CBEE 102 (3 Cr.) – Engineering Problem Solving and Computations
Winter Quarter 2016
School of Chemical, Biological, and Environmental Engineering
Oregon State University
Updated 2016.01.25 11:50
PROJECT DESCRIPTION: Devil's Tower (Monte Carlo Simulation)

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Due Date: 2016.02.29 1700
(Absolutely no late projects will be accepted without pre-arranged consent of the instructors.)

Additional Information: Please refer to the syllabus for further information.

Team Project Grading: *20% of course grade*

MATLAB Code	60% of the project grade
Project Report	30% of the project grade
Administrative Tasks	10% of the project grade

If you determine that a regrade is necessary, the entire assignment will be regraded.

Timeline

- lec01: during the first lecture of the course (2016.01.04), a brief overview of the project will be given during the introduction of the course.
- ws01a: prior to the end of the first workshop section (2016.01.05), you will be required to complete a homework assignment surveying your interests and skills. This survey will help the instructors organize the students into teams.
- ws01b: during the second workshop section (2016.01.07), you will be organized into teams based on the results of the survey.
- lec04: during the fourth lecture of the course (2016.01.25), a theoretical background of the Monte Carlo method and a theoretical background of the diffusion problem will be given.
- ws04: during the fourth week of workshop exercises (ws04b), you will complete a brief experiment with your team to collect brute force data.
- lec05: at 1700 on 2016.02.01, the minutes of your required meeting with acknowledgement of the assigned tasks will be due.
- ws05: during the fifth week of workshop exercises, you will have your first project checkpoint meeting during one of your workshops with your instructor, where you will need to present an outline of your plan for completing the project.
- lec06: at 1700 on 2016.02.08, a penultimate flow chart of your project code will be due.

- ws07: during the seventh week of workshop exercises, you will have your second project checkpoint meeting during one of your workshops with your instructor, where the first draft of your report will be due.
- lec09: at 1700 on 2016.02.29, your team project will be due. Absolutely no late projects will be accepted.
- lec10: by 1700 on 2016.03.07, your team project assessments will be due to Charlotte Williams in the CBEE Main Office (Gleeson 103).

MATLAB Code: 60%

The MATLAB Code will be the major portion of your project. This MATLAB Code will produce a simple Monte Carlo simulation where a number of 2D random walkers (or "particles") will diffuse from a center origin radially outward. The random walk of these particles will be tracked, and a number of statistical values will be compared to the theory presented including the mean number of steps necessary for a particle to walk a set distance from the origin and the average final concentration of particles after a set number of steps.

The following list gives requirements for the code. Note that the *length scale* is give as one "stride" or motion of the particle, the *time scale* is give as one "step" or time between individual motions, and the *mass scale* is give as one "part" or an individual particle. This list should provide you a clear path toward creating a flow chart. Also, please realize that the following statement includes all of the parts of the code that were used to make the figures show in lec04; however, you may be able to write a working code that does not use the same set of steps. Further, in writing the solution used in lec04, the following pieces were not written in the order that they are presented here.

- Create one *m-file* script called "devil.m" that will be the only submission.
  - Explicitly required: make a header comment describing the program and giving overview of use/syntax to run it.
  - Explicitly required: use in-line comments describing the purpose of any non-trivial code.
  - Explicitly required: define a comment block containing description of each variable parameter and its physical significance.
- Create a set of non-dimensional values defining the number of particles (M), the number of steps (N), and the length of the stride (δr). Also, a (pseudo-)bound (B) is defined to calculate the average number of steps that are needed to reach a certain distance.
- Calculate the diffusivity ($\mathscr{D}$) from the information given, such that

$$\mathscr{D} = \frac{1}{4}\frac{[\delta r]^2}{\delta t}, \tag{1}$$

  where δt is exactly equal to the time to take one step, and we assume that each step is taken over the same time period. Note that $\mathscr{D}\,[=]\,\frac{\mathrm{L}^2}{\mathrm{T}}$ has units of $\frac{\text{stride}^2}{\text{step}}$.

