ChE class and home problems

ENERGY BALANCE ON AN E-CIGARETTE DEVICE

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PROBLEM STATEMENT

As part of the Mass and Energy Balances course at The Ohio State University, students are asked to generate their own problem as part of the final homework for the course. The homework problem can cover any of the material presented in the course and must include a well-defined problem statement, a worked out solution, and a linkage to specific topical areas in the course text.[1] A particularly intriguing problem was submitted by a student, and the problem was augmented for this submission. The problem statement was:

> *Over the last few years, many people have been switching from smoking cigarettes to 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[2] 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.***

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Eric Collins *started his Chemical Engineering degree at Ohio State in 2014. He learned incredible problem solving skills as well as conceptual thinking skills. He was heavily involved in the school's AIChE chapter, where he met a lot of great and supportive people. After graduating from Ohio State in 2018, he moved out west to work for one of the largest investment management companies in the world. Chemical Engineering left him fascinated by how take advantage of economies of scale and how to make processes more efficient, which is a great skill set to bring to a financial institution.*

This problem was unique for several reasons. First, it was more complex and involved than most of the student submissions. It required knowledge of multiple different aspects from the course. It referenced at least five different chapters and a minimum of nine sections in the text and linked to seven high-level learning objectives. Second, it had a worked-out solution, but had 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.

SOLUTIONS

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. An algorithm for the step-by-step solution is provided below, with several of the simplifying assumptions clearly stated. 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.

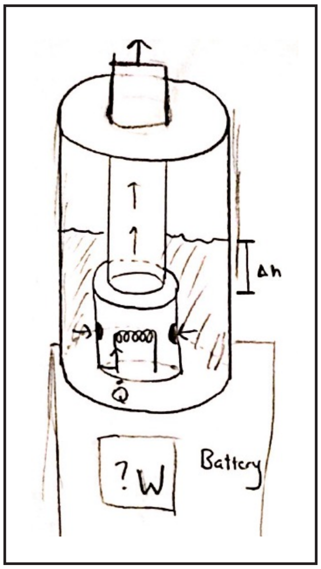

Figure 1. *Student Schematic of the Reservoir on an e-Cigarette Device*

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 NIST[3] 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
$\rho_A = 1.261$ g/cm^3 [4]
$\rho_B = 1.036$ g/cm^3 [4]

Heat Capacity
C_{pA} (liquid) = 221.2 J/(mol-K)
C_{pB} (liquid) = 189.9 J/(mol-K)
C_{pA} (vapor) = 167.6 J/(mol-K) [4]
C_{pB} (vapor) = 152.1 J/(mol-K) [4]

Boiling Point
T_{bpA} = 290°C
T_{bpB} = 187°C

Heat of Vaporization
ΔH_{vapA} = 91.7 kJ/mol
(value at normal boiling point)

ΔH_{vapB} = 66.5 kJ/mol
(value at normal boiling point)

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

Calculate the volume change over the observed time.

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

$$\pi\left(\left(\frac{1.6\text{cm}}{2}\right)^2-\left(\frac{1.3\text{cm}}{2}\right)^2\right) \tag{1a}$$

$$A = 0.6833\ \text{cm}^2 \tag{1b}$$

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

$$\Delta V = A\Delta h \tag{2a}$$

$$\Delta V = (0.6833\ \text{cm}^2)(0.4\ \text{cm}) \tag{2b}$$

$$\Delta V = 0.2733\ \text{cm}^3 \tag{2c}$$

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

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

e. **Calculate the mass fractions and mole fractions 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 behaves as an ideal solution, 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 0.8827g of glycerin and 0.3108g of propylene glycol, or 1.1935g total. To convert from mass fractions to mole fractions, a basis of 100g can be assumed.

$$\omega_A = \frac{0.8827\text{g}}{1.1935\text{g}} = 0.7396 \tag{4a}$$

$$\omega_B = \frac{0.3108\text{g}}{1.1935\text{g}} = 0.2604 \tag{4b}$$

$$x_A = 0.701 \tag{4c}$$

$$x_B = 0.299 \tag{4d}$$

The concentrations of glycerin and propylene glycol in the reservoir will change over time as the liquid evaporates. This is similar to a batch distillation problem that will be covered in more detail in Separations.

