Effective Implementing Total Differential Calculus to UW-Green Bay Thermodynamics Class

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2011-2012 Teaching Scholar Presentation

Project Goal

- The goal for this teaching scholar project is to develop teaching methods effectively <u>integrating</u> partial differential equation (multivariate calculus) into physical chemistry <u>in the context and language of thermodynamics.</u>

Background

- Multivariate calculus is an integral part of Thermodynamics.
  - Thermodynamics is a science to study equilibrium and spontaneity.
  - Spontaneity criteria are based on entropy change ΔS or Gibbs free energy change ΔG.
  - However, the experimental variable are heat capacity C_p , and enthalpy change ΔH.
  - Multivariate calculus allows us to relate experimental variables to variables for predicting spontanety.

Background

- Students are generally not mathematically prepared for the thermodynamics class.
  - The material on partial differential calculus was covered only very lightly even in mathematics curriculum.
  - Even students who have taken multivariate calculus still have difficulties of translating from mathematics context into physical chemistry context. Students are generally not skillful enough to translate dx, dy, and dz into dU, dH, and dS.

Context difference between math calculus and thermodynamics calculus

Rule 3; Maxwell Relation: If f=f(x,y),

$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy = M(x,y)dx + N(x,y)dy \qquad \text{Eq [6]}$$

then

$$\left(\frac{\partial M}{\partial y}\right)_x = \left(\frac{\partial N}{\partial x}\right)_y \qquad \text{Eq [7]}$$

Context difference between math calculus and thermodynamics calculus

Exercise 3: Using Equation [5] as a starting point:

$$\begin{aligned} dH &= TdS + Vdp \\ dA &= -SdT - pdV \\ dG &= -SdT + Vdp \end{aligned} \qquad \text{Eq [5]}$$

Show that:

$$\begin{aligned} \left(\frac{\partial S}{\partial V}\right)_T &= \left(\frac{\partial p}{\partial T}\right)_V \\ \left(\frac{\partial S}{\partial p}\right)_T &= -\left(\frac{\partial V}{\partial T}\right)_p \end{aligned} \qquad \text{Eq [8]}$$

Background

- Thermodynamics textbooks usually introduce multivariate calculus to relate heat capacity to entropy only after both the first and the second law of thermodynamics are introduced which is about at the 6–7th week of the semester.
  - This left only 7–8 weeks for intensive mathematical drills to prepare students mastering the subject.

Background

- I have prepared 7 modules of multivariate calculus in physical chemistry context with the intention to teach students in the first 3 weeks of the semester about 2 years ago.
  - It was not successful because of its intensity that has caused great anxiety in students. Students responded by dropping the class at the very beginning of the semester.

Approaches (2011–2012)

- I begin to introduce the calculus module at the second week of the semester asking students to accept both the first and the second law of thermodynamics are true without proving.
  - $dU = T\,dS - p\,dV;\ \delta q_{rev} = T\,dS$
- At the first module, I gave intensive lectures orienting students to dS (entropy), dH (enthalpy), and dU (internal energy) instead of dx, dy, and dz which most students in the mathematics curriculum are familiar with.

Approaches (2011-2012)

- These seven modules are spread out through the semester by introducing these modules one-by-one every two weeks. Applications of these calculus equations to the real world are emphasized throughout the semester.

Module-3

- Students are asked to prove:

Exercise 2: Using Eq.[2], derive:

$$C_V = C_p - \frac{TV\beta^2}{\kappa} \qquad \text{Eq [3]}$$

Note: Eq.[3] is the same equation, Eq[3.38] in Engel's textbook, page 52.

Exercise 3: Recall β=1/T and κ=1/p for ideal gas, show that in one-mole of ideal gas,

$$C_V = C_p - R \qquad \text{Eq [4]}$$

Module-4

- Students are asked to solve:

Exercise 1: Set up a proper thermodynamic relation for the following problem:

Calculate the change in entropy of 50 g of nickel when it is heated from 0 to 500 C at one atmospheric pressure.

Which thermodynamic properties are needed for numerical calculation of this problem?

Note: Nickel is not an ideal gas. Students cannot simply copy textbook equation for solving this problem.

Approaches (2011-2012)

- Students are asked to prepare a 3-ring-binder to organize these calculus modules. They are encouraged to use the organized material for problem solving in the real world.

