

# Interactive Computing Activities as Chemical Engineering Educational Tools in University and Informal Learning Environments



**AIChE CAST Division Himmelblau Award 2022**

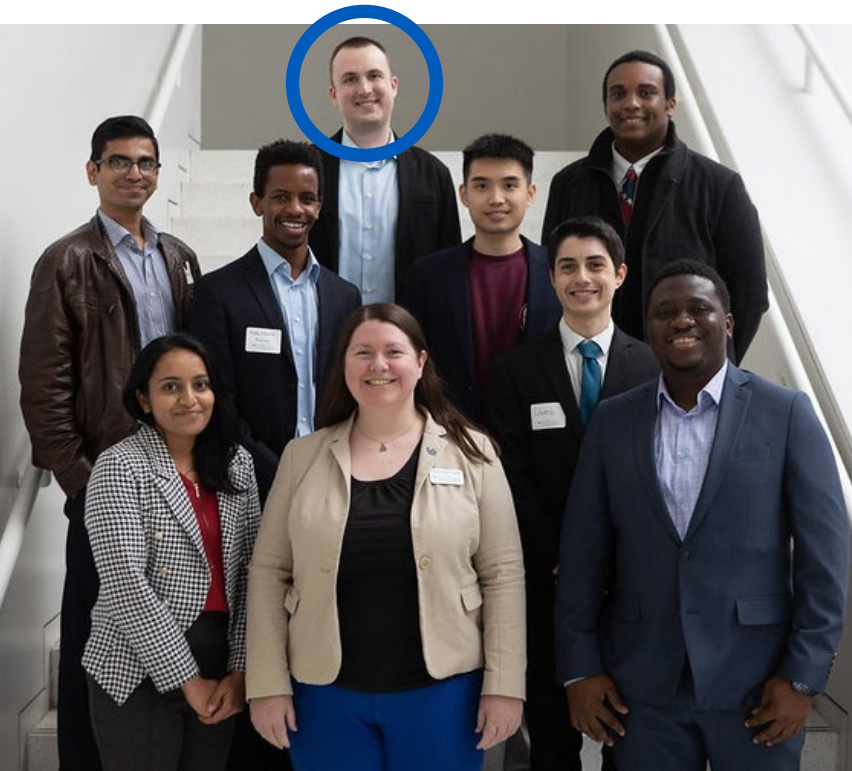
**Ashlee N. Ford Versypt, Ph.D.**  
**Chemical & Biological Engineering**  
**University at Buffalo, SUNY**  
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 **University  
at Buffalo**  
The State University of New York  
Download slides at [PSEcommunity.org/LAPSE:2022.XXXX](https://PSEcommunity.org/LAPSE:2022.XXXX)

# Goals for this webinar

- Showcase some computer-based tools we made broadly accessible to computing non-experts: students, educators, and lay people
  - graphical user interfaces (GUIs)
  - interactive notebooks (e.g., Jupyter Notebooks and MATLAB Live Scripts)
  - GitHub repositories
- Highlight examples of computational tools we have used in outreach/informal learning environments outside structured courses
- Share tips and lessons learned in designing and deploying outreach activities for non-university audiences
- Further disseminate materials for faculty and university student training

# Ford Versypt Lab: outreach volunteers & engineering education scholars



CACHE Corporation





# ASEE & CEE peer-reviewed publications

## AICHE Virtual Communities of Practice – Supporting Faculty during the COVID-19 Pandemic

Matthew W. Liberatore, Daniel Lepek, Laura P. Ford, Tracy Carter, Jennifer Pascal, Monica Lamm, Christi Patton Luks, David L. Silverstein, Ashlee N. Ford Versypt, Stephanie Butler Velegol, Troy Vogel, Neha Raikar, Matt J. Kipper, Christy Wheeler West

2021-11-05

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**Collection** 2021 ASEE Virtual Annual Conference Content Access  
**Authors** Ashlee N. Ford Versypt, *University at Buffalo*; Samantha Lyn Carpenter, *Oklahoma State University*; Troy Lamarr Adkins II, *Oklahoma State University*; Ted Anderson Sperry, *Oklahoma State University*; Yu Feng, *Oklahoma State University*

## Apps for Chemical Engineering Education: Off the Shelf and Do It Yourself Development Options

Ashlee N. Ford Versypt, Jason E. Bara, Rachel B. Getman, Chris A. Kieslich, Roman S. Voronov

2020-07-15

### Clean Water through Chemical Engineering: Introducing K-12 Students to ChE Using Filtration

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2019-03-06

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# Themes in these publications

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## Outreach/underserved populations

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## Skills development for university students and/or faculty

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# Outreach venues for our computational tools

- Chemical engineering design module
  - OSU College of Engineering, Architecture and Technology Summer Bridge Program for incoming freshmen
  - UB Chemical Engineering Camp for high school students
- Hands-on experiential “biomedical engineering major”
  - OSU Grandparent University for middle student students and their grandparents
- Expo booth
  - Oklahoma EPSCoR Women in Science Conference for junior high and high school girls and their teachers



# Pharmaceutical drug dosing for chemical engineering design

Pharmaceutical Drug Dosing

|                           |                         |           |
|---------------------------|-------------------------|-----------|
| Dose Size                 | 10                      | mg        |
| Dose Frequency            | 1                       | doses/day |
| Drug Options              | Patient Kidney Function |           |
| Drug 1: Benazepril        | Normal                  |           |
| Treatment Duration (Days) |                         |           |
| 1                         |                         |           |

