

Material and Energy Balances
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Lecture - 48

Energy Balances on Nonreactive Processes with Phase Change: Tutorials - 1

Welcome to today's lecture for Energy Balances on Nonreactive Phase Change Processes. We already looked at some of the fundamentals associated with such processes and we solved a couple of simple example problems. Today, we will have a tutorial session. We will look at problems which are a little more complicated, try to address them from all different angles, so that we can actually get a full feel for how these problems need to be solved.

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Problem #1

- A mixture that contains 46 weight % acetone (CH_3COCH_3), 27% acetic acid (CH_3COOH), and 27% acetic anhydride [$(\text{CH}_3\text{CO})_2\text{O}$] is distilled at $P = 1$ atm. The feed enters the distillation column at $T = 348$ K at a rate of 15,000 kg/h. The distillate (overhead product) is essentially pure acetone, and the bottoms product contains 1% of the acetone in the feed. The vapor effluent from the top of the column enters a condenser at 329 K and emerges as a liquid at 303 K. Half of the condensate is withdrawn as the overhead product, and the remainder is refluxed back to the column. The liquid leaving the bottom of the column goes into a steam-heated reboiler, in which it is partially vaporized. The vapor leaving the reboiler is returned to the column at a temperature of 398 K, and the residual liquid, also at 398 K, constitutes the bottoms product. A flowchart of the process and thermodynamic data for the process materials follow.
- Calculate the molar flow rates and compositions of the product streams.
- Calculate the condenser cooling requirement \dot{Q}_c (kJ/h).
- Use an overall energy balance to determine the reboiler heating requirement \dot{Q}_r (kJ/h).
- If the reboiler heat is provided by the condensation of saturated steam at 10 bar gauge, at what rate must steam be fed?

Problem adapted from Felder and Rousseau, Elementary Principles of Chemical Processes, 3rd edition, Wiley-India

A mixture that contains 46 weight percent acetone and 27% acetic acid and 27% acetic anhydride is distilled at pressure 1 atmosphere. The feed enters the distillation column at temperature of 348 Kelvin at a rate of 15,000 kg/hour. The distillate, which is the overhead product, is essentially pure acetone and the bottom product contains 1% of the acetone, which is sent through the feed.

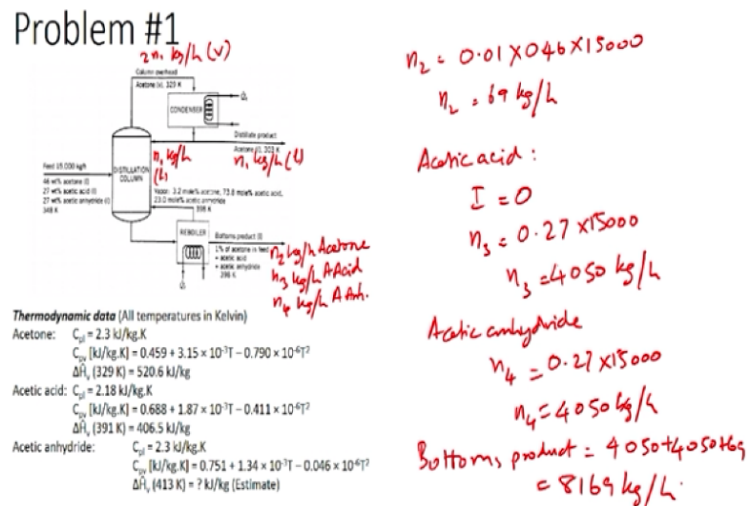
The vapour effluent from the top of the column enters a condenser at 329 Kelvin and emerges as a liquid at 303 Kelvin. Half of the condensate is withdrawn as the overhead product and the remainder is refluxed back to the column. The liquid leaving the bottom of the column goes to a

steam heater reboiler, in which it is partially vapourised. The vapour leaving the reboiler is returned to the column at a temperature of 398 Kelvin and residual liquid also at 398 Kelvin constitutes the bottom product.

A flow chart of the process and the thermodynamics data of the process materials are given here and based on that you are likely expected to calculate the molar flow rates and the composition of the product stream, the condenser cooling requirement and using the overall energy balance to determine the reboiler heating requirement QR and if the reboiler heat is provided by the condensation of saturated steam at 10 bar, at what rate should the steam be fed.

Now we have multiple things that we need to calculate. We have the flow chart given and the thermodynamic data given.

