

Integration of Industrially Relevant Examples in ChE Courses

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Integration of Industrially Relevant Examples in ChE Courses Energy Balance on an e-Cigarette Device

Abstract

Identifying industrially relevant and/or real-world examples is an excellent technique to enhance the student learning experience. Linking theory and calculations from the lecture to something concrete to which the students are routinely exposed provides relevancy and can successfully reinforce key aspects of the topic. This paper illustrates the integration of a practical example into a chemical engineering curriculum, with the example pulled from a Mass and Energy Balances course.

The problem involves calculation of the power required to vaporize the liquid in an electronic cigarette (e-cigarette or vaporizer). Solution of this problem requires a coupled mass and energy balance and requires some knowledge of vapor-liquid equilibrium. Obviously, some assumptions are required to analyze this problem. Even with these assumptions, a reasonable estimate of the power required for the unit is obtained. Extensions of the problem include student speculation on how their assumptions impact the calculated power and why the calculated estimate is slightly lower than the actual power delivered by a vaporizer. Properly implemented, this problem can touch on multiple learning objectives, including lower-level skills such as estimation up to critical analysis of key assumptions required to solve the problem.

Background

Generating a problem that addresses multiple course learning objectives can be a challenging, but worthwhile exercise for a professor. These types of problems are particularly useful late in a course to help students tie together seemingly disparate concepts to solve an integrated problem that requires them to review concepts mastered throughout the course. Relating the problem to something that the student experiences on a day-to-day basis enhances the utility of the problem. This paper provides an overview of one such problem, an energy balance for an e-cigarette device.

The mass and energy balance course is the first department-specific course to which chemical engineers are exposed. The range of topics covered is quite broad and bridges to gap between basic calculations introduced in freshman chemistry and physics courses to the fundamental chemical engineering design equations that will be further pursued in the chemical engineering curriculum. The mass and energy balance course is often divided into two parts, per the course title, with the mass balance portion including summaries of process variables and simple vapor-liquid equilibrium. The learning objectives for a typical mass and energy balance course are quite extensive and cover a wide range of topics. This is not unexpected, since the course forms the foundation on which the chemical engineering problem solving approach and tools are further built during the rest of the undergraduate curriculum.

The mass and energy balance course is a problem-intensive course, with the most effective student learning occurring in an environment in which students perform numerous calculations that reinforce key course topics. Ideally, a problem can link to multiple course learning objectives, showing the student how solving real-world problems requires integration of various tools and techniques learned throughout the course. A recent problem, submitted by a student as part of a homework assignment in which students were asked to generate their own homework problem, met this objective and serves as the basis for this submission. It is focused on an energy balance for an e-cigarette device.

Problem Statement

The draft of the problem being submitted was initially put forth by a sophomore in the Mass and Energy Balances (ChBE 2200) course. As part of the final homework assignment in the course, students generated problems that covered any of the material presented in the course. The following problem statement was submitted by Eric M. Collins:

Over the last few years, many people have been switching from smoking cigarettes to a healthier alternative, e-cigarettes, sometimes called vaporizers. Instead of using tobacco, they use a mixture of Glycerin and Propylene Glycol liquid to create the vapor.

You decide you want to build your own vaporizer, but aren't sure of the minimum power needed for the device. You know that the liquid comes pre-mixed in a volumetric ratio of 70/30 glycerin to propylene glycol, and can be considered well mixed. Three (3) ml of liquid is poured into the main tank of the device, where it flows into a smaller tank that is connected to the mouth piece through a small tube. A coil inside of the small tank is connected directly to the battery, in which a voltage is applied as a button is held down to heat up the coil, providing the energy needed to vaporize the liquid.

You measure the large tank, which is a cylinder, to have a diameter of 1.6 cm. The smaller tank (also a cylinder) sits inside the large tank and has a diameter of 1.3 cm.