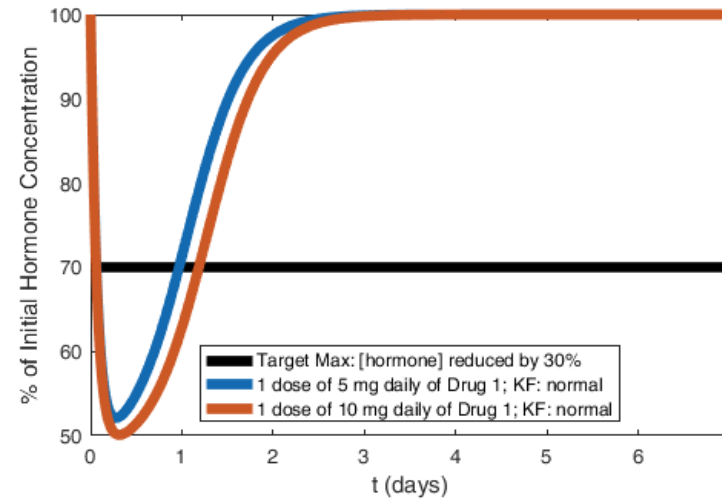
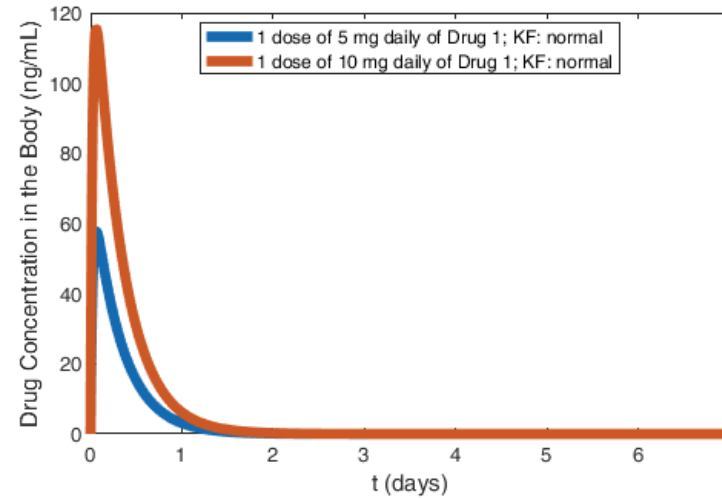
- Background Information
- Goal of the Project
  - About the Pharmaceutical Drugs
  - What is an ACE Inhibitor?

Plot Options

Layer Plots

Clear Plots

Save Top Plot    Save Bottom Plot



Run Simulation

# OSU Summer Bridge Camp for Engineering Freshmen

# UB ChemE Camp for HS Jrs & Srs

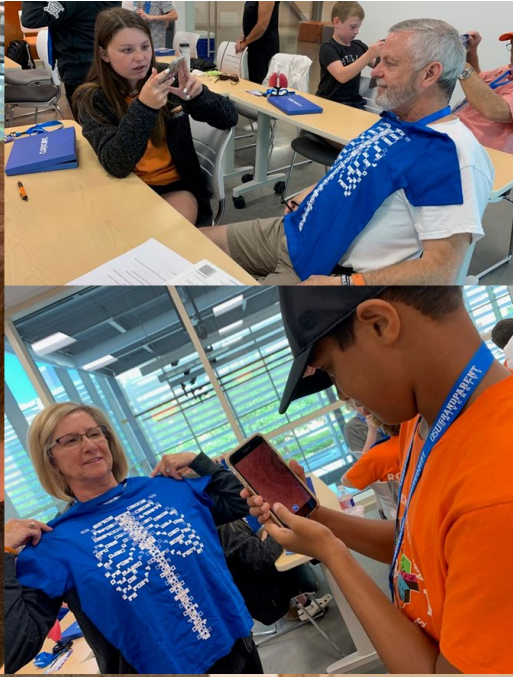


## Outline for the 90 minute session

- Section 1
  - Introductions
  - Introduction to design project topic: treating high blood pressure
  - Engineering design process
- Section 2
  - Use MATLAB app to simulate drug dosing and blood pressure regulation
  - Work on design project assigned case
  - Expand design project to additional cases
  - Compare cases
- Section 3
  - Chemical engineering of manufacturing of pharmaceuticals