Approaches (2011-2012)

- Students' ability to use those organized information is assessed at the 13th week of the semester in which a one-hour calculus test is given to all students who are allowed to bring the organized materials to the test.
  - Additional assessment is given in terms of three take-home examinations which include calculus problems that required students using the organized materials for writing correct answers.

Final Calculus Test

- 20 points. 5 problems, 1 hr.
- Students are allowed (encouraged) to bring the organized calculus modules in 3-ring binder to the test.

Calculus Test—Fall, 2011—Name________________________________

Students are only allowed to bring the 3-ring-binder for the test.

1. Show that $(\frac{\partial U}{\partial V})_T = T\left(\frac{\beta}{k}\right) - p$

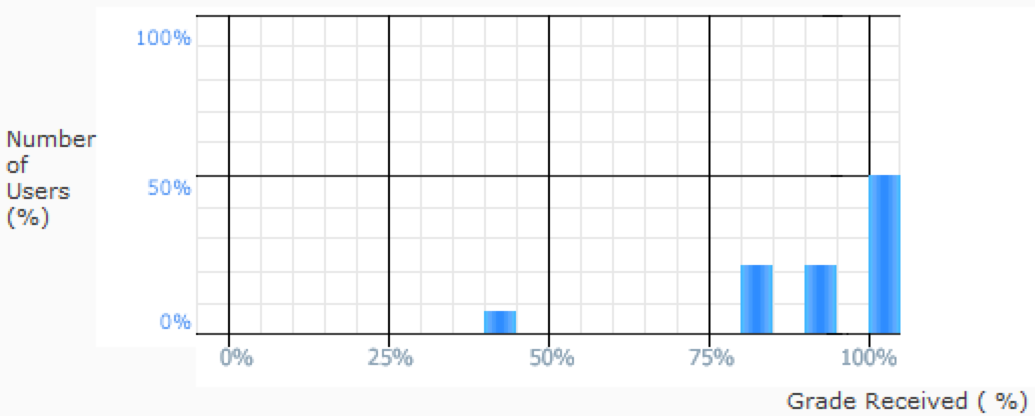
2. Show that for ideal gas, $(\frac{\partial U}{\partial V})_T = 0$, What is the physical meaning for this equation?

Final Calculus Assessment Results

Calculus Final Assessment Class Statistics

Number of submitted grades: 14 / 18
Minimum: 40 %
Maximum: 100 %
Average: 89.29 %
Mode: 100 %
Median: 95 %
Standard Deviation: 15.8 %