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Let us look at how we would go about solving this problem. The first part of the problem is only material balance and it is reasonably simple material balance that we need to perform. Before we start performing the material balance calculations, let us first label all the unknowns. We have all the information about the feed stream. We know that the column overhead basically contains only acetone vapour, which is condensed and half of it is sent back as recycle.

And the other half is removed as the distillate product. The column overhead let us assume that it is $2n_1$ kg/hour. So this would be a vapour phase and you have a distillate product, which would be n_1 kg/hour, which is a liquid product and you would also have n_1 kg/hour of recycle, which is also a liquid sent back into the system. We also have been given the temperature conditions, which is 329 Kelvin for the column overhead and 303 Kelvin for the distillate product and the recycle stream.

So the bottom enters into a reboiler and you have a bottoms product, which is recovered and this bottoms product contains 1% of the acetone, which is fed to the system. The rest is acetic acid and acetic anhydride at 398 Kelvin. Let us call this contains n_2 kg/hour of acetone and n_3 kg/hour of acetic acid and n_4 kg/hour of acetic anhydride. So these are the mass flow rates of these components, which are leaving the system through the bottoms product.

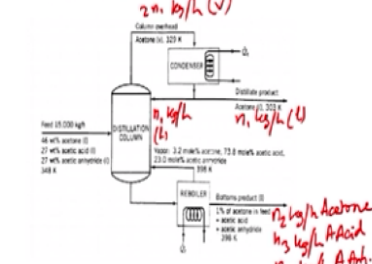
Now let us perform the required material balance calculations. The first information that we have directly is 1% of the acetone fed to the system is actually recovered through the bottoms product, which means we can calculate n_2 directly. So $n_2 = 0.1 * 0.46$, which is the mass fraction of acetone in the feed * the mass flow rate of the feed, which 15,000 kg/hour. Therefore, you get n_2 as 69 kg/hour.

Now we need to calculate how much of acetic acid and acetic anhydride are actually leaving through this stream. We need to write an acetic acid balance. Acetic acid balance would be input = output, which would be $n_3 = 0.27 * 15,000$. As acetic acid and acetic anhydride are leaving only through the bottoms product for the overall system, this calculation is simple and we can get n_3 as 4,050 kg/hour.

Similarly writing an acetic anhydride balance, we would be able to calculate the n_4 , which is $0.27 * 15,000 = 4050$ kg/hour. From this, we can calculate what the bottoms product is. So bottoms product is basically the summation of these masses, which is $4050 + 4050 + 69$ giving a total mass of 8169 kg/hour. Using the total mass balance, we can actually calculate the distillate product also.

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Problem #1



Thermodynamic data (All temperatures in Kelvin)

Acetone: $C_{p,i} = 2.3 \text{ kJ/kg.K}$
 $C_{p,i} \text{ [kJ/kg.K]} = 0.459 + 3.15 \times 10^{-7}T - 0.790 \times 10^{-9}T^2$
 $\Delta H_i \text{ (329 K)} = 520.6 \text{ kJ/kg}$

Acetic acid: $C_{p,i} = 2.18 \text{ kJ/kg.K}$
 $C_{p,i} \text{ [kJ/kg.K]} = 0.688 + 1.87 \times 10^{-7}T - 0.411 \times 10^{-9}T^2$
 $\Delta H_i \text{ (391 K)} = 406.5 \text{ kJ/kg}$

Acetic anhydride: $C_{p,i} = 2.3 \text{ kJ/kg.K}$
 $C_{p,i} \text{ [kJ/kg.K]} = 0.751 + 1.34 \times 10^{-7}T - 0.046 \times 10^{-9}T^2$
 $\Delta H_i \text{ (413 K)} = ? \text{ kJ/kg (Estimate)}$

Total : Distillate
 $15000 = \text{Distillate} + \text{Bottoms}$
 Distillate = 6831 kg/L

Bottoms :
 $\left(\frac{69}{8169} \times 100\right)\%$ Acetone
 $\left(\frac{4050}{8169} \times 100\right)\%$ Acetic acid & Acetic anhydride
 0.8% , 49.6% AA & AAH.