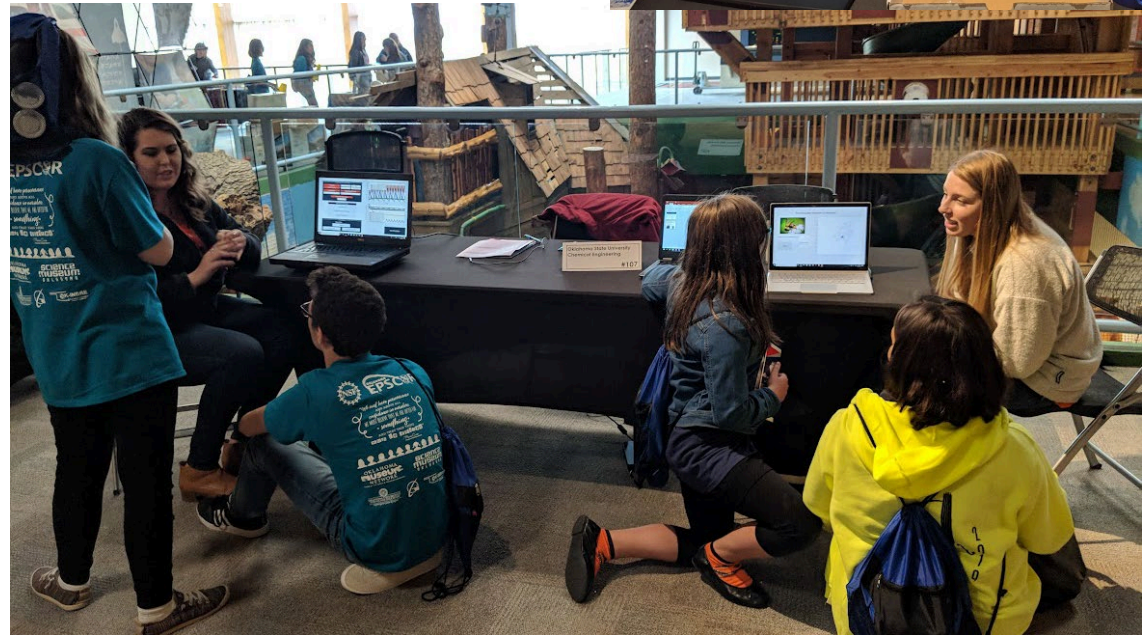
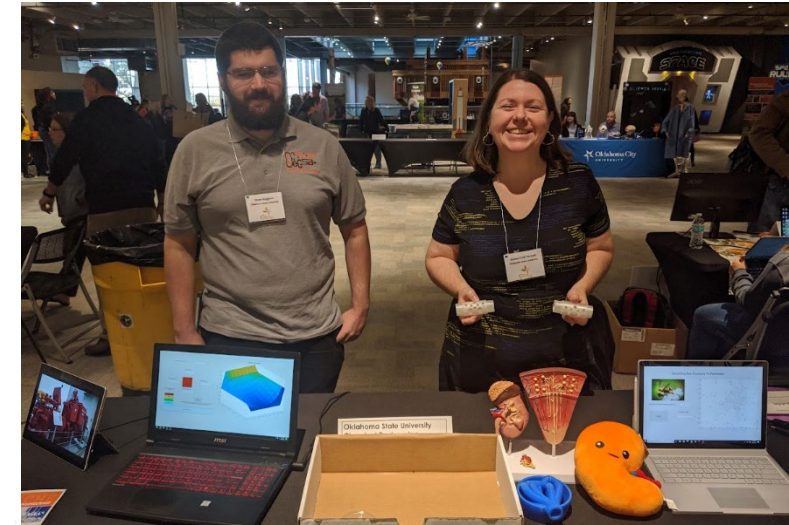


