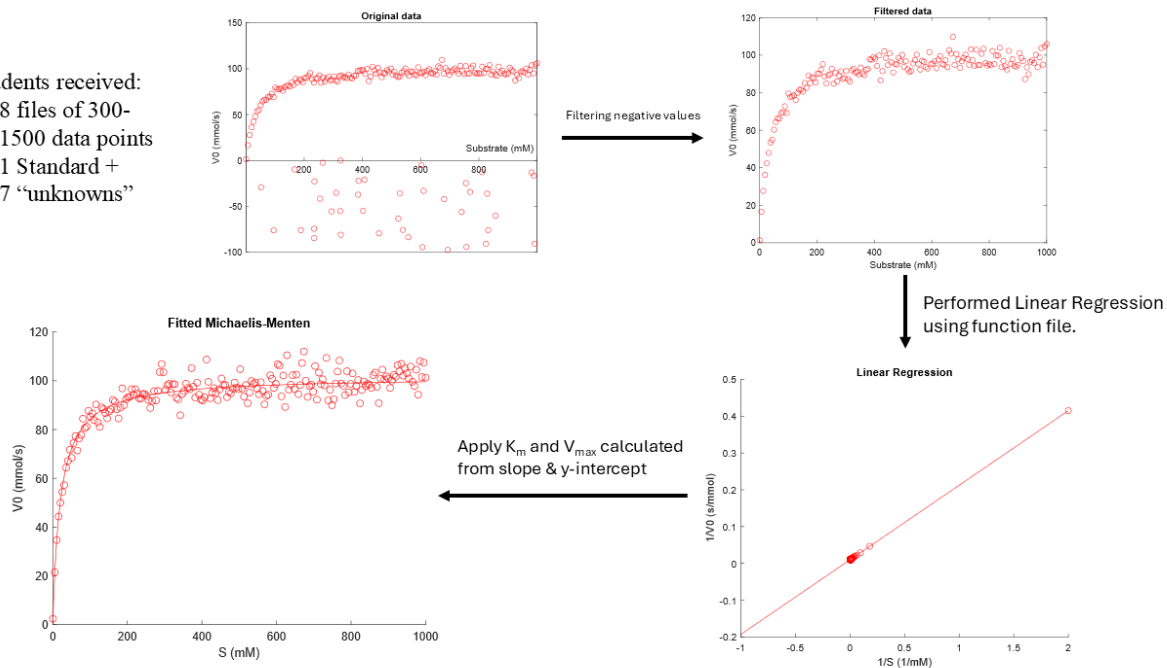


Figure 1. A step-by-step diagram to perform fitting for a Michaelis-Menten curve.

Table 1. An example of categorization of inhibition based on K_M (mM) and V_{max} (mmol/s) calculations. Yellow highlights signified a significant difference in either K_m or V_{max} values from the experimental batch file with respect to the standard file.

<u>File Name</u>	K_m (mM)	V_{max} (mmol/s)	Type of Inhibition
Standard	20.59	101.66	Standard
Batch 1	35.01	101.73	Competitive
Batch 2	6.01	85.17	Uncompetitive
Batch 3	20.62	75.99	Noncompetitive
Batch 4	20.53	61.17	Noncompetitive
Batch 5	46.07	101.85	Competitive
Batch 6	12.97	49.90	Uncompetitive
Batch 7	20.59	58.49	Noncompetitive

An overview guideline for students performing their Michaelis-Menten curve fitting in MATLAB was shown in **Figure 1**. Briefly, each given .csv file contains 2 columns, the first column is the substrate concentration (S, mM), and the 2nd column is the initial velocity (V_0 , mmol/s). Students started by importing the data to MATLAB using *readmatrix()* function, then used the for loop with a nested-if statement with logical indexing to filter the “outliers” values, in this case defined in the project description as the negative values of initial velocity, as “NaN”. “NaN”, in MATLAB, is defined as Not a Number value. The “NaN” was also applied to the same substrate concentration value with the filtered substrates columns and the filtered initial velocity of all 8 filtered files subsequently being combined into one singular variable. Both of the filtered variables were then inverted and the slope and y-intercept were calculated by applying the provided .m linear regression function file with a *for* loop. Students used mathematics and their understanding of linear regression to calculate K_M and V_{max} with V_{max} being the inverse of the y-intercept, and K_M being the slope multiplied by V_{max} . K_M and V_{max} were then applied into a *for* loop that allowed students to further calculate the initial velocity with substrate concentrations ranging from 0.1 mM to the maximum substrate concentration provided in the .csv files. Subsequently students were asked to plot each file’s Michaelis-Menten and its consequent Lineweaver-Burk in one figure window, resulting in 8 total figures, of which an example solution was presented in the Appendix. Subsequently, from the K_M and V_{max} values calculated, students can create a table and compare the experimental batch results to the standard file in order to categorize and justify the enzyme inhibition mechanism, as shown in **Table 1**.