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

First, the average density must be calculated assuming volume additivity:

$$\frac{1}{\bar{\rho}} = \frac{\omega_A}{\rho_A} + \frac{\omega_B}{\rho_B} \tag{5a}$$

$$\frac{1}{\bar{\rho}} = \frac{0.7396}{1.261\ \frac{\text{g}}{\text{cm}^3}} + \frac{0.2604}{1.036\ \frac{\text{g}}{\text{cm}^3}} \tag{5b}$$

$$\frac{1}{\bar{\rho}} = 0.8379\ \frac{\text{cm}^3}{\text{g}} \tag{5c}$$

$$\bar{\rho} = 1.1935\ \frac{\text{g}}{\text{cm}^3} \tag{5d}$$

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

$$\dot{m} = \dot{V}\bar{\rho} \tag{6a}$$

$$\dot{m} = (0.001981\ \frac{\text{cm}^3}{\text{s}})(1.1935\ \frac{\text{g}}{\text{cm}^3}) \tag{6b}$$

$$\dot{m} = 0.002364\ \text{g/s} \tag{6c}$$

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:

$$\dot{m}_A = \dot{m}_{tot}\,\omega_A \tag{7a}$$

$$\dot{m}_B = \dot{m}_{tot}\,\omega_B \tag{7b}$$

$$\dot{m}_A = 0.001748\ \text{g/s} \tag{7c}$$

$$\dot{m}_B = 0.000616\ \text{g/s} \tag{7d}$$

g. **Calculate the bubble point and dew point of the mixture, assuming Raoult's Law is valid. Note that the mole fractions must be used with Raoult's Law.**

$$P_{tot} = x_A P_{vapA} + x_B P_{vapB} \tag{8a}$$

$$P_{vapA} = 10^{\left(A-\frac{B}{T+C}\right)} \tag{8b}$$

$$P_{vapB} = 10^{\left(A-\frac{B}{T+C}\right)} \tag{8c}$$

In these equations, P_{vapA} is the vapor pressure of Component A, and P_{vapB} is the vapor pressure of Component B.

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

$$P_{tot} = x_A P_{vapA} + x_B P_{vapB} \tag{9a}$$

$$Obj\ Fxn = P_{atm} - P_{tot} \tag{9b}$$

An Excel spreadsheet was set up to solve for the temperature when the objective function ($Obj\ Fxn$) was equal to zero. The calculated bubble point temperature was 225.1°C.

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

$$\frac{y_A P}{P_{vapA}(T)} + \frac{y_B P}{P_{vapB}(T)} = 1 \tag{10}$$

The calculated dew point was calculated to be 273.9°C.

An alternate means of obtaining these temperatures is through the use of a Txy diagram. Reviewing a Txy diagram from the system provides a means of validating the calculated answers. A Txy diagram for the glycerin/propylene glycol system is provided for reference (Figure 2).

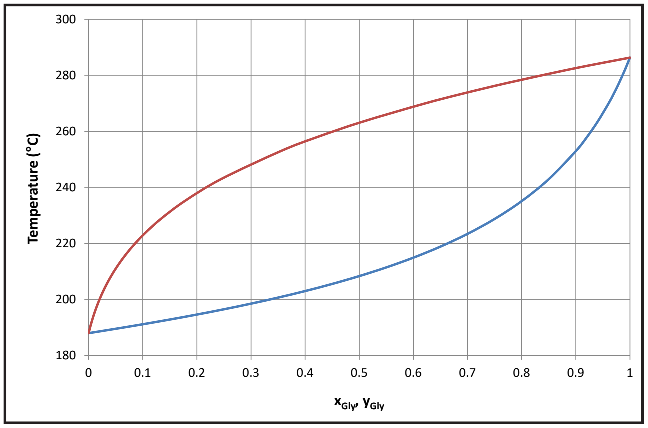

Figure 2. *Txy Diagram for Glycerin and Propylene Glycol*

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

This is a semi-batch system, so an overall mass balance should be performed first, with the mass accumulation in the reservoir related to the mass flow rate out of the system. In its most general form, the energy balance would be:

$$\frac{d}{dt}\left\{m\left(\hat{U} + \frac{v^2}{2} + gh\right)\right\} = 0 - \dot{m}\left(\hat{H}_{out} + \frac{v_{out}^2}{2} + gh_{out}\right) + \dot{W}_s + \dot{W}_{EC} + \dot{Q} \tag{11}$$