# Grandparent University





# Oklahoma Women in Science Conference



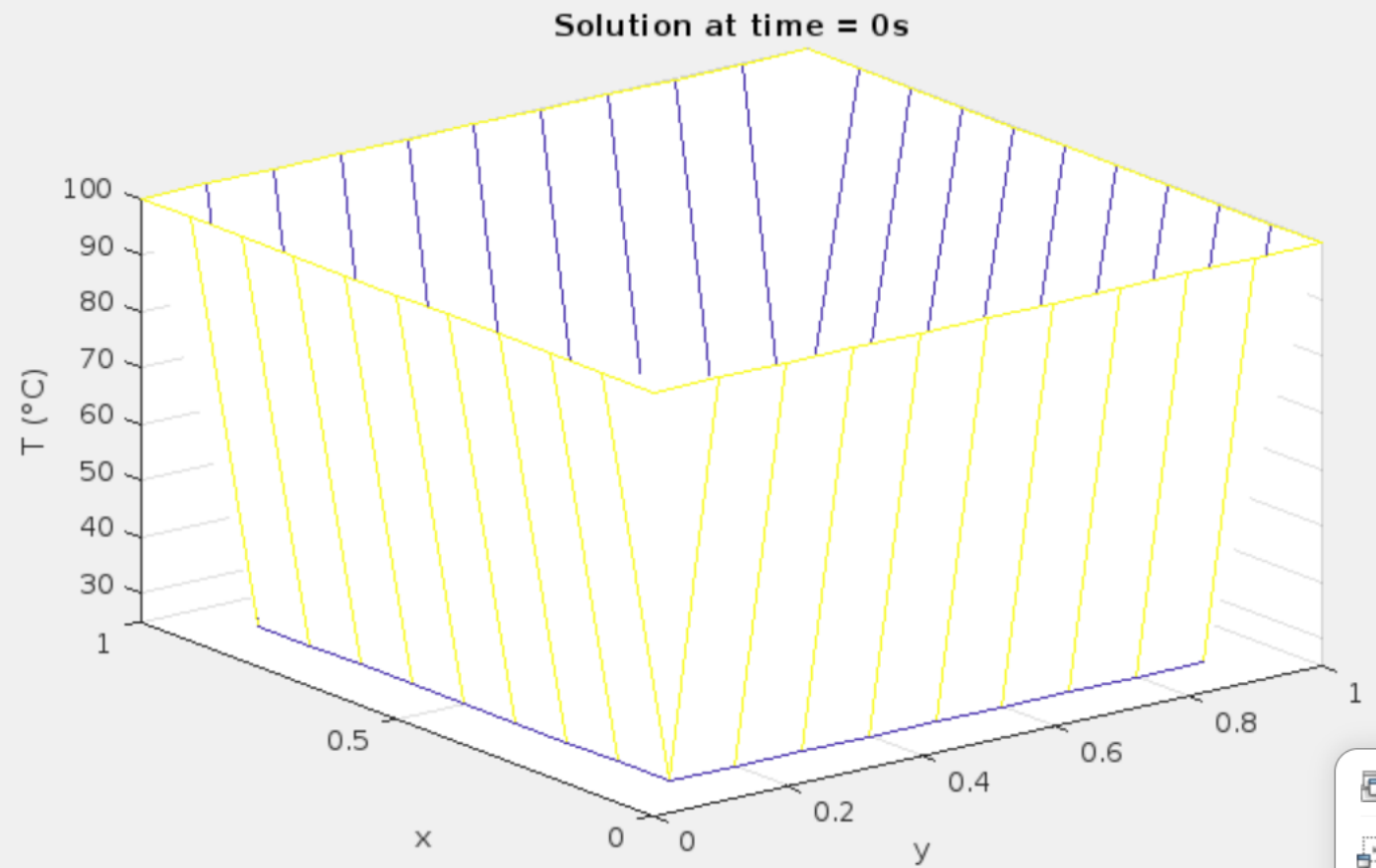


# 2D dynamic heat conduction

HeatTransfer\_2D

|   |                                   |
|---|-----------------------------------|
| Length of X = Length of Y:                        | <input type="text" value="1"/>    |
| Alpha Value                                       | <input type="text" value="0.25"/> |
| Delta Time:                                       | <input type="text" value=".01"/>  |
| Delta X = Delta Y:                                | <input type="text" value=".1"/>   |
| Left Boundary Condition:                          | <input type="text" value="100"/>  |
| Right Boundary Condition:                         | <input type="text" value="100"/>  |
| Bottom Boundary Condition:                        | <input type="text" value="100"/>  |
| Top Boundary Condition:                           | <input type="text" value="100"/>  |
| Uniform Initial Condition:                        | <input type="text" value="25"/>   |
| Current Fourier Number:                           | 0.25                              |
| Number of time intervals<br>displaved in the plot | 0                                 |

Calculate next time interval of 3 Delta t



# 2D dynamic heat conduction

HeatTransfer\_2D



Solution at time = 0.09s

Initial Temperature Inside the Square:

Cold T = 40 F

Top Edge Temperature:

Hot T = 100 F

Left Edge Temperature:

Warm T = 80 F

Right Edge Temperature:

Cold T = 40 F



Color key for Temperatures in the 2D rectangle

- Hot
- Warm
- Cool
- Cold

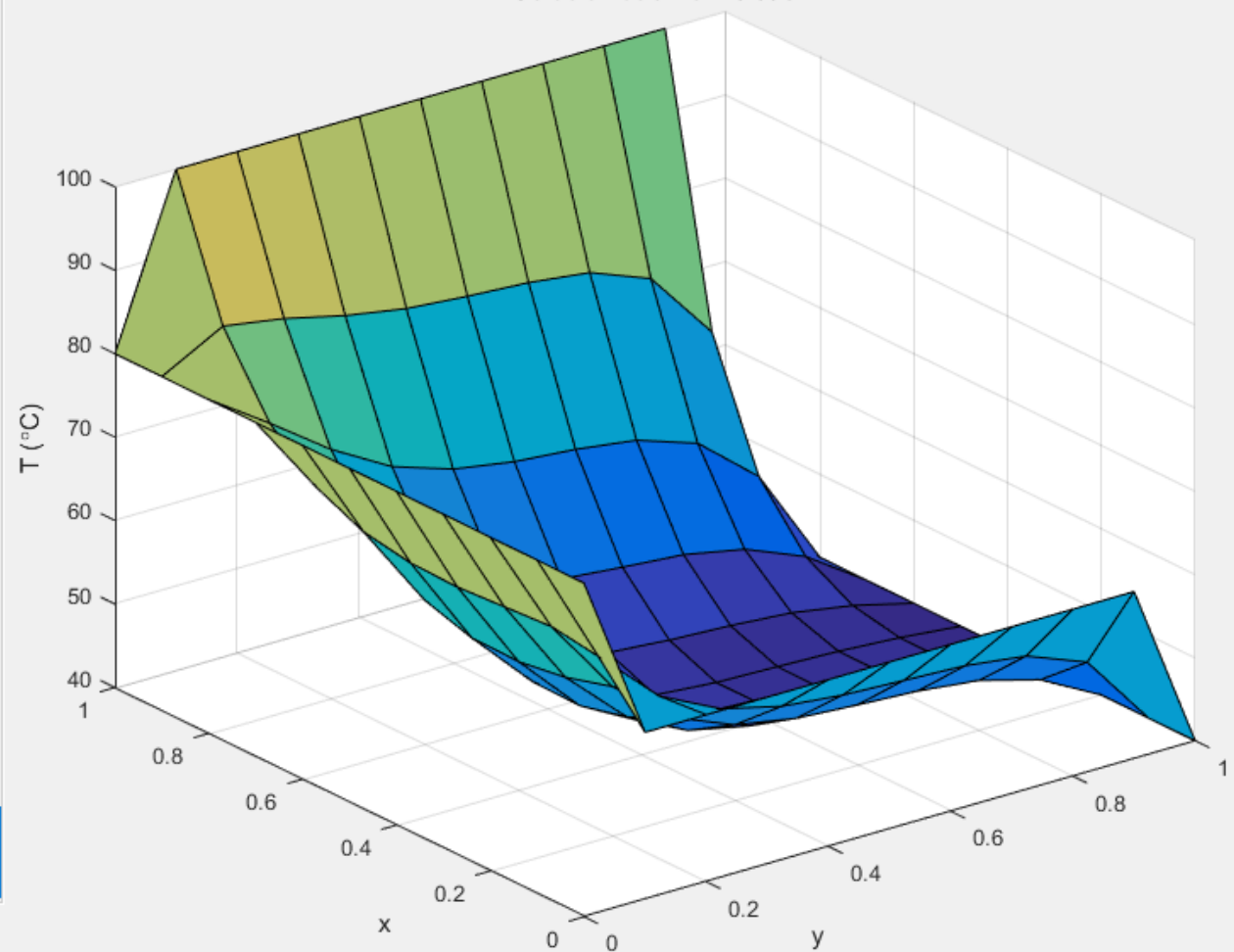
Bottom Edge Temperature:

Cool T = 60 F

Reset

NOTE: Reset will change all the temperatures (inside and edges) to 100 F as the starting point. However, the numbers displayed on the pop-up menu bar may not change