- Calculate the estimate for the number of steps necessary to cross the bound, such that

$$\tilde{N} \approx \left[\frac{B}{\delta r}\right]^2. \tag{2}$$

- Initialize the arrays that will be used to store the location of the particles and the number of steps necessary to cross the predefined bound.
- Use a *random number generation* using `rand` to define the angle at which the particle will take its next step.
- Use a `for`-loop to track each particle that will be introduced.
- Use a `for`-loop to make each step that a particle will take.
- Calculate the new position of the particle based on the previous position, the step size, and the angle, using trigonometric functions.
- Use an `if`-statement to conditionally test for the number of steps that the particle takes to cross the boundary.
- Calculate the position of the particles in radial distance from the origin, the maximum radial position of all particles, and the standard deviation of the final position.
  - You are required to identify the first time step when they cross the bound.
  - The random walkers are allowed to continue beyond the bound.
- Calculate the maximum ring size that is needed to calculate the average concentration per concentric ring. Note that these rings will be integer scalers of the initial bound.
- Initialize an array having a length equal to the number of rings for storing the average concentration.
- Use a `for`-loop to calculate the final concentration as a function of radial distance (i.e., number of particles per area), based on the number of particles found in each ring.
- Remove all particles that did not cross the boundary from the Figure 4 statistics.
- Find the mean number of steps and the standard deviation necessary for the particles to cross the bound.
- Create the following figures.
  - Figure 1: create a *plot* of the solution (concentration versus radial position) to the 2D time-dependent diffusion equation as a function of time, such that

$$\hat{C} = \frac{M}{\pi\,(4\mathscr{D}t)} \exp\left[-\frac{r^2}{4\mathscr{D}t}\right], \tag{3}$$

    where $\hat{C}$ is a two-dimensional concentration (i.e., $\hat{C} = HC$, where H is the height, and C is the 3D concentration), r is the coordinate system in strides, and t is time in number of steps.
  - Figure 2: create a *scatter plot* representation of the ability of the function `rand` to provide an unbiased input using the data associated with the angle of the randon walk. This plot should show the angle divided by 2π as a function of the step for a given particle.
  - Figure 3: create a *cartoon* representation (MATLAB-generated plot) of the path of each particle past a ring at the desired bound distance. This plot should represent the particle paths as lines of different colors, and the plot should designate the end of the each particle's path with a red 'x'.

An m-file called `circle.m` has been added to Canvas at `<Files/project>`. You will be able to use this file to draw your circles on your plots.

- Figure 4: create a *histogram* (using the function `hist`) binning the total steps necessary for each particle to initially pass the desired bound, quoting the mean and the standard deviation of the set of trials in the legend or in a text label. Also, note the expected number of steps $\left(\tilde{N}\right)$.

$$\tilde{N} \approx \left[\frac{B}{\delta r}\right]^2 \tag{4}$$

- Figure 5: create a *cartoon* representation (MATLAB-generated plot) of the final position of each particle with rings at incremental distances.
- Figure 6: create a *scatter plot* representation of the concentration of particles in each annulus (s) after a certain amount of time, and compare this Monte Carlo prediction to the solution to Fick's second law of diffusion, where (M_s) is the number of particles in the s-annulus, and r_s is the radius of the outer edge of the s-annulus, respectively:

$$\hat{C} = \frac{M_s}{\pi\left(r_s^2 - r_{s-1}^2\right)}. \tag{5}$$

Note that $r_0 = 0$ in Equation (5) (i.e., the area of the first "annulus" is just the area of the circle with radius r_1).

- Print figures 1, 2, 4, 5, and 6 to PDF.
- Print figure 3 to JPEG.

In an effort to relieve confusion, please check back to this portion of the problem statement to find useful hints.

- No updates are available at this time.

Project Report: 30%

In addition to an electronic submission of your project code, a Project Report will be required. The Project Report should be no longer than five (5) pages for sections 1-7 listed below, including figures. A printout of the final flow chart will be added as an appendix. A printout of the MATLAB Code will be added as an appendix. The printed code is to be monospaced font with a minimum size of 72 columns, formatted by MATLAB "Print" output, NotePad++, or another syntax-highlighting program. An optional one-page appendix comparing and contrasting the use of `rand` versus `randn` can be added for extra credit with direct inference to the use of `randn` with the angle of the step and an accompanying speculation on its effect on the angle. No further content should be included. Please see the handout entitled "`CBEE_Technical_Writing_Guidelines_2013.pdf`" as a guide in writing your report and the handout entitled "`CBEE414ReportTemplate.pdf`" as an example of the expected professionalism. The project grade will include neatness and attention to formatting as given in the Technical Writing Guidelines. Also, note that the report must be typed, while any color figures must be printed in color. We understand that this report may be your first opportunity to experience technical writing, and we will take this generalization into consideration during the grading.

