Sky Chrastina
CHEN 4090
180511

Summary of work for CHEN 4090 Independent Study from 180115 to 180511:

1. Thermodynamic spreadsheets (5)
2. Web-based simulation/exercise engine
3. Web-based exercise (1)

Thermodynamic Spreadsheets

Several spreadsheets created by Elliot & Lira (https://chethermo.net) and in use by students in CHEN 3320 Thermodynamics were modified:

1. Antoine.xlsx (calculation of saturation pressure by Antoine's equation)
2. Kcalc.xlsx (calculation of equilibrium constant K of a given reaction)
3. Preos.xlsx (calculation of properties using the Peng-Robinson equation of state (1 component))
4. PrMix.xlsx (calculation of properties using the Peng-Robinson equation of state (3 components))
5. PrFug.xlsx (calculation of properties using the Peng-Robinson equation of state (3 components))

Major improvements across all sheets are:

1. Improved color/line formatting: Using Microsoft Excel cell templates for Note, Input, Calculation, and Output cells to clarify user interactions. Modified Calculation style to a blue font instead of orange to improve readability. (see Fig. 1 and Fig. 2 to compare)
2. Standardized property reference sheet: All material properties and parameters were taken from their various sheets and compiled into one master list.
3. List lookup features: Instead of needing to copy-paste cells from another sheet, properties are now retrieved automatically by typing the name of the desired compound.
4. Name completion: Compounds can be selected from a drop-down list (Fig. 3) or will autocomplete if a match is found (Fig. 4)

	A	B	C	tMin[oC]	tMax[oC]	Source	P^{sat} (mmHg)		
methanol	8.08097	1582.271	239.726	15	84	3	2651.419	T(°C)	100
ethanol	8.1122	1592.864	226.184	20	93	3	1693.832		
1-propanol	7.74416	1437.686	198.463	60	106		845.6573		

Figure 1: Old Antoine.xlsx (only first four rows shown)

Saturation pressures calculated from Antoine equation

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For use with "Introductory Chemical Eng
http://chethermo.net
Modified 2018, Paul JS Chrastina

Enter temperature in Celsius

T(°C) = 105

Type names of compounds in cells below (case-insensitive, full list on Antoine data worksheet)

						Saturation pressure (P^{sat})				
Name	A	B	C	Min T	Max T	mmHg	kPa	bar	psi	Warnings
water	8.07131	1730.63	233.426	1	100	906.88	120.91	1.21	17.54	Warning: Temperature outside range
1-propanol	7.74416	1437.686	198.463	60	106	1015.22	135.35	1.35	19.63	

Figure 2: New Antoine.xlsx with color/ border formatting

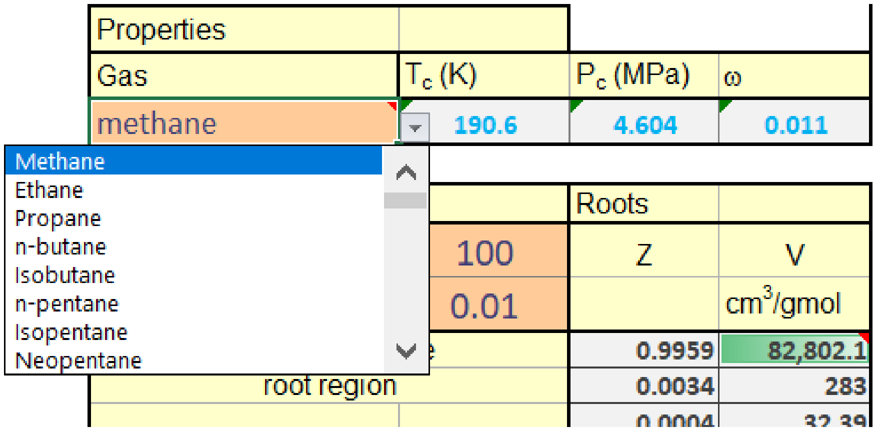

Figure 3: Drop-down list for selecting compounds

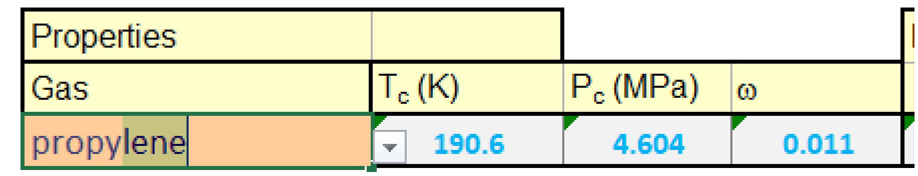

Figure 4: Autocomplete for selecting compounds

These modifications should make the use of these spreadsheets much easier by reducing copy/paste busywork and reducing information overload through clear formatting.