Calculate next time interval



# Bee responses to pesticides

BeeAttraction



## Simulating Bee Exposure to Pesticides



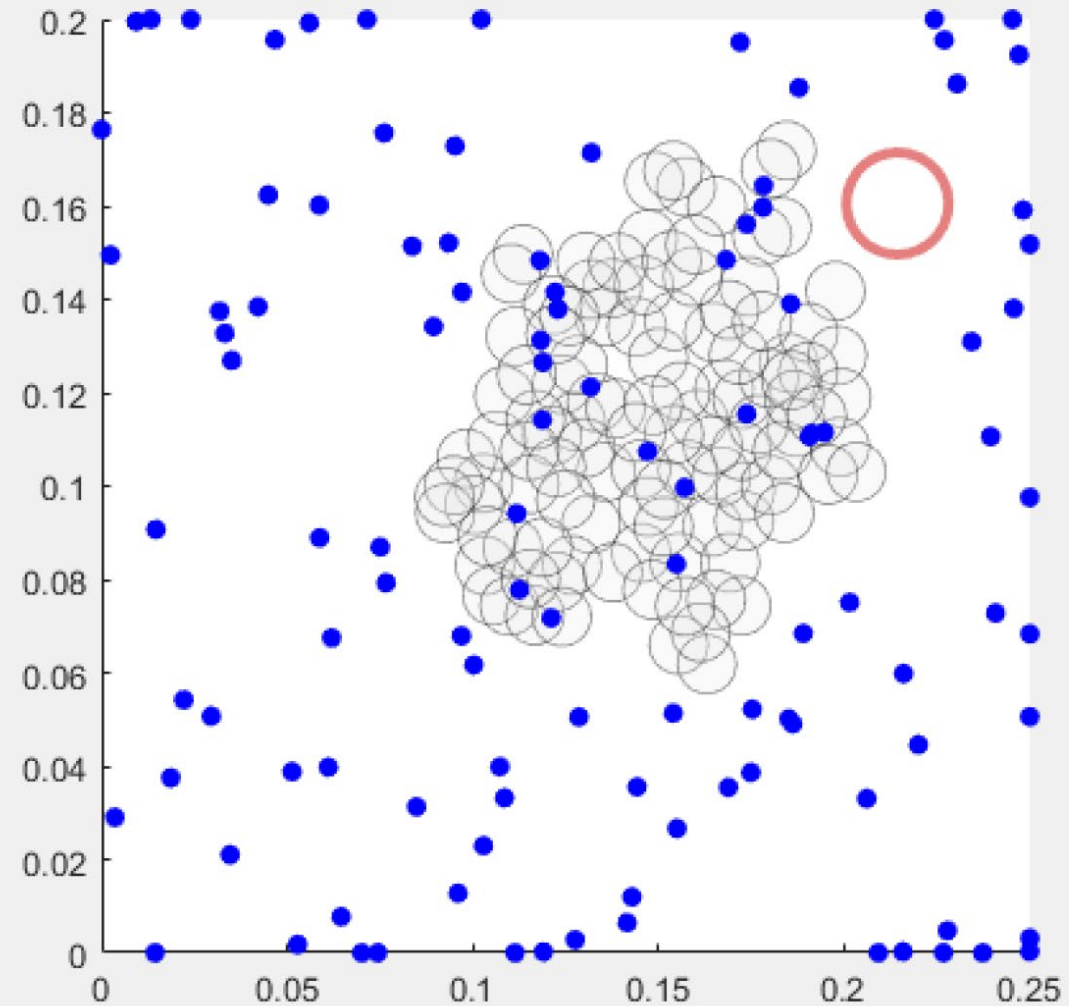
Strength of attraction between bees (%)

Simulation length

Short



Run



# Educational GitHub repositories

From research into outreach

- <https://github.com/ashleefv/ACEInhibPKPD>
- <https://github.com/ashleefv/BeeNestABM>

For classes

- <https://github.com/ashleefv/ApplNumComp>
  - Lessons 14-16 on GUIs
  - FV Lab GUIs deep dive: [https://youtu.be/k\\_JD7kmkeTM](https://youtu.be/k_JD7kmkeTM)
- <https://github.com/ashleefv/MEBLinearSystems>

For educator training

- <https://github.com/ashleefv/ChESS2022>



# Linear systems lesson for Material & Energy Balances

**<https://github.com/ashleefv/MEBLinearSystems>**

## MEBLinearSystems

---

Includes instructions and examples of solving systems of linear equations with computing software.

This repository is designed for use in CE 212: Fundamental Principles of Chemical Engineering at the University at Buffalo, The State University of New York. Instructor: Dr. Ashlee N. Ford Versypt @ashleefv. Content provided here is developed by Dr. Ford Versypt and Austin Johns @austin-johns.

The course textbook is the Material and Energy Balances zyBook by Matthew Liberatore available from <https://www.zybooks.com/catalog/material-and-energy-balances/>.

The material developed here supplements the section in the zyBook titled Systems of linear equations, specifically as a MATLAB Live Script-based alternative to the subsection titled "Solving systems of linear equations in a spreadsheet." This main file is [Systems\\_of\\_Linear\\_Equations.mlx](#), with a corresponding solution to the worked example available in [Systems\\_of\\_Linear\\_Equations\\_sol.mlx](#). We also have created an explanatory youtube video: [Solving Systems of Linear Equations Using a MATLAB Live Script](#)

# Linear systems lesson for Material & Energy Balances

<https://github.com/ashleefv/MEBLinearSystems>

Systems\_of\_Linear\_Equations\_sol.mlx x +

## Systems of Linear Equations

The examples in this MATLAB Live Script are adapted from examples from the Systems of linear equations section from M. W. Liberatore, Material and Energy Balances ZyBook. Electronic, interactive textbook: ZyBooks, 2019.