To evaluate students’ ability to understand the module topic, a technical report and PowerPoint presentation was required per individual student team with such reports providing both theoretical information and practical analysis of concepts related to enzyme implementation. Briefly, the students needed to answer a set of questions developed to demonstrate the fulfillment of the project and students understanding of the given topics, with completion-assessed based on teams’ ability to answer predefined questions, namely:

1. Why are enzymes (in general) important in the specific industry / process you are working with?
2. What does the enzyme assigned to your group specifically do?
3. Aside from the specific enzyme, are there any other additional enzymes being used in the process? Provide information on names, roles and functions.
4. What are the other factors (aside from enzymes in general) that engineers need to account for to ensure the viability of the given enzyme-based application?
5. What are some of the inhibitors of the specific enzyme-based application? Give 2 or 3 specific examples of how the inhibitors slow down or interfere with the respective process.

Critical thinking analysis of MATLAB integration/ implementation was assessed to demonstrate understanding of enzyme applications in synthetic environments through the written report integration of responses to the following questions:

1. Why use “NaN” instead of marking it as a zero?
2. Why use “NaN” instead of removing that specific line of data? (This was asked in the context of a matrix: What happens when you are combining uneven vectors, would it work?)

3. Why was the student instructed to create a variable called S_LB containing values ranging from -1 to $\max(S_1)$?
4. Function file: what does $x(\sim \text{isnan}(x))$ mean?
5. How were K_M and $V_{\max}$ values calculated based on the equations given above?
6. What other way rather than using a nested-for loop analysis can be performed? For instance, one can reduce the number of loops from 2 to 1. How can that be accomplished?

Future Works

While this Work in Progress focused on understanding kinetics of enzymes involved in a variety of practical applications was carefully designed, it has some limitations. One limitation is that the study overlooked student familiarity with the concepts being introduced which could significantly affect their overall participation and report evaluation. As such, further assessment and analysis of the individual student's ability to integrate prompted knowledge is needed in future offerings of this class module to ensure transparent evaluation of their work in teams. For this, pre- and post-module familiarity will be assessed using structured surveys and analysis based on the Likert scale. Evaluating students' backgrounds at the start of the module can also inform the instructor of the students' abilities to understand and assess the topic, contribute appropriately to teams, while allowing them to identify weaknesses, or areas needing additional learning as related to the topic of the module.

The second limitation of this current study consists of lack of assessment of student integration in teams and their perception of the teams' dynamics in relation to their overall team contribution and evaluation for this project. Introducing pertinent and descriptive analysis of student participation in the team and how that leads to overall teamwork is very important for future offering to ensure a "team- focused" experience. As such, a summative assessment will be introduced to evaluate the collaborative skills among the team members along with their perception for team integration, with Likert-scale survey analysis to be integrated in future studies.

The third limitation of this study consists of the assessment of engineering identity development over the course of this project. The population of students that took part in the CHE 102 courses are predominantly students who have declared their major, specifically chemical engineering and biomedical engineering. The student's engineering identity can be further explored and compared between CHE 102 and other engineering majors with similar course structure design as well as projects related to linear regression application in future studies.

Furthermore, this study aims to expand by addressing the limitations acknowledged above for future studies, pending approval from the Institutional Review Board (IRB).

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Appendix

Table A1. Course topics introduced in CHE 102 with respect to project deliverables.

Week #	Topic Introduced	Project Progression and Deliverables
Week 1	Introduction to the course, Chemical and Biomedical Engineering majors	
Week 2	Basics of MATLAB - Creating variables and script files - Understand commonly used built-in functions - Relational (==, ~=, >, <, etc.) and logical (&&, , ~) operators	
Week 3	Order of precedence Indexing 1D arrays (vectors) - Vectors and matrices as function arguments - Scalar operations on vectors and matrices - Element-wise calculation Spreadsheet interface with Excel	
Week 4	Logical vectors and logical indexing Indexing 2D arrays (matrices) Linear algebra - Matrix multiplication - Solving systems of linear equations	
Week 5	Input and Output	
Week 6	2D Plotting	
Week 7	Conditional (if) Statements	
Week 8	Nested-if Statements Switch-case Statements	- Instructor provided background knowledge and project deliverables, - Students formed teams of 4, - Teams received .csv files related to the enzyme application of interest. <u>Project deliverable #1:</u> team charter and Gantt chart
Week 9	For loops	- Students were asked to perform a background research on the application of enzymes. - Students simultaneously began and performed their MATLAB coding. <u>Project deliverable #2:</u> Background Research Summary