Web-based simulation/exercise engine

An engine was built to allow the construction of simulations/exercises that have been previously made in Wolfram to be made in JavaScript instead. Major improvements are:

1. No additional software requirements: JavaScript runs natively on any modern browser, while Wolfram files (whether .nb or compiled to .cdf) require additional software to be installed to access.
2. Grading support: Wolfram simulations, as standalone files, do not have the ability to transmit grade information and thus cannot be reliably used for assignments. The use of JavaScript allows secure data to be submitted to the LearnChemE website which can be used for grading of exercises in CU classes.
3. Customization: Wolfram simulations are cumbersome to customize, as the developer is limited to the pre-defined structures (Module, Manipulate, Plot, etc.). Using html, css, and JavaScript, customization is flexible, modular, and easy to create new structures.

The Wolfram engine offers great usability with little configuration, and handles the busywork of calculation/graphics behind the scenes, allowing the user to focus on finding answers and visualizing systems. The goal of this JavaScript-based engine is to allow the same usability in a web interface.

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The format is an object-oriented class hierarchy that follows the following structure. Each Problem consists of a variable number of Questions. Each Question contains a variable number of Elements. Some possible Elements are Graphs, Text, Textboxes, etc. One Question will be displayed to the user at a time, where they can interact with the Elements on the page. When they have finished, the user clicks Submit, which reports all of the user input back to the Problem. The Problem checks each answerable Element against its correct answer, then shows the user the correct answers along with their grade. The user then clicks Next to proceed to the next Question in the Problem.

To create problems, a JSON structure is submitted to the engine, which constructs the relevant objects and html to interact with the user. JavaScript Object Notation (JSON) is a standard data format that is known for being human-readable. A snippet of JSON structuring is shown below:

```
"questionelements": [
        {
            "type": "text",
            "label": "1) Drag the line to the pressure where three phases coexist. <br>",
            "style": "prompt"
        },
        {
            "type": "text",
            "label": datalabel,
            "style": "data"
        }
]
```

Figure 5: An example of JSON formatting

By using this structure, creation of problems is as straightforward as choosing the pieces one wants, then filling out a template for each piece to describe it. This means that no JavaScript knowledge is necessary to create problems, and in the future a GUI could be created to ease problem creation even further. This format also allows simple addition of new features, as unused properties will do no harm, and defaults can be assigned for newly added properties that did not exist previously.

Web-based exercise

To showcase the engine, a copy of an exercise already made in Wolfram was created to easily compare the two methods. The JavaScript version functions the same, but with the added features mentioned earlier. Screenshots are shown below:

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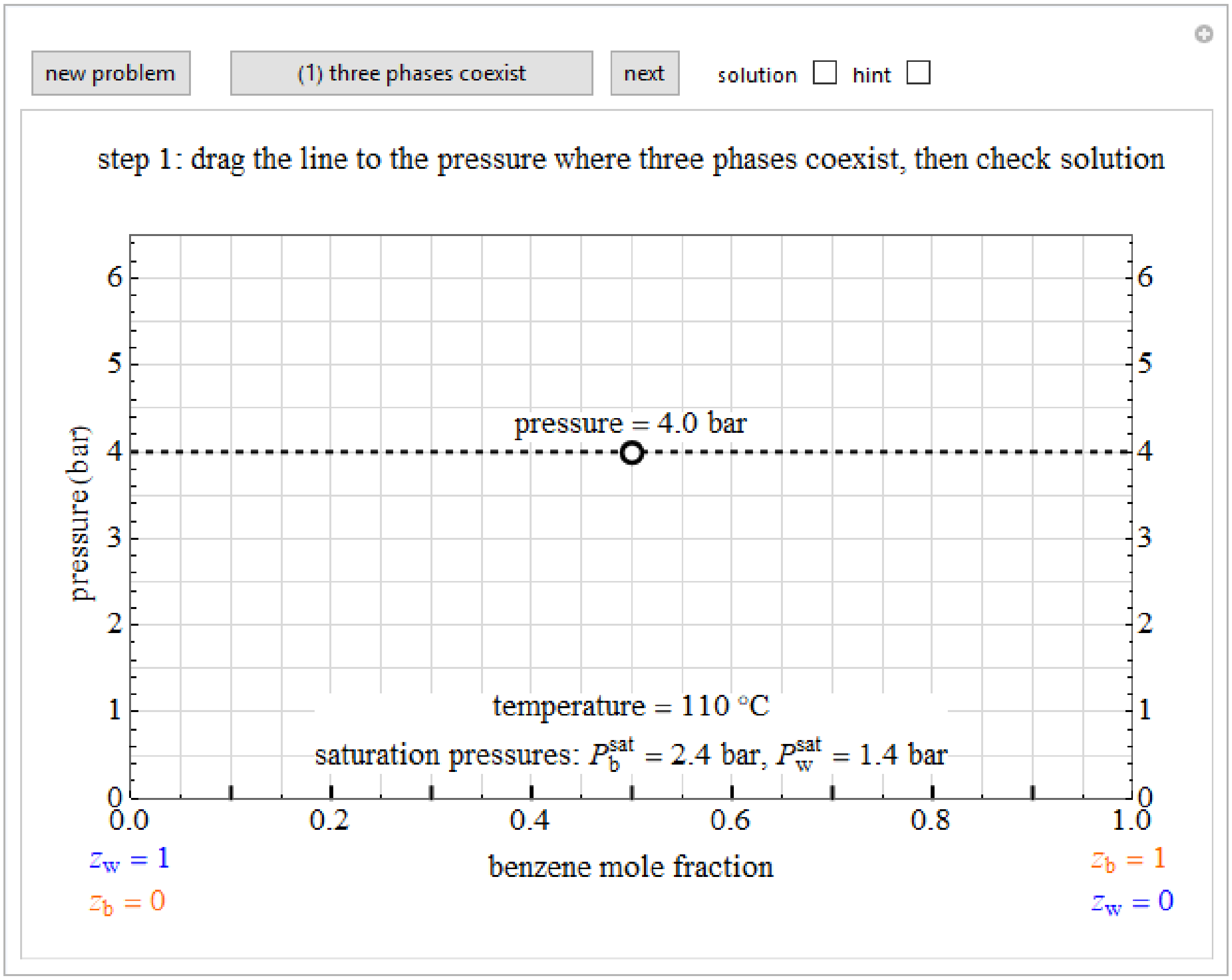

Figure 6: Wolfram exercise (step 1)

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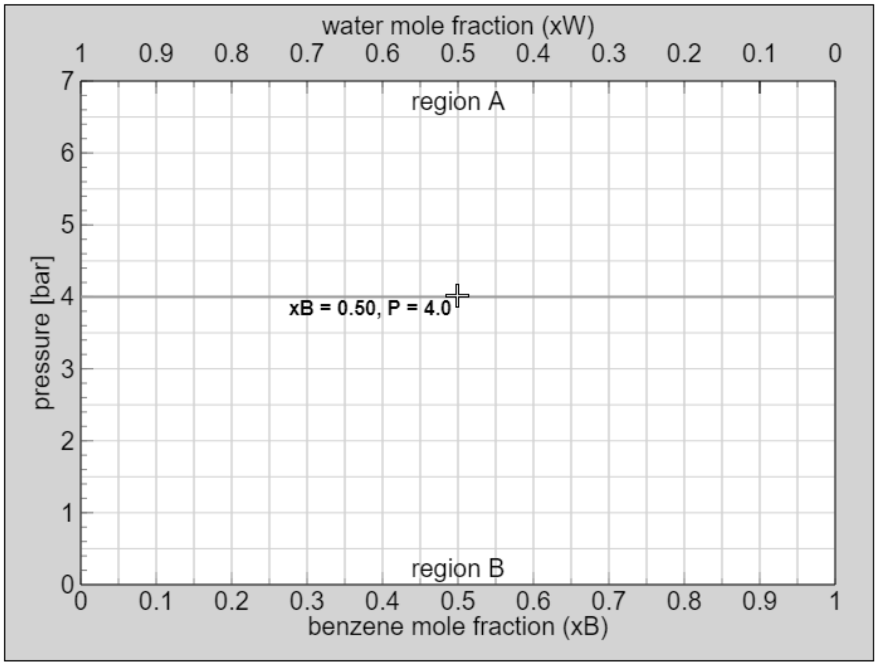
Construct a Pressure-Composition Diagram for Immiscible Liquids

1) Drag the line to the pressure where three phases coexist.

temperature = 109 C

saturation pressures: P_W^{sat} = 1.4 bar, P_B^{sat} = 2.3 bar



SCORE

Part	Points	Total	Pct
1	0	20	0%
2	0	20	0%
3	0	10	0%
4	0	20	0%
Total	0	70	0%

Which region has two liquids in equilibrium and no vapor?