Code authors: Dr. Ashlee Ford Versypt and Austin Johns

Corresponding author: [ashleefv@buffalo.edu](mailto:ashleefv@buffalo.edu)

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[Learning Objectives](#)

[Systems of Linear Equations in MATLAB](#)

[Worked Example](#)

[Interactive Example / Template](#)

# Linear systems lesson for Material & Energy Balances

<https://github.com/ashleefv/MEBLinearSystems>

Systems\_of\_Linear\_Equations\_sol.mlx × +

## Learning Objectives

- Solve a system of linear equations using the backslash operator in MATLAB.

## Systems of Linear Equations in MATLAB

Systems of linear equations consist of coefficients, constants, and variables, which can be arranged into matrices. The matrix form to express a system of linear equations is matrix  $A$  for the coefficients, matrix  $x$  for the variables, and matrix  $b$  for the constants, which yields the formula  $Ax = b$ . Solving for the variables involves taking the transpose of  $A$  multiplied by  $b$ , or  $A^{-1}b = x$ . Solving for the variables of a system of linear equations in MATLAB involves using the backslash operator,  $\backslash$

$x = A \backslash b$  will return the solution to  $x = A^{-1}b$ .

# Linear systems lesson for Material & Energy Balances

<https://github.com/ashleefv/MEBLinearSystems>

Systems\_of\_Linear\_Equations\_sol.mlx × +

## Interactive Example / Template

This example can be used as a template to solve system of linear equations of any size. Using the same procedure as the worked example, solve the following system of linear equations.

$$2x_2 + 7x_4 = 5 - 5x_1 - 8x_3$$

$$2x_1 + 6x_2 = 2 + 4x_3 + 4x_4$$

$$-4x_1 - 3x_2 - 7x_3 + x_4 - 1 = 0$$

$$-9x_2 + 6x_3 - 3 = 2x_1 - 2x_4 + 4$$

The system of linear equations above can be rearranged as follows:

$$5x_1 + 2x_2 + 8x_3 + 7x_4 = 5$$

$$2x_1 + 6x_2 - 4x_3 - 4x_4 = 2$$

$$-4x_1 - 3x_2 - 7x_3 + x_4 = 1$$

$$-2x_1 - 9x_2 + 6x_3 + 2x_4 = 7$$



# Linear systems lesson for Material & Energy Balances

<https://github.com/ashleefv/MEBLinearSystems>

Systems\_of\_Linear\_Equations\_sol.mlx x +

As there are four equations and four unknowns,  $A$  will have four rows and four columns,  $b$  will have four rows, and  $x$  will return the solutions to the four unknown variables. Enter in the corresponding values below (expanding the number of rows or columns, if needed for new problems) and press run.

```
17 A = [ 5  2  8  7;  
18      2  6 -4 -4;  
19      -4 -3 -7  1;  
20      -2 -9  6  2]
```

A = 4x4

```
    5    2    8    7  
    2    6   -4   -4  
   -4   -3   -7    1  
   -2   -9    6    2
```

```
21 b = [5;  
22      2;  
23      1;  
24      7]
```

# Linear systems lesson for Material & Energy Balances

<https://github.com/ashleefv/MEBLinearSystems>

Systems\_of\_Linear\_Equations\_sol.mlx x +

```
-4 -3 -7 1  
-2 -9 6 2
```

```
21 b = [5;  
22     2;  
23     1;  
24     7]
```

b = 4x1

```
5  
2  
1  
7
```

```
25 x = A\b
```

x = 4x1

```
8.0912  
-4.5927  
-2.8663  
-0.4772
```

# Numerical Problem Solving across the Curriculum with Python and MATLAB Using Interactive Coding Templates

## Presenters:

Ashlee N. Ford Versypt, University at Buffalo

Matthew D. Stuber, University of Connecticut

Robert P. Hesketh, Rowan University

Assisted by Austin Johns, University at Buffalo



<https://github.com/ashleefv/>

[ChESS2022](#)



# Learning objectives for the workshop

By the end of this workshop, participants will be able to

- Create interactive coding templates (MATLAB Live Scripts or Jupyter Notebooks using Python) for teaching chemical engineering concepts and problem-solving
- Select, run, and interact with a MATLAB Live Script or Jupyter Notebook template applied to a chemical engineering topic of their choice

# Example interactive coding templates

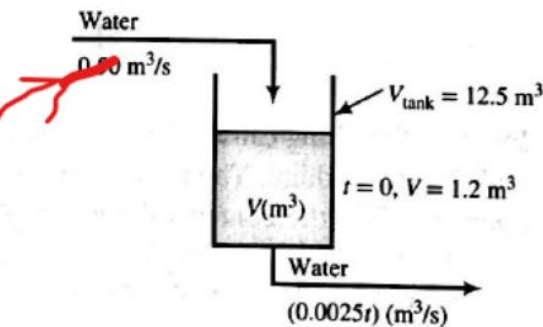
- Ex. 10.2-1 from MEB book by Felder, Rousseau, & Bullard
- Jupyter Notebook (Python) version: [J6 TankDrainage.ipynb](#)
- MATLAB version: [M6 TankDrainage.mlx](#)

## Example 10.2-1

### Mass Balance on a Water Storage Tank

A 12.5-m<sup>3</sup> tank is being filled with water at a rate of 0.050 m<sup>3</sup>/s. At a moment when the tank contains 1.20 m<sup>3</sup> of water, a leak develops in the bottom of the tank and gets progressively worse with time. The rate of leakage (m<sup>3</sup>/s) can be approximated as 0.0025*t*, where *t*(s) is the time from the moment the leak begins.

$$\text{ODEfun}(t, y_i's)$$
$$\frac{dV}{dt} = \dot{v}_{in} - \dot{v}_{out}$$



1. Write a mass balance on the tank and use it to obtain an expression for  $dV/dt$ , where  $V$  is the volume of water in the tank at any time. Provide an initial condition for the differential equation.
2. Solve the balance equation to obtain an expression for  $V(t)$  and draw a plot of  $V$  versus  $t$ .



