CADET _____ SECTION _____TIME OF DEPARTURE _____

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2025-2026
Machine Learning Bonus
10 October 2025

TEXT: Smith, Van Ness, Abbott & Swihart
SCOPE: Mathematica and AI
TIME: ~60-120 minutes

References Permitted: Open notes, book, internet, CHEMCAD, Mathematica, Excel.

INSTRUCTIONS

1. This is a BONUS exercise and is due **Friday 2359 10 October 2025**.
2. There are 2 problems on 1 page in this exercise (not including the cover page).
3. Upload all electronic work and cover page to CANVAS.

(TOTAL WEIGHT: 30 POINTS)

DO NOT WRITE IN THIS SPACE

PROBLEM	VALUE	CUT
A	15	
B	15	
TOTAL BONUS	30	

Cadet:_____

Problem:	Weight:
A	15

In the Beer Day Bonus, you used the Beattie-Bridgeman equation of state (EOS) to model the PVT behavior of xenon gas. The assignment was to use the EOS to calculate pressures given volumes and temperatures and compare the results to experimentally measured data. In this assignment, you will build a machine learning (ML) model from the same data set. In the ML approach, the measured PVT data are fed to the computer without providing an EOS. The computer will then derive its own "surrogate" model. This is known as data-based modeling and is an important emerging area of chemical engineering.

Table I in the paper by Beattie, Barriault, and Brierley (attached in CANVAS) contains experimentally measured pressures of xenon gas as a function of temperature and molar density. A spreadsheet accompanies this assignment with the experimental values typed in. However, this spreadsheet is organized differently than Table I. In the spreadsheet, the data are re-arranged into three columns, molar volume, temperature, and pressure, with descriptive column headers. In this assignment, you are asked to import this Excel data into Mathematica as a data set, build associations into the data set, and then use Mathematica's AI tools to create a predictive model that calculates pressure as a function of temperature and volume.

The assignment is to create this data-based predictive model, then plot the model predictions and actual data on the same axes to make a visual comparison. A video tutorial is linked on CANVAS to help you get started.

To receive full credit, you must create Mathematica "list" PV plots of experimental and predicted data at 289.8 K and one other temperature from the spreadsheet. These plots must show measured and predicted data as symbols (circles, triangles, etc.) and not smooth curves and on the same set of axes (two sets of axes, two list plots on each set of axes).

Problem:	Weight:
B	15

Going back to the original excel file from the Beer Day Bonus, complete the green and yellow shaded regions using your ML model and data transfer through Mathematica Link for Excel. Compare the total average percent deviation for the ML model to the value in Table I in the paper.