type A or B

New Problem | Hint | Submit Answers

Figure 7: JavaScript exercise (step 1)

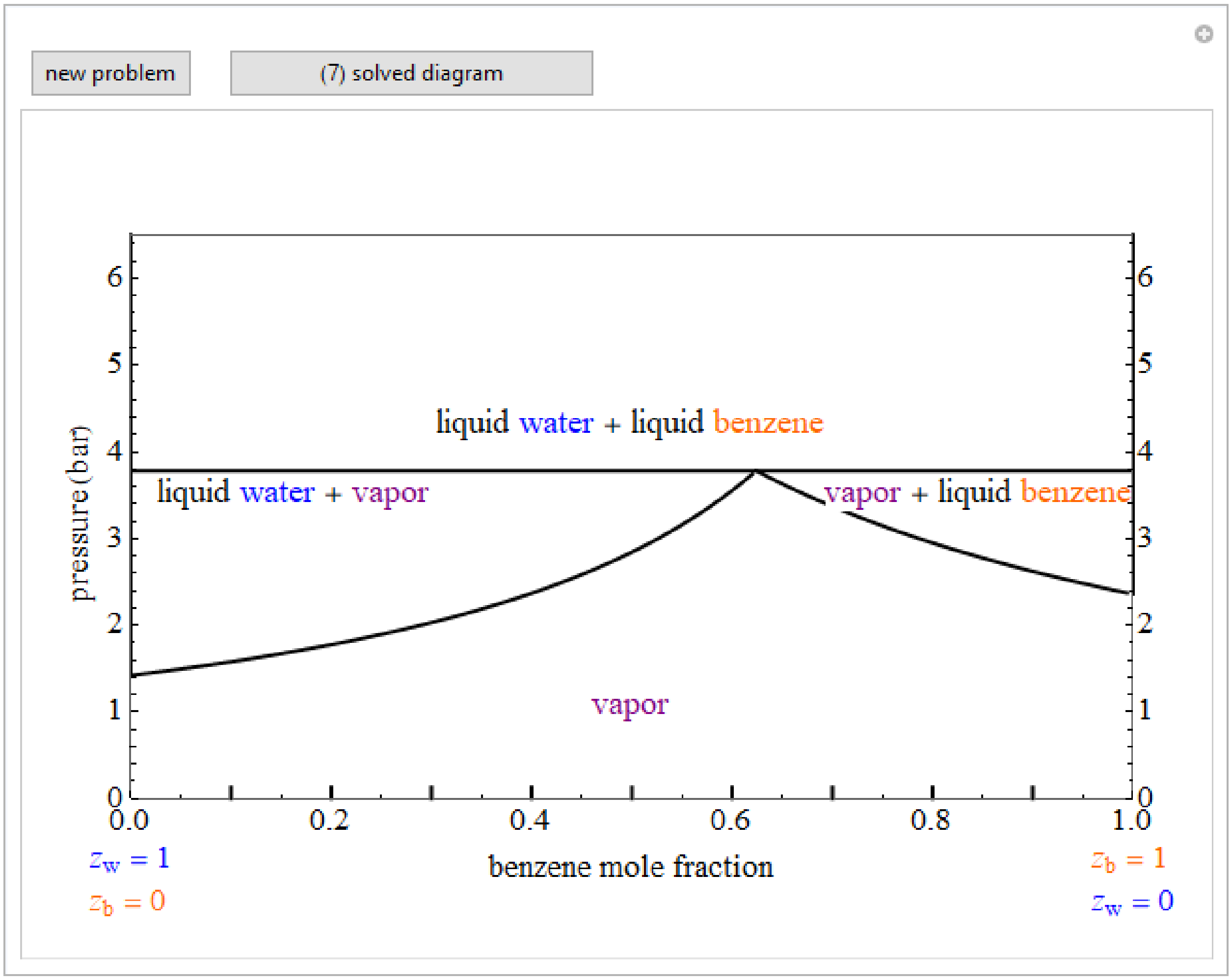


Figure 8: Wolfram exercise (final step)