In this equation, m is the mass in the system, $\hat{U}$ is the specific internal energy of the fluid in the reservoir, v is the velocity, g is the gravitational constant, h is the height, $\dot{m}$ is the mass flow rate out of the system, $\dot{H}$ out is the specific enthalpy, $\dot{W}_s$ is the shaft work, $\dot{W}_{EC}$ is expansion/contraction work, and $\dot{Q}$ is the energy transferred to the system as heat. To simplify the energy balance, kinetic and potential energy changes, shaft work, and expansion/constraction work are neglected. Applying these simplifications results in the following energy balance:

$$\frac{d(m\hat{U})}{dt} = -\dot{m}\hat{H}_{out} + \dot{Q} \tag{12}$$

The equation can be further simplified by using the product rule, incorporating the result of the overall mass balance (dm/dt = -$\dot{m}$) and using the assumption that $d\hat{U}/dt$, the change in specific internal energy with time, is equal to zero. For liquids, the specific internal energy in the reservoir is approximately equal to the specific enthalpy in the reservoir. Therefore, the final form of the energy balance with the stated assumptions is:

$$\Delta\dot{H} = \dot{Q} \tag{13}$$

If the device can be assumed to have negligible heat loss from the system to the surroundings, then the heat added to the system by the heater element is equal to the change in enthalpy. Heat loss to the environment (non-adiabatic operation) would increase the magnitude of the $\dot{Q}$ term.

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

TABLE 1
References: Glycerin and propylene glycol liquids at 25°C and 1.01325 bar

Substance	$\dot{m}_{in}$	$\widehat{H}_{in}$	$\dot{m}_{out}$ (g/s)	$\widehat{H}_{out}$ (J/g)
Glycerin (A)	0	0	0.001748	$\widehat{H}_1$
Propylene glycol (B)	0	0	0.000616	$\widehat{H}_2$

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 go to the final temperature. The final temperature, T_f , was assumed to be the average of the bubble point and dew point temperatures (249.5°C for this example). Note that this simplified analysis assumes that the liquid and vapor heat capacities are independent of temperature.

$$\widehat{H}_1 = C_{pA,liquid}(T_{bpA} - 25°C) + \Delta H_{vapA} + C_{pA,vapor}(T_f - T_{bpA}) \tag{14a}$$

$$\widehat{H}_1 = 56.62 + 91.7 - 6.79 = 143.5 \text{ kJ/mol} \tag{14b}$$

$$\widehat{H}_1 = \left(143.5\ \frac{\text{kJ}}{\text{mol}}\right)\left(\frac{1000\ \text{J}}{1\ \text{kJ}}\right)\left(\frac{1\ \text{mol}}{92\ \text{g}}\right) = 1560.1\ \text{J/g} \tag{14c}$$

$$\widehat{H}_2 = C_{pB,liquid}(T_{bpB} - 25°C) + \Delta H_{vapB} + C_{pB,vapor}(T_f - T_{bpB}) \tag{15a}$$

$$\widehat{H}_2 = 30.76 + 66.5 + 9.50 = 106.8 \text{ kJ/mol} \tag{15b}$$

$$\widehat{H}_2 = \left(106.8\ \frac{\text{kJ}}{\text{mol}}\right)\left(\frac{1000\ \text{J}}{1\ \text{kJ}}\right)\left(\frac{1\ \text{mol}}{76\ \text{g}}\right) = 1404.8\ \text{J/g} \tag{15c}$$

$$\dot{Q} = \dot{m}_A\widehat{H}_1 + \dot{m}_B\widehat{H}_2 \tag{16a}$$

$$\dot{Q} = \left(0.001748\ \frac{\text{g}}{\text{s}}\right)\left(1560.1\frac{\text{J}}{\text{g}}\right) + \left(0.000616\frac{\text{g}}{\text{s}}\right)\left(1404.8\frac{\text{J}}{\text{g}}\right) \tag{16b}$$

$$\dot{Q} = 3.59\ \text{J/s} = 3.59\ \text{W} \tag{16c}$$

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. There are a variety of designs for e-cigarette devices, but a typical device will use a 3.7 volt battery and power from 5 to 10 watts.[5] The predictions made in this analysis are slightly lower than the power delivered by the battery, which makes sense since we assumed the device did not lose heat to the environment. Heat loss to the environment would add a heat term to the energy balance and would result in an increase in the required power to provide a heat input of 3.6 watts to the liquid in the device. In addition, the power supplied to an e-cigarette device needs to power LED lights, and the control system.

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?

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. The problem has been successfully used in two semesters as part of an in-class jigsaw problem, in which different groups of students work on different parts of the problem. The small groups summarize their work on a whiteboard in the classroom and present it to the class. The entire scope of the problem is demonstrated as the sum of the group contributions.

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