1. Abstract
2. Background
3. Experimental Materials and Methods
4. Experimental Results and Discussion
5. Computational Materials and Methods
6. Computational Results and Discussion
7. Conclusions

I. Appendix 1: Flow Chart
II. Appendix 2: MATLAB Code
III. Appendix 3 (optional): Random Number Generators

Administrative Tasks: 10%

- Survey
- Team meeting outside of class with assigned tasks
- First project checkpoint meeting
- Penultimate flow chart
- Second project checkpoint meeting
- Team assessment

FORM FOR PROJECT TEAM ASSESSMENT

A form entitled `2016w_cbee102_team_assessment.pdf` has been uploaded to the Project module. Every person must submit an assessment to receive credit for completing the project. The assessments are due Friday, 2016.03.04, to Charlotte Williams in the CBEE Main Office (Gleeson 103). We will go over this assessment during class on Monday (2016.02.29).

Project Submission

A physical version of your report is due at the start of class on Monday, 2016.02.29, at 1700. A digital version of your one MATLAB function file (devil.m) will be submitted through T.E.A.C.H. by Monday, 2016.02.29, at 1700. Information regarding how to submit a file through T.E.A.C.H. is provided below.

Submission to T.E.A.C.H.

Please submit your main MATLAB function file (one file) using the assignment submission system of the OSU Engineering T.E.A.C.H. website, which is located at the following website.

`https://secure.engr.oregonstate.edu:8000/teach.php`

Once you have accessed this web page, please do the following steps to submit your files (successful completion of these steps is part of this assignment):

1. Log into the T.E.A.C.H. system using your Engineering username and password.
2. Select "Submit Assignment" (under the "Class Tools" heading) in the menu on the right side of the screen.
3. Choose the "`project_matlab_script`" assignment from the pull-down menu that is displayed; then, select "Submit Query" to continue.
4. Select the "Browse..." buttons to upload one (1) files. Please upload your MATLAB function file (devil.m).
5. Select the "Submit Query" button to submit your files.

Note that, if you use MATLAB through Citrix, you will need to upload the files from your engineering home directory (i.e., Z: drive). Directions for accessing your ENGR home directory from your personal computer are available at the following website.

`http://engineering.oregonstate.edu/computing/fileaccess/windows_file_sharing/#map_network_drive`

If you need help submitting your MATLAB files, please see one of the TAs or the instructor.

Submit your completed project MATLAB files by 1700 on Monday, 2016.02.29.

Important Dates:

Midterm	2016.02.08 1100-1250
Project Deadline	2016.02.29 1700
Final Exam	2016.03.14 2000-2150

TECHNICAL WRITING GUIDELINES
CHE 334 (where appropriate) and CBEE 414-416

Unacceptable basic mistakes:

- Misspelled words
- Lack of introduction for a figure/table/equation in the preceding text
- Lack of title and/or detailed caption on a figure or table
- Unreasonable number of significant figures reported in Abstract/Conclusions
- Decimal written without leading zero
- Incomplete web site reference (site, date accessed, comments if appropriate)

Writing

- PROOFREAD YOUR WORK BEFORE YOU SUBMIT IT.
- Don’t write in the first person.
- Avoid starting sentences with prepositions, thereby being more direct and avoiding commas.
- No figures, tables, equations, or footnotes in the abstract.
- Introduce figures, tables, equation, etc., in the preceding text.
- All figures need a title below, e.g. "Figure 1", and caption that explains the figure. Make the caption summarize the relevance to somebody who has not read the report, i.e. it can stand alone.
- Titles for figures, tables, equations, etc., should be capitalized in the text, e.q. “Equation 1”.
- Don’t regurgitate/retype detailed information that is provided in a cited reference, e.g. a standard operating procedure (SOP). Provide sufficient details, but use a proper citation.
- Spell names correctly. If unsure, find out.
- Spell correctly and use the correct word: spellcheck may indicate a word is correctly spelled even if it is the wrong word. Some examples from previous years: “Miss counting”, “out liar”, “descent data”, “asses”, “ingrate”, “verse”.

Calculations and Technical Stuff

- Do not use unusual terms without introducing them first.
- Abbreviations and acronyms need be defined either at first use or in an appendix with reference.
- Use good judgment in deciding how many significant figures to report, e.g. if you’re using a rotometer to measure flow, don’t report 5 significant figures.
- Embrace terms like "prototype", "testbed" and "benchtop system". For example, you might use a prototype gas absorption column to assess mass transfer properties, then "scale up" to an actual system design.