Week 10	For loops with conditionals	Students progressed in their MATLAB coding project.
Week 11	While loops	Students finalized their MATLAB coding project. <u>Project deliverable #3:</u> Final MATLAB .m script file
Week 12	Loops with vectors and matrices (vectorizing)	Students wrote their technical report. <u>Project deliverable #4:</u> Technical Report
Week 13	Function files	Students prepared their presentation files and their oral presentation. <u>Project deliverable #5.1:</u> PowerPoint presentation files.
Week 14	<u>Project deliverable #5.2:</u> PowerPoint Presentation	
Week 15	Finals Week	

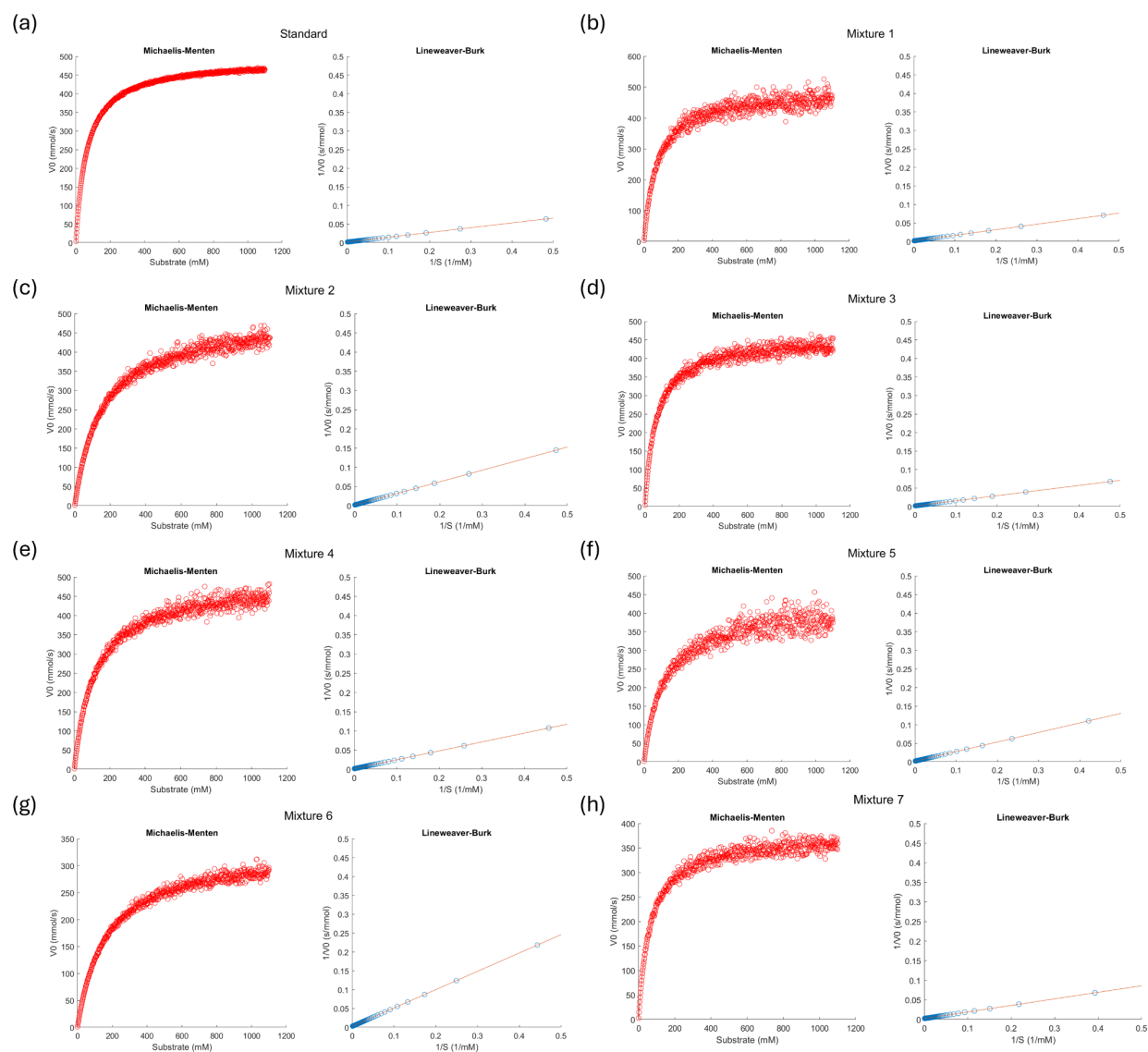


Figure A1. An example of the MATLAB coding project's solution with the "fitted" Michaelis-Menten (right) and Lineweaver-Burk linear regression (left) for the (a) Standard file, and (b-h) Mixture 1-7 files.