# MATLAB Live Script (.mlx)

- MathWorks literate programming
- Works using online and standalone client
- MATLAB code + Simplified Markdown
  - LaTeX available for equations
- Functions defined at end of document
- Interactive elements

## Net rates for each species

$$r_A = r_{1A} + r_{2A} = -k_{1A}C_A - k_{2A}C_A^2$$

$$r_B = r_{1B} = k_{1A}C_A$$

$$r_C = r_{2C} = \frac{1}{2}k_{2A}C_A^2$$

## Mole Balances

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_B}{dV} = r_B$$

$$\frac{dF_C}{dV} = r_C$$

## PFR Energy Balance

$$\text{Part a: } \frac{dT}{dV} = 0$$

$$\text{Part b: } \frac{dT}{dV} = \frac{U_a(T_a - T) + (-r_{1A})(\Delta H_{R1A}) + (-r_{2A})(\Delta H_{R2A})}{F_A C_{P_A} + F_B C_{P_B} + F_C C_{P_C}}$$

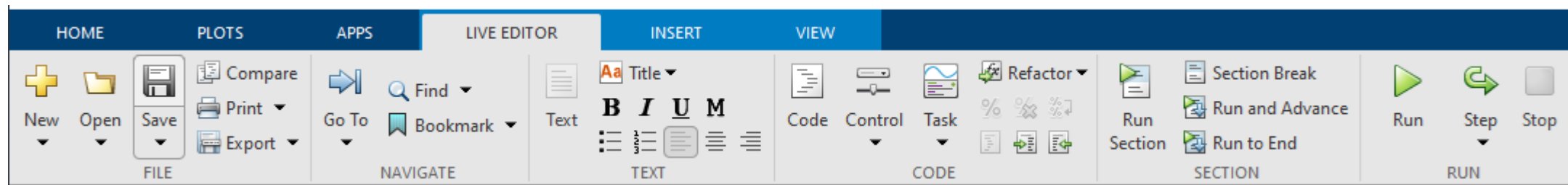
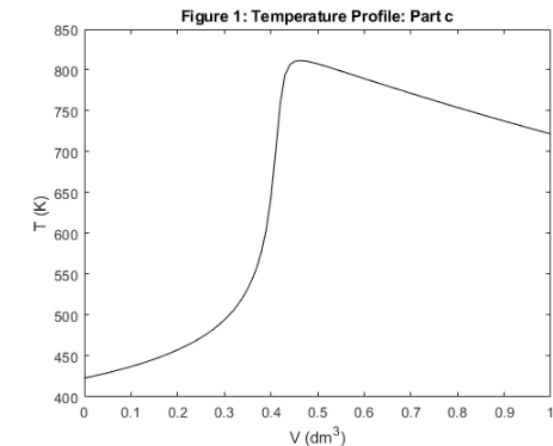
$$\text{Part c: } \frac{dT}{dV} = \frac{U_a(T_a - T) + (-r_{1A})(\Delta H_{R1A}) + (-r_{2A})(\Delta H_{R2A})}{F_A C_{P_A} + F_B C_{P_B} + F_C C_{P_C}}$$

Using the default parameter values and the PFR energy balance from Part c, the plots should resemble the following

Note that we have different line styles and colors in the plots. The general plot formatting options are

- Colors: black 'k', green 'g', red 'r', blue 'b', magenta 'm', cyan blue 'c', yellow 'y'.
- Line types: '-' solid line, '--' dashed line, '-.' dash-dot line, '...' dotted line.
- Colors and line styles can be combined as 'r:' or 'k-.' for a red dotted line or a black dash-dot line.
- See this webpage for more details: <https://www.mathworks.com/help/matlab/ref/plot.html>

```
figure(1) % Plot T vs. V graph
plot(V_eval, T_soln, 'k-')
title('Figure 1: Temperature Profile: Part ' + Part)
xlabel('V (dm^3)')
ylabel('T (K)')
```



# Jupyter Notebook (.ipynb)

- Open-source literate programming option
- Works using online and standalone client
  - Google Colab opens directly from Google Drive
- Python code + Markdown default
  - >40 programming languages available
- Functions must run before called
- Notebooks render directly on GitHub
  - Non-interactive / Read-only



## Import Packages and Functions

The following packages need to be imported for solving ODE models, formatting, and plotting results.

```
[ ] import numpy as np
    from math import exp
    from scipy.integrate import solve_ivp
    import matplotlib.pyplot as plt
    from IPython.display import display, Math, Latex
```

The screenshot shows a Jupyter Notebook interface. The top part is a code cell with the following Python code:

```
## Problem Statement
 $\require{mhchem}$ 
The following gas-phase reactions occur in a nonisothermal PFR:
<p> Reaction 1:  $A \rightarrow B$   $r_{1A} = k_{1A}C_A$  <br>
<p> Reaction 2:  $2A \rightarrow B$   $r_{2A} = k_{2A}C_A^2$  <br>

Pure A is fed at a rate of 100 mol/s, a temperature of 150degC, and a concentration of 0.1 mol/dm<sup>3</sup>. Determine the temperature and molar flow rate profiles down the reactor.
```

The bottom part is a rendered markdown cell with the following content:

**Problem Statement**

The following gas-phase reactions occur in a nonisothermal PFR:

Reaction 1:  $A \xrightarrow{k_1} B \quad -r_{1A} = k_{1A}C_A$

Reaction 2:  $2A \xrightarrow{k_2} B \quad -r_{2A} = k_{2A}C_A^2$

Pure A is fed at a rate of 100 mol/s, a temperature of 150°C, and a concentration of 0.1 mol/dm<sup>3</sup>. Determine the temperature and molar flow rate profiles down the reactor.