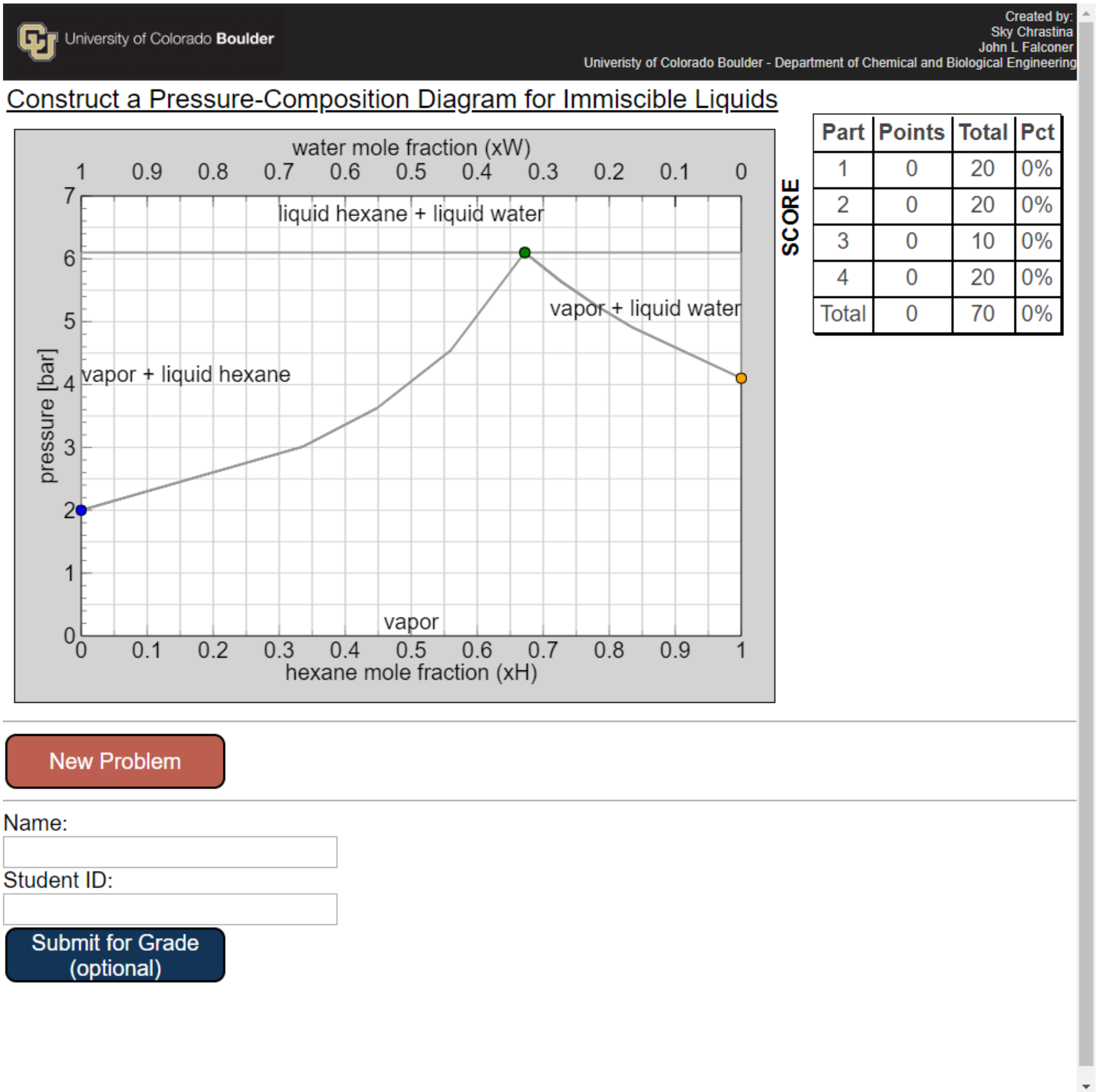


Figure 9: JavaScript exercise (final step)

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Conclusion

I found this independent study to be very fruitful for all parties. Starting with the spreadsheet modifications allowed me to use my existing knowledge to improve a section of a class in our department while developing my user interface skills and thinking about formatting more than I usually do.

During this time I also began learning JavaScript to discover whether it would be possible/feasible to create simulations and exercises that could be hosted and interacted with directly on the LearnChemE site instead of using Wolfram .cdf files. I was able to learn the language well enough and create a working engine and proof of concept exercise during the semester, providing a new direction for LearnChemE development to expand in. It also provided me a great opportunity to learn a new language that is very widely used, and practice using it in a real user-facing project. By working with my advisors, I learned how to better take an outside perspective that I don't often apply to my own personal projects.

This project has improved my skills as a developer, deepened my understanding of the covered material, and aided the department in the pursuit of improving Chemical Engineering education.