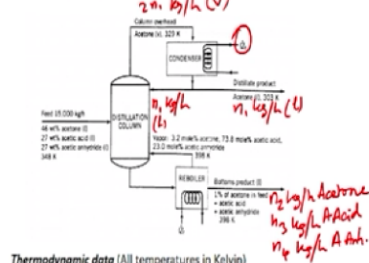
Distillate product can be calculated here. So what we need to do is the total mass balance would be $15,000 = \text{distillate} + \text{bottoms}$. Now we already know the bottoms is 8169, so we can calculate distillate as 6831 kg/hour. With this, we have the mass flow rates of the distillate and the bottoms product and also the composition of the bottoms product can be identified because we know the individual components and the mass flow rates of the individual components.

So the bottoms product composition would be $69/8169 \times 100\%$ for acetone and it would be $4050/8169 \times 100\%$ for both acetic acid and acetic anhydride. You can calculate this and the values are 0.8% acetone and 49.6% acetic acid and acetic anhydride. With that, we have performed the required material balance calculations. We can now move on to the second part of the problem. In the second part of the problem, we have been asked to calculate Q_c , which is the cooling requirement of the condenser. So this Q_c needs to be calculated.

For identifying Q_c , we can actually use the condenser as the system and perform energy balances.

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Problem #1



Thermodynamic data (All temperatures in Kelvin)

Acetone: $C_{p,l} = 2.3 \text{ kJ/kg}\cdot\text{K}$
 $C_{p,v} \text{ (kJ/kg}\cdot\text{K)} = 0.459 + 3.15 \times 10^{-7}T - 0.790 \times 10^{-9}T^2$
 $\Delta \hat{H}_v \text{ (329 K)} = 520.6 \text{ kJ/kg}$

Acetic acid: $C_{p,l} = 2.18 \text{ kJ/kg}\cdot\text{K}$
 $C_{p,v} \text{ (kJ/kg}\cdot\text{K)} = 0.688 + 1.87 \times 10^{-7}T - 0.411 \times 10^{-9}T^2$
 $\Delta \hat{H}_v \text{ (391 K)} = 406.5 \text{ kJ/kg}$

Acetic anhydride: $C_{p,l} = 2.3 \text{ kJ/kg}\cdot\text{K}$
 $C_{p,v} \text{ (kJ/kg}\cdot\text{K)} = 0.751 + 1.34 \times 10^{-7}T - 0.046 \times 10^{-9}T^2$
 $\Delta \hat{H}_v \text{ (413 K)} = ? \text{ kJ/kg (Estimate)}$

$$Acetone (v, 329 K) \rightarrow Acetone (l, 303 K)$$

$$\dot{H}_c (v, 329 K) \rightarrow \dot{H}_c (l, 329 K)$$

$$\downarrow$$

$$Ac (l, 303 K)$$

$$\hat{H} = -\Delta \hat{H}_v + \int_{329}^{303} (C_p)_l dT$$

$$= -520.6 + 2.3(-26)$$

$$\hat{H} = -580.4 \text{ kJ/kg}$$

$$\dot{Q}_c = \Delta \dot{H} = (2 \times 6831 \times -580.4) \text{ kJ/h}$$

$$\dot{Q}_c = -7.93 \times 10^6 \text{ kJ/h}$$

So what we have is acetone, which is coming in as vapour at 329 Kelvin. This is getting condensed to form acetone liquid at 303 Kelvin. So this is the overall process. Looking at the thermodynamic data provided, we have that the heat of vapourisation for acetone at 329 Kelvin is given, which means we can use that heat of vapourization for performing these calculations.

This can actually be broken down into two steps, which would be acetone vapour at 329 Kelvin going to acetone liquid at 329 Kelvin and then getting cooled further to form acetone liquid at 303 Kelvin. This would be condensation process where you have the delta H cap V can be used and this would be a change in temperature where you can use integral CPdT. The total change in enthalpy for this process, which will be calculated as delta H cap would be.

This would be the total change in the specific enthalpy of the process for the condenser, so this would be equal to $-\Delta \hat{H}_{cap V}$. Because it is a condensation process, we will be using the negative of heat of vapourization + integral of 329 Kelvin to 303 Kelvin CP acetone liquid dT. So using the CP of acetone liquid, we would be able to calculate these values. We know that the CP of acetone liquid is 2.3 k joules/kg Kelvin.

So using that value, we can directly calculate what this would be. So this is $-520.6 + 2.3 \times -26$. So your H cap value = $-580.4 \text{ k joules/kg}$. So \dot{Q}_c can be obtained using simple energy balance. This is an open system. So the equation would get simplified to form $\dot{Q}_c = \Delta \dot{H}$. Delta H

dot would be = mass flow rate*change in specific enthalpy. So the mass flow rate is $2 \cdot n_1$, which is $2 \cdot 6831 \cdot -580.4$, which would be in terms of kilo joules per hour.