The screenshot shows a GitHub repository page for a Jupyter Notebook. The repository is named "Chemical\_Engineering\_Analysis\_Notebooks" and is located in the "tutorial / julia / Tutorial 1 - Linear Algebra / J1\_LAsystems.ipynb" directory. The repository is owned by "MatthewStuber" and has 2 contributors. The notebook file is 498 lines long, 498 sloc, and 21 KB in size. The notebook content is displayed below the repository information, showing the title "Linear Algebraic Systems" and the section "Learning Objectives".

## Linear Algebraic Systems

### Learning Objectives

*Setting up a linear system*

- Be able to distinguish a linear system from a nonlinear system.
- Learn to write a linear system in a matrix-vector format.
- Input a linear system into a program
- Write applicable engineering models in a linear format.

# Ways to use interactive coding templates in ChE classrooms across the curriculum

- Reinforce computational thinking
- Introduce/enhance familiarity with MATLAB and/or Python
- Student use cases
  - Lecture notes with in-class activities
  - Pre-class readings with embedded activities
  - Worked example case studies
  - In-class problems
  - Homework or project problems

# Modeling a student use case: reading with embedded interactive activities

- Choose either MATLAB Live Script or Jupyter Notebook (Google Colab)
- Open [M0\\_HowToCreate.mlx](#) or [J0\\_HowToCreate.ipynb](#) file on How to create a MATLAB Live Script/How to create a Jupyter Notebook
- Read through the file and complete the interactive activities
- We will circulate to answer your questions

# Your turn to build your own interactive coding template

- Choose either MATLAB Live Script or Jupyter Notebook (Google Colab)
- Find a partner who is interested in using the same language (MATLAB or Python)
- Work together to build a notebook for students to solve an equation of your choice. The notebook must include code blocks for numerical computation (solving) and the following text blocks (in any order)
  - learning objectives
  - problem statement
  - mathematical equation(s)
  - an image



# Going further: case study examples to explore

- We have prepared a set of interactive coding templates that correspond to mathematical topics and chemical engineering topics across the curriculum.
- Pick a file from our set of templates. Play with the interface and reflect on how to adapt for your purposes: lecture/in-class activity, homework, group projects, other.

[Interactive coding templates](#)

# 5.0 MATLAB Live Script and Jupyter Notebook Tutorials

---

## 5.0.1 M0\_HowToCreate.mlx & J0\_HowToCreate.ipynb

---

[M0\\_HowToCreate.mlx](#) covers how to create MATLAB Live Scripts. [J0\\_HowToCreate.ipynb](#) covers how to use Google Colab to create Jupyter Notebooks.

## 5.1 Linear Equations

---

### 5.1.1 M1\_MassBalance.mlx (separate solution file available)

---

- Intended student use case: This file is designed as a homework problem.
- Numerical technique: Format mass balances as a linear algebraic system in matrix-vector form. Explore the Gauss elimination algorithm implementation.
- ChemE application: Linear mass balances on a reaction/separation system with recycle. Material and energy balances (MEB)
- Workshop activity: Explore a Live Script formatted as a homework assignment. Possibly solve the problem.

## 5.2 Nonlinear Equations

---

### 5.2.1 M2\_NonlinearSystems.mlx (separate solution file available)

---

- Intended student use case: This file contains three fully worked examples and a case study that requires students to input a single vector of initial guesses to solve the problem.
- Numerical technique: Newton's method, Picard's method, and Newton-Raphson
- ChemE application: Nonlinear mass balances on a reaction/separation system with recycle. Material and energy balances (MEB), reaction engineering
- Workshop activity: Explore a Live Script formatted as a worked example and complete the Case Study. Reflect on how this might be modified for deployment in a class other than numerical methods.

# Computational educational materials from the workshop presenters

- Video highlighting key features of MATLAB Live Scripts and Jupyter Notebooks (Austin Johns, Ford Versypt Lab):  
<https://youtu.be/u5YkzFI6FbE>
- Ford Versypt: <https://github.com/ashleefv/AppINumComp>
- Hesketh: <https://github.com/heskethrp>
- Stuber:  
[https://github.com/PSORLab/Chemical Engineering Analysis Notebooks](https://github.com/PSORLab/Chemical_Engineering_Analysis_Notebooks)

Shareable Handout

# Ford Versypt previously recorded publicly available materials

- *Engaging Instructional Practices*  
Institute for Teaching & Learning Excellence interview:  
<https://player.vimeo.com/video/141915144>
- *Active Learning Exercises for Teaching Reactor Design*  
Keynote, Survey Results & Best Practices: Reactor Design Session,  
Education Division, 2020 AIChE Annual Meeting:  
<https://youtu.be/qms5YEPOhbY>
- *Teaching Computational Skills for Chemical Engineers*  
Webinar, AIChE Education Division, Feb 2020:  
<https://www.aiche.org/academy/webinars/teaching-computational-skills-chemical-engineers>
- *Applied Numerical Computing*  
Online course materials including recordings:  
<https://github.com/ashleefv/AplNumComp>

# Interactive Computing Activities as Chemical Engineering Educational Tools in University and Informal Learning Environments



**AIChE CAST Division Himmelblau Award 2022**

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