When using the vaporizer with a premade battery, you measure the height change of the liquid in the large tank to be 4mm over a time of 2.3 minutes of use. You also approximate the room temperature to be 77°F. Specific heats, densities, heats of vaporization, and Antoine coefficients may need to be found for the two components in order to solve the problem.

Solve for the power required to vaporize the liquid mixture.

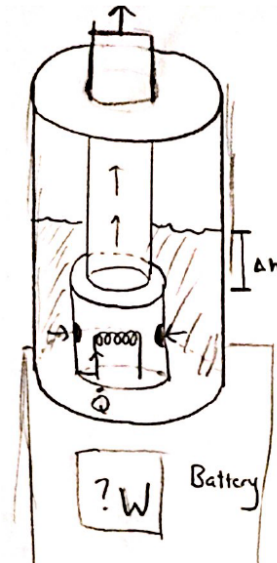
This problem was unique for several reasons. First, it was more complex and involved that most of the student submissions. It required knowledge of multiple different aspects from the course. It referenced at least five (5) different chapters and a minimum of nine (9) sections in Felder and Rousseau and links to seven (7) high-level learning objectives. Second, it had a worked-out solution, but included many aspects that could be open-ended. The problem was amenable to numerous extensions. Third, the problem was relatable to the students, linking the calculations

and technical material in the course to something observed daily. Students working out this problem would establish a direct linkage between the course material and how it could be applied to solve a real world problem.

Solution

There is a lot of information presented in the problem statement, and it is recommended that a roadmap for the solution be provided to the students to guide them in solving this problem. Based on discussions with Eric, the problem statement was augmented to break the solution into multiple parts. The revised problem statement and an algorithm for the step-by-step solution are provided below, with several of the simplifying assumptions clearly stated. As noted previously, this problem is somewhat open-ended, and some students may obtain alternate numeric values for some variables, depending on the assumptions made during their solution.

- a) **Draw a schematic of this problem, labeling the fluid reservoir in the vaporizer the heater, and key dimensions required to solve the problem.**



- b) **Identify the process type (batch, semi-batch, or continuous).**

The system is defined as the fluid reservoir. Therefore, this is a semi-batch process, since mass will leave the system but no mass enters the system.

- c) **Use various resources to obtain the molecular weight, density, heat capacity, normal boiling point, and heat of vaporization for the two components in the liquid reservoir.**

Data obtained from webbook.nist.gov unless otherwise noted

Molecular Weight

Glycerol (A) = $C_3H_8O_3$, $MW_A = 92$ g/mol

Propylene glycol (B) = $C_3H_8O_2$, $MW_B = 76$ g/mol

Density

$\rho_A = 1.261 \text{ (g/cm}^3\text{)}$ (source: Properties of Gases and Liquids, 4th ed. Reid, Prausnitz, and Poling)

$\rho_B = 1.036 \text{ (g/cm}^3\text{)}$ (source: Properties of Gases and Liquids, 4th ed. Reid, Prausnitz, and Poling)

Heat Capacity

$C_{pA} \text{ (liquid)} = 221.2 \text{ J/(mol}\cdot\text{K)}$

$C_{pB} \text{ (liquid)} = 189.9 \text{ J/(mol}\cdot\text{K)}$

$C_{pA} \text{ (vapor)} = 167.6 \text{ J/(mol}\cdot\text{K)}$ (source: Properties of Gases and Liquids, 4th ed. Reid, Prausnitz, and Poling)

$C_{pB} \text{ (vapor)} = 152.1 \text{ J/(mol}\cdot\text{K)}$ (source: Properties of Gases and Liquids, 4th ed. Reid, Prausnitz, and Poling)

Boiling Point

$T_{BPA} = 290^\circ\text{C}$

$T_{BPB} = 187^\circ\text{C}$

Heat of Vaporization

$\Delta H_{\text{vap}A} (\Delta H^\circ) = 91.7 \text{ kJ/mol}$

$\Delta H_{\text{vap}B} (\Delta H^\circ) = 66.5 \text{ kJ/mol}$

- d) Calculate the average volumetric flow rate of the vapor, based on the observed reduction in the liquid level over the observation time.**

