

Material and Energy Balances
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Module No # 09

Lecture No # 41

Introduction to Nonreactive Processes Without Phase Change

Welcome to today's lecture on energy balances so in the last lecture we looked at procedures and objectives in which we would approach energy balance problem during that time we actually discussed that we can calculate change in internal energy and