Formatting

- Never write a decimal without a leading zero to ensure it's not mistaken as an integer: 0.62, not .62.
- Never start a sentence with a number, instead use “Thirty mL were delivered using a pipette.”
- Always put a space between a number and its units. It's easier to read and avoids alphanumeric confusion, e.g. If I write 6 liters as 6l, it sure looks like the number 61.
- Indent titles and captions on tables and figures and consider using smaller font, e.g. 10 pt, to make them stand out from the surrounding text. Some even use italics.
- Figures and tables should be centered on the page.

- Use "Ca^{2+}", "Na^{+}", etc. to represent ions. Elemental sodium (not ionic) would be "Na", and explosive when added to water!
- One often sees "Enclosure" at the bottom of the page. Is that not from the old days, when you "enclosed" something in the envelope?
- Many struggle in Equation Editor without the ability to put in spaces between numbers and units, etc. Try hitting Ctrl+space bar to put in spaces, or convert the entire equation to text style, which allows spaces.
- Italicize variables, e.g. t_b. It makes them stand out better to the reader.

TECHNICAL REPORT GUIDELINES

- *Abstract*
- *Background*[1]
- *Materials and Methods*
- *Results and Discussion*
- *Acknowledgements*
- *Appendices*

Some guidance about what these sections look like:

- *No Cover Page.*
- *Abstract* is a high-level summary and includes (1) objectives, (2) methods, and (3) results. The goal is 4-6 sentences. Emphasize *content*: settings, ranges, numbers, units. No references, equations, etc.
- *Background* should be shorter for CBEE 414 lab reports, with brief theoretical background, then broaden as you move to more open-ended labs and senior projects. Look for previous work on the subject, e.g. have others measured that mass transfer coefficient? How? What did they find? Use footnote references liberally.
- *Materials and Methods* provides details about what you did. It is written in past tense, a story of what was done, <u>not</u> in first person, not as instructions, and not as bullets. The level of detail should be sufficient to allow another worker to repeat your work without having you physically there. Include equipment, manufacturer, model, equipment schematics/pictures.[1] Cite provided documents/SOP.
- *Results and Discussion* is the section in which you present data, calculations performed, error analysis performed, and what you observe and conclude (trends, issues, etc.). It is where you compare experimental results with theory (or manufacturer-supplied) information. Most plots will be in this section. If there is a design component to your lab, include it in this section.
- *Acknowledgements*[1] are included to (1) thank those that helped you setup equipment, explained equipment, etc., but also to (2) provide a record of who helped you so that your readers might use that information, e.g. Jill knows how to run the gas chromatograph. Be succinct.
- *Appendices*[1] are a location for supporting details. Sample calculations are <u>required</u> and must include assumptions, unit, etc., so the reader can follow and check your computations. They can be hand-written if legible. A spreadsheet printout is not enough. Other content might include copies of raw data, equipment calibration data, non-critical charts, etc.

[1] Not necessary for CHE 334 reports.

Josephine Hornsnogger CBEE 414, Lab Section M 1300-1550 April 19, 2010

<u>Tornado Eddy Investigation</u>

Abstract

The objective of this lab was to write a bunch of jibberish to provide students with a formatting template. Chemical engineering, bioengineering, and environmental engineering are "process engineering" disciplines. Good abstracts contains real content, such as 560 mL/min, 35 deg, and 67 percent yield. Ideal degreed graduates are technically strong, bring broad system perspectives to problem solving, and have the professional "soft skills" to make immediate contributions in the workplace. The senior lab sequence is the "capstone" opportunity to realize this ideal by integrating technical skills and developing professional soft skills to ensure workforce preparedness. The best conclusions are objective and numerical, such as operating conditions of 45 L/min at 32 deg C with expected costs of $4.55/lb.

Background

Insect exchange processes are often used in bug filtration, as they are effective at removing either positive or negative insects from water. An insect exchange column is a packed or fluidized bed filled with resin beads. Water flows through the column and most of the insects from the water enter the beads, but some of them pass in between the beads, which makes the exchange of insects non-ideal. Insectac 249 resin is a cation exchange resin, as it is being used to attract cationic Ca^{2+} from the toxic waste stream. This means the resin is negatively charged, and needs to be regenerated with a solution that produces positively charged insects, in this case, salt water which contains Na^{+} insects. The resin contains acidic styrene backbones which capture the cationic insects in a reversible process.