First, calculate the volume change over the observed time

The area of the annulus can be obtained from the given diameters:

$$\text{Area} = \pi * \left(\frac{1.6\text{cm}^2}{2} - \frac{1.3\text{cm}^2}{2} \right)$$
$$\text{Area} = 0.6833 \text{ cm}^2$$

Next, use the change in height over the observed time to convert the area to volume:

$$\Delta V = \text{Area} * \Delta h$$
$$\Delta V = 0.6833 \text{ cm}^2 * 0.4 \text{ cm}$$
$$\Delta V = 0.2733 \text{ cm}^3$$

The average volumetric flow rate is the change in volume divided by the observation time:

$$\dot{V} = \frac{\Delta V}{\Delta t} = \frac{0.2733 \text{ cm}^3}{138 \text{ s}} = 0.001981 \text{ cm}^3/\text{s}$$

- e) **Calculate the mass fraction of the glycerol and the propylene glycol in the liquid reservoir based on the given volume fraction.**

The liquid composition has been given in volume fraction. Assuming the mixture is ideal, the total volume is the sum of the individual volumes. Using 1 ml as a basis, the volume of glycerin would be 0.7 ml, and the volume of propylene glycol would be 0.3 ml. With the given densities, this would equate to 0.8827 g of glycerin and 0.3108 g of propylene glycol, or 1.1935 g total.

$$x_A = \frac{0.8827}{1.1935} = 0.7396$$

$$x_B = \frac{0.3108}{1.1935} = 0.2604$$

- f) **Calculate the mass flow rate of the vapor using the average density of the liquid mixture.**

First, the average density must be calculated:

$$\frac{1}{\bar{\rho}} = \frac{x_A}{\rho_A} + \frac{x_B}{\rho_B}$$

$$\frac{1}{\bar{\rho}} = \frac{0.7396}{1.261 \frac{\text{g}}{\text{cm}^3}} + \frac{0.2604}{1.036 \frac{\text{g}}{\text{cm}^3}}$$

$$\frac{1}{\bar{\rho}} = 0.8379$$

$$\bar{\rho} = 1.1935 \frac{\text{g}}{\text{cm}^3}$$

The mass flow rate is equal to the volumetric flow rate times the density:

$$\dot{m} = \dot{V} * \bar{\rho}$$

$$\dot{m} = 0.001981 \text{ cm}^3/\text{s} * 1.1935 \frac{\text{g}}{\text{cm}^3}$$

$$\dot{m} = 0.002364 \text{ g/s}$$

The mass flow rates of glycerin (A) and propylene glycol (B) can be obtained by multiplying the total mass flow rate by the mass fractions of the components:

$$\dot{m}_A = \dot{m}_{tot} * x_A$$

$$\dot{m}_B = \dot{m}_{tot} * x_B$$

$$\dot{m}_A = 0.001748 \text{ g/s}$$

$$\dot{m}_B = 0.000616 \text{ g/s}$$

- g) Calculate the bubble point and dew point of the mixture, assuming Raoult's Law is valid.

$$P_{tot} = x_A * P_{vapA} + x_B * P_{vapB} \text{ (Raoult's Law)}$$

$$P_{vapA} = 10^{\left(A - \frac{B}{T+C}\right)} \text{ (Antoine Equation)}$$

Solve for the temperature at which the total pressure is equal to the atmospheric pressure