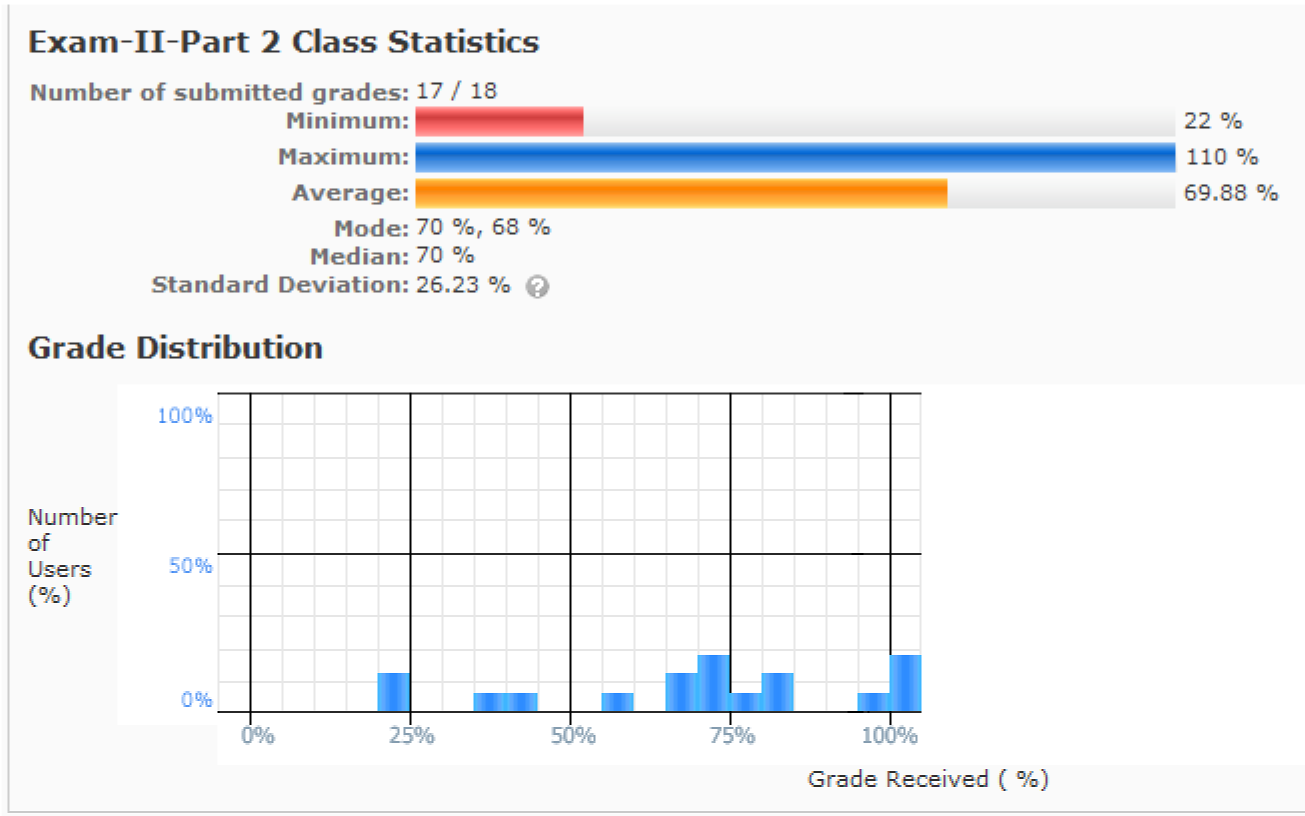
Grade Distribution



Final Calculus Assessment Results Summary

- 14 out of 18 students took the calculus exam.
- The class average was 89.26%.

Other Assessment Results– Exam 2 that include calculus

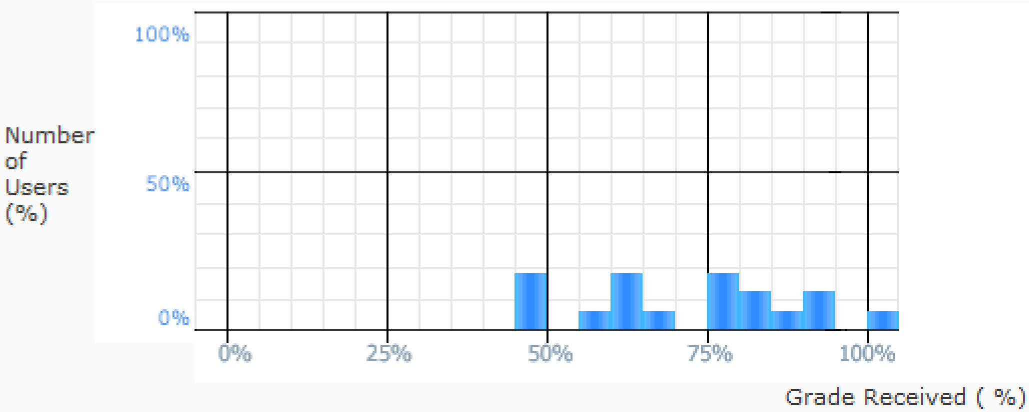


Other Assessment Results– Exam 3 that include calculus

Exam-3 Class Statistics

Number of submitted grades: 17 / 18
Minimum: 46 %
Maximum: 100 %
Average: 71.29 %
Mode: 46 %, 75 %
Median: 75 %
Standard Deviation: 16.41 %

Grade Distribution



Summary and Conclusions

- Calculus modules (in the context of thermodynamics) can be introduced before formerly proving the 1st and the 2nd laws.
- By spreading out 7 modules throughout a whole semester alleviating students' anxiety on learning calculus.
  - No students were dropping.
- By asking students to organize the calculus modules in 3-ring binder help students solve real-world problems after leaving UW-Green Bay.

Summary and Conclusions

- Initial assessment results suggest that the approach taken in this teaching scholar project is effective.