A curve of Ca^{2+} concentration concentration vs. time was obtained after a standard curve was made to determine how many drops from the low cost barium test kit from Aquarium Pharmaceuticals (API)[1] bottle #2 would correspond to a certain concentration in solution. A standard curve works by preparing solutions with known concentrations and testing these concentrations using the kit to create a curve of number of drops from bottle #2 (obtained result) vs. concentration of Ca^{2+} in solution (desired response). The standard curve can then be used for every test on the prototype and in the field, to quickly and accurately obtain a concentration from the test kit.

The barium concentration vs. time curve can be used to calculate the exchange capacity of the resin and, in later tests, the regeneration efficiency. The curves must be used to get the total amount of barium removed from the water, *m*. Seen in Equation 2, the volumetric flow rate of water, $\dot{V}$, is multiplied by the integral from $t_{initial}$ to t_{final} of the total concentration of Ca^{2+} absorbed by the resin as a function of time, *C*.

$$m = \dot{V} * \int_{t\ initial}^{t\ final} C\ dt \qquad (2)$$

[1] *http://aquariumpharm.com/Products/Product.aspx?ProductID=72 , date accessed: 11/26/10*

A graphical trapezoid method was used to evaluate the integral and get the final solution in equivalents of Ca^{2+} per L, it must be noted that there are 2 equivalents per mole of barium, as the charge of the barium insect is +2. An initial exchange capacity was calculated for the virgin resin, and an adjusted exchange capacity was calculated once the resin was regenerated. The regenerated resin capacity was found by multiplying the virgin resin capacity by the regeneration efficiency, expressed in Equation 3.

$$Regeneration\ Efficiency = \frac{Ca^{2+}\ ejected\ during\ regeneration}{Ca^{2+}\ absorbed\ by\ virgin\ resin} \times 100\ \% \qquad (3)$$

See Appendix A for the calculation of the exchange capacities and the regeneration efficiency.

Materials and Methods

Rosalie and Peter Johnson of Corvallis established the Linus Pauling Chair in Chemical Engineering to honor Oregon State University's most famous graduate. Peter Johnson, former President and owner of Tekmax, Inc., a company which revolutionized battery manufacturing equipment, is a 1955 graduate of the College of Engineering.[2] The Chair, also known as the Linus Pauling Distinguished Engineer or Linus Pauling Engineer (LPE), was originally designed to focus on the traditional “capstone” senior lab sequence in the former Department of Chemical Engineering. The focus is now extended to all the process engineering disciplines. The LPE is charged with establishing strong ties with industry, ensuring current and relevant laboratory experiences, and helping upperclass students develop skills in communication, teamwork, project management, and leadership.

Include details about lab procedures not sufficiently detailed in the SOP, problems you had, etc.

The bulk solution prepared to create the standard curve was used in the second day of testing to obtain the exchange capacity of the insectac 249 resin. The solution was pumped through a bathroom scale into the prototype insect exchange column. 45 mL of resin was rinsed and added to the column. The bed was fluidized as the solution was pumped through the resin, but for the creation of the Ca^{2+} concentration vs. time curve, the solution was pumped down through the column, as illustrated in the process flow diagram seen in Figure 1.

Figure 1. Process sketch of the insect exchange column used for the project. Ref: http://www.generon.co.uk/acatalog/Chromatography.html

[2] *Harding, P. Viscosity Measurement SOP, Spring, 2010.*

A bathroom scale calibration curve was created to ensure that the 150 mL/min, used to calculate the breakthrough time, would be delivered to the resin. The bathroom scale used was a Dwyer brand with flowrates between 0 and 300 cc/min of water. Originally, values between 120 and 180 mL/min were chosen for the calibration, with three runs for each flowrate, however the bathroom scale values were so far away from the measure values the range was extended to 100 to 200 mL/min. The regeneration experiment was performed using a method similar to that used in the water softening experiment, however instead of using a 640 ppm Ca^{2+} solution to fill the resin, a 6000 ppm Na^{+} solution was used to eject the Ca^{2+} from the resin. Twelve samples times were chosen and adjusted as the experiment progressed, with more than half of the samples taken at times less than 10 minutes, and the last sample taken at 45 minutes. The bulk exit solution was also tested to determine the regeneration efficiency.