$$P_{tot} = x_A * P_{vapA} + x_B * P_{vapB}$$

$$Obj\ Fxn = P_{atm} - P_{tot}$$

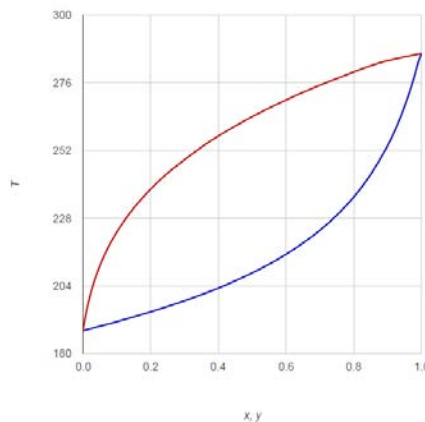
An Excel spreadsheet was set up to solve for the temperature when the objective function was equal to zero. The calculated bubble point temperature was 229.2°C.

Similar to the calculation of the bubble point, the dew point is calculated when the temperature satisfies the following condition:

$$\frac{y_A P}{P_{vapA}(T)} + \frac{y_B P}{P_{vapB}(T)} = 1$$

The calculated dew point was calculated to be 275.7°C.

The dew point and bubble point can be verified by obtaining vapor-liquid-equilibrium (VLE) data. For example, a Txy diagram at atmospheric pressure can be used to directly obtain the two relevant temperatures. The diagram below was obtained from the website, vle-calc.com and presents the phase envelope as a function of mole fraction at a pressure of 1.01325 bar.



- h) Set up the energy balance for the system identified in part a, justifying any simplifying assumptions.

The open system energy balance is applicable for this problem. Neglecting kinetic and potential energy changes and shaft work, the energy balance simplifies to the following:

$$\Delta\dot{H} = \dot{Q}$$

If the device can be assumed to be adiabatic, then the heat added to the system by the heater element is equal to the change in enthalpy.

- i) **Set up an enthalpy table for the system, clearly identifying the reference conditions.**

References: Glycerin and propylene glycol liquids at 25°C and 1.01325 bar				
Substance	\dot{m}_{in}	\hat{H}_{in}	\dot{m}_{out} (g/s)	\hat{H}_{out} (J/g)
Glycerin (A)	0	-	0.001748	\hat{H}_1
Propylene glycol (B)	0	-	0.000616	\hat{H}_2

- j) **Fill in the enthalpy table and use the results to calculate the heat required to run the vaporizer. Approximate the final temperature of the system as the midpoint between the dew point and bubble point for the liquid mixture.**

The process path for both materials is for the liquid to be heated from the reference temperature (25°C) up the normal boiling point, vaporizing, and the vapor to be go to the final temperature.

$$\hat{H}_1 = C_{pA,liquid}*(T_{BPA}-25C) + \Delta H_{vapA} + C_{pA,vapor}*(T_f-T_{BPA})$$

$$\hat{H}_1 = 637.2 + 996.7 - 68.4 = 1565.5 \text{ J/g}$$

$$\hat{H}_2 = C_{pB,liquid}*(T_{BPB}-25C) + \Delta H_{vapB} + C_{pB,vapor}*(T_f-T_{BPB})$$

$$\hat{H}_2 = 404.7 + 875 + 131.0 = 1410.8 \text{ J/g}$$

$$\dot{Q} = \dot{m}_A \hat{H}_1 + \dot{m}_B \hat{H}_2$$

$$\dot{Q} = 0.001748 \frac{g}{s} * 1565.5 \frac{J}{g} + 0.000616 \frac{g}{s} * 1410.8 \frac{J}{g}$$

$$\dot{Q} = 3.605 \frac{J}{s} = 3.605 \text{ W}$$

Remarkably, even with the assumptions made in solving this problem, the predicted heat input compares very well against actual values for batteries used in these devices.

Standard e-cigarette devices often use 3.7 volt batteries and use 5.5 watts of power (www.vaportrain.com). The predictions made in this analysis are slightly lower than the power delivered by the battery, which makes sense since we assumed the device was adiabatic. Heat loss to the environment would increase the required power to provide a heat input of 3.6 watts. In addition, the power supplied to an e-cigarette device needs to power LED lights, and the control system. Our solution has been validated by comparing it against an actual situation.