So $Q_c \text{ dot} = -7.93 \cdot 10^6$ kilo joules/hour. So the rate of cooling, which needs to be done for this system, which is the condenser is $-7.93 \cdot 10^6$ kilo joules per hour. So we have the negative sign, because it is a cooling process, where heat is being removed from the system. now that we have performed the calculation for the second part, we can move on to the third part, where we have been asked to calculate the Q_r , which is the heat supplied to the reboiler and this has to be done using the overall system as the system to be studied for energy balance.

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Problem #1

Overall:

Ref: 348 K, l	\hat{H}_{in}	n_{out}	\hat{H}_{out}
Ac (l, 303K)	0	6831	-103
Ac (l, 398K)	0	69	115
Ac. Acid (l)	0	4050	109
Ac. Anh (l)	0	4050	113

$\dot{Q} = \dot{Q}_c + \dot{Q}_r = \Delta \dot{H}$

$\dot{Q}_c + \dot{Q}_r = \sum n_{out} \hat{H}_{out}$

$\dot{Q}_r = -\dot{Q}_c + \sum n_{out} \hat{H}_{out}$

$= 8.13 \times 10^6 \text{ kJ/h}$

Thermodynamic data (All temperatures in Kelvin)

Acetone: $C_{p,l} = 2.3 \text{ kJ/kg.K}$
 $C_{p,v} [\text{kJ/kg.K}] = 0.459 + 3.15 \times 10^{-7} T - 0.790 \times 10^{-9} T^2$
 $\Delta \hat{H}_v (329 \text{ K}) = 520.6 \text{ kJ/kg}$

Acetic acid: $C_{p,l} = 2.18 \text{ kJ/kg.K}$
 $C_{p,v} [\text{kJ/kg.K}] = 0.688 + 1.87 \times 10^{-7} T - 0.411 \times 10^{-9} T^2$
 $\Delta \hat{H}_v (391 \text{ K}) = 406.5 \text{ kJ/kg}$

Acetic anhydride: $C_{p,l} = 2.3 \text{ kJ/kg.K}$
 $C_{p,v} [\text{kJ/kg.K}] = 0.751 + 1.34 \times 10^{-7} T - 0.046 \times 10^{-9} T^2$
 $\Delta \hat{H}_v (413 \text{ K}) = ? \text{ kJ/kg (Estimate)}$

Let us look at the overall system. So the overall system would basically have acetone liquid at 303 Kelvin leaving the system, acetone liquid at 298 Kelvin leaving the system, acetic acid and acetic anhydride at 398 Kelvin leaving the system. We need to have these streams as the outlet streams and we would have an inlet stream, which would be acetone, acetic acid and acetic anhydride liquids entering the system at 348 Kelvin.

We can choose reference state either as the inlet or the outlet conditions. For these calculations, I have used the inlet condition as the reference state. So the reference state for this problem would be 348 Kelvin and liquid as the phase. Now let us write down all the components. Here we have

acetone, which is leaving in two different streams at two different conditions. So we will write these separately, so that we can calculate the specific enthalpies for these two things separately.

The substances we would have would be acetone liquid, which is at 303 Kelvin and acetone liquid at 398 Kelvin. You also have acetic acid which is liquid and acetic anhydride, which is also a liquid leaving the system, both are 398 Kelvin. The inlet conditions have been assumed to be the reference state. Because of this, all the enthalpies associated with the inlet streams would be equal to 0. So we do not have to worry about the inlet stream enthalpies for this calculation.

We have to however, account for the outlet enthalpies. So the outlet enthalpy $H_{cap out}$ would have to be calculated. Now we need to identify the flow rates for the individual components, which have been entered in the enthalpy table. We have 6831 kg of acetone liquid leaving at 303 Kelvin and 69 kg of acetone liquid leaving at 398 Kelvin and we also have 4050 kg of acetic acid and acetic anhydride liquids leaving at 398 Kelvin.

Now we need to calculate the specific enthalpy changes for each of these processes. We have acetone liquid at 348 Kelvin going to acetone liquid at 303 Kelvin and acetone liquid at 398 Kelvin. We have acetic acid liquid from 348 Kelvin going to 398 Kelvin and acetic anhydride liquid from 348 Kelvin goes to 398 Kelvin. Now we need to calculate these enthalpies using the CP values that we have.