Results and Discussion

The senior lab sequence has its roots in the former Department of Chemical Engineering. CHE 414 and 415 were taught in Winter and Spring and included 6 hours of lab time per week. The School has endeavored to incorporate the courses into the BIOE and ENVE curriculum, and this will be complete in 2008-2009. Recent development of the senior lab course sequence is shown chronologically in Fig. 1. In 2006-2007, CHE 414 and 415 were moved to Fall and Winter to enable CHE 416, an elective independent senior project course. Also that year, BIOE students took BIOE 414 in the Fall and BIOE 415 was developed and taught. No BIOE students enrolled in the optional CHE. In 2007-2008, the program transitioned in a new Linus Pauling Engineer and ENVE 414 was offered. Also, approximately 30 percent of BIOE students enrolled in the optional CHE 416. Accommodating the academic calendars of the three disciplines required a reduction in weekly student lab time from 6 to 3 hours. The expected relationship between coughing rate, *y*, and length of canine, *x*, is

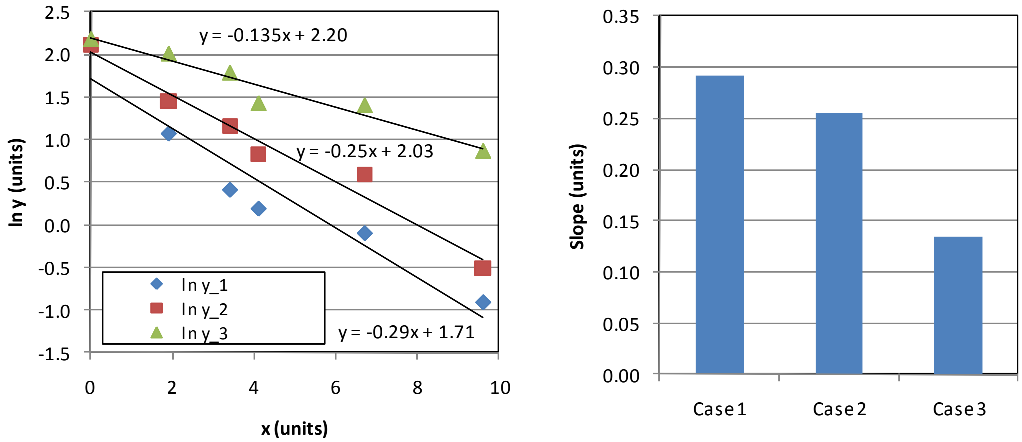
$$y = Fe^{-\frac{Bx}{z}} \qquad (1)$$

where *F* is a pre-exponential constant, *B* is vitamin B concentration and *z* is the height of an average trapeze artist.[3]

The 2008-2009 brings the challenge of the dramatic enrollment increase shown in Fig. 1 and the first offering of ENVE 415. The result, shown on the right in Fig. 1, is the delivery of the senior lab sequence uniformly across the process engineering disciplines. CBEE 416 is expected to drawn approximately of the students that take the 415 courses. In 2007-2008, 414 and 415 were required for CHEs, 414 and 415 for BIOEs, and only 414 for ENVEs. CHE 416 is ostensibly an elective for all disciplines. In 2008-2009, 414 and 415 is required for all disciplines and CHE 416 will be an elective. The content of 414 is essentially

[3] Fundamentals of Momentum, Heat, and Mass Transfer, Welty, J.R. et al., 4th edition, John Wiley & Sons, Inc.

identical for all three disciplines, 415 has discipline-specific labs, and 416 consists of senior projects with potentially cross-discipline teams of 2 to 4 students. Tremendous labor and struggling with the lab equipment resulted in the data shown in



(a) (b)

Figure 1. (a) Data for y and x plotted for various values of z and (b) a comparison of slopes for the 3 cases investigate. The log plot slope yields the vitamin B concentration. The slopes were shown to be significantly at the 90% confidence level, but the instructor ran out of time and did not include error bars.

The slope changed as predicted by the Snirtenhoffer equation. Improvements to the lab might include advice on how to legally change my name to something less embarrassing. My whole life I have been forced to repeat and spell it. I really feel that this has affected my psychologically.

This was perhaps the worst lab I have ever done in my academic career, primarily due to the fact that there was no lab time. I simply typed in this entire report and filled it with jibberish. Some might think nobody will notice, but I know that …… Harding reads every word.

Acknowledgments

The author acknowledges his elementary teacher for providing truly foundational instruction in addition and subtraction. Jenny Burninbalm was instrumental with guidance on use of the RT-345 dog scratching device.