Potential Problem Extensions

The open-ended nature of this problem lends itself to various problem extensions. Several inductive based learning questions that can be applied to this problem include the following:

- a) Do you expect the rate of vaporization (calculated in part b) to be constant? Why or why not? If your answer is that it is not expected to be constant, what is the expected variation and does the assumption of a constant average vaporization rate dramatically impact the results?
- b) The problem statement assumed that the fluid reservoir reached a temperature between the bubble point and dew point during vaporization. How would you expect the actual temperature to vary during the process? Do you expect your calculated result for the required power to be dramatically impacted by this assumption? Why or why not?
- c) The power required to vaporize the liquid mixture was calculated based on the given set of conditions. Research the power delivered by different batteries. What type of battery would you recommend be used for this application? What would be the factors involved in making this selection (e.g. think of size, cost, safety, packaging, and reliability)? What is the efficiency of a typical battery?

Planned Problem Assessment

This problem provides an ideal opportunity for assessing student comprehension of critical topics late in the Mass and Energy Balances course. The problem will be given to students in the current spring semester course, with an assessment implemented to evaluate the learning impact of this problem. The format of the assessment will be as follows. First, a general, open-ended problem statement will be provided to the students as a seed, and the students will be asked to identify key variables required to perform the calculations and assumptions required to enable solution. Students will be asked to submit an outline of their solution strategy and a quantitative ranking of their confidence in their ability to solve the problem. Second, students will be divided into small groups to work together on gathering required data. The instructor and teaching assistants will circulate amongst the groups, using directed questions to break through barriers and guide groups towards performing a quantitative analysis of this problem. Third, the groups will present their solution to the class after working on the problem over a span of two (2) days. Finally, a post-assessment will be administered. Each student will update their ranking of their confidence in solving similar problems and will be asked one of the three problem extensions. The goal of the pre- and post-test assessment is to determine if the small group exercise and guided discovery increased student comprehension of these types of complex problems.

Conclusions

Often, student-generated problems can be a pleasant surprise for the instructor, with the core of a problem offering some useful insights and linkages to defined learning objectives for a course. Even if the stated problem cannot be used directly for future course assessments such as a homework, quiz, or exam problem, the student-generated problems can serve as a kernel around which a useful assessment problem can be derived. In a recent mass and energy balance course, an intriguing problem was posed by a student that was used to develop a useful assessment problem that linked diverse topics throughout the course and was directly relevant to a real world design problem. The power required for an e-cigarette device was calculated based on some experimentally measured parameters and physical property data. The problem offers numerous extension possibilities and can be adapted for multiple purposes by a professor teaching this course.

Nomenclature

C_{pA}, C_{pB}	Heat capacity of components A and B (J/(mol*K) or J/(g*K))
MW_A, MW_B	Molecular weights of components A and B (amu)
T_{BPA}, T_{BPB}	Normal boiling points of components A and B (°C)
x_A, x_B	Mass fractions of components A and B
P_{vapA}, P_{vapB}	Vapor pressures of components A and B (mm Hg)
A	Antoine coefficient A
B	Antoine coefficient B
C	Antoine coefficient C
Area	Cross-sectional area of cylinder in vaporizer (cm ²)
h	Height of fluid in vaporizer reservoir (cm)
Δh	Change in height of fluid in vaporizer reservoir (cm)
Δt	Observation time (s)
\dot{V}	Volumetric flow rate (cm ³ /s)
\dot{m}	Mass flow rate (g/s)
ρ_A, ρ_B	Density of components A and B (g/cm ³)
$\bar{\rho}$	Average density of mixture (g/cm ³)
Q	Heat (W)
\hat{H}	Specific enthalpy (W)
ΔH	Enthalpy change (W)
$\Delta H_{vapA}, \Delta H_{vapB}$	Heat of vaporization for components A and B (W)