As all these components are simple enough to calculate, we are able to directly use the CP values and fill out this table, so please go ahead and do these calculations. I will give you the answers, which I have here, which is -103 k joules/kg and 115 k joules/kg and 109 k joules/kg and 113 k joules/kg. So the first acetone liquid alone, you have cooling from 348 Kelvin, which is the inlet to 303 Kelvin, which is the outlet.

Because of this, you have a negative change in enthalpy. The other ones you are actually increasing the temperature by 50 Kelvin, so you end up with values, which are positive. We can calculate the total change in enthalpy using this and we would have to plug it into the general

energy balance, the overall energy balance equation to get Q_R . Assuming that there is no energy, which is being used in the distillation column, you will only account for Q_R and Q_C .

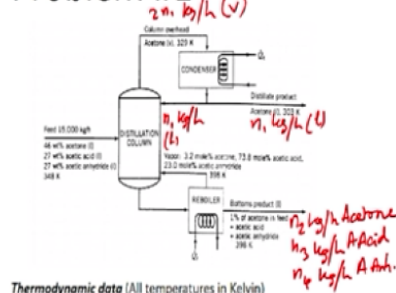
Because those are the only terms, which have been given to us as the terms where heat is being supplied. So using that assumption, we will calculate Q dot as Q_C dot + Q_R dot and fitting it back into the general energy balance equation, this would be equal to ΔH dot. Now we can have Q_C dot + Q_R dot = $\sum n_{out} H_{cap out}$. As all the values for H_n are 0, we can ignore the inlet stream and we will be able to perform calculations using this.

So we would get Q_R dot as $-Q_C$ dot + $\sum n_{out} H_{cap out}$. This value comes out to be 8.13×10^6 k joules/hour. This is the amount of heat rate at which heat needs to be transferred to the reboiler, so that you have the process according to the parameters given. With this, we can move on to the fourth part of the problem where we have been told that the heat for the reboiler is supplied using steam.

It is coming in as steam, which is saturated at 10 bar. Using the heat of vapourization for steam, which is saturated at 10 bar that can be obtained from the steam tables, we can calculate, how much would be the mass of steam, which is required for generating that amount of energy, just by condensation. Using the steam tables, we can identify the enthalpy associated with condensation or vapourization of saturated steam at 10 bar as 1999 k joules/kg.

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Problem #1



$$\Delta \hat{H}_v = 1999 \text{ kJ/kg}$$

$$\frac{\dot{Q}_r}{\Delta \hat{H}_v} = 4070 \text{ kg/h}$$

Thermodynamic data (All temperatures in Kelvin)

Acetone: $C_{p1} = 2.3 \text{ kJ/kg.K}$
 $C_{p1} [\text{kJ/kg.K}] = 0.459 + 3.15 \times 10^{-7}T - 0.790 \times 10^{-9}T^2$
 $\Delta \hat{H}_1 (329 \text{ K}) = 520.6 \text{ kJ/kg}$

Acetic acid: $C_{p2} = 2.18 \text{ kJ/kg.K}$
 $C_{p2} [\text{kJ/kg.K}] = 0.688 + 1.87 \times 10^{-7}T - 0.411 \times 10^{-9}T^2$
 $\Delta \hat{H}_2 (391 \text{ K}) = 406.5 \text{ kJ/kg}$

Acetic anhydride: $C_{p3} = 2.3 \text{ kJ/kg.K}$
 $C_{p3} [\text{kJ/kg.K}] = 0.751 + 1.34 \times 10^{-7}T - 0.046 \times 10^{-9}T^2$
 $\Delta \hat{H}_3 (413 \text{ K}) = ? \text{ kJ/kg (Estimate)}$

This means condensation of 1 kg of steam, which is saturated at 10 bar would generate close to 2000 k joules of energy. To calculate the mass of steam required, we would have to calculate $\dot{Q}_r / \Delta \hat{H}_v$, which would be roughly equal to 4070 kg of steam/hour. By condensing 4070 kg of steam, which is saturated at 10 bar/hour, we will be able to generate the amount of heat required by the reboiler.

So this gives us a way to calculate the energy balances and we have tried to use multiple concepts, which we have learnt over the last few lectures to apply here. In the next lecture, we will talk about similar calculations, however we will look at a closed system. Until now, all the calculations that we have performed are for open systems. We will look at how energy balances can be applied for closed systems in the next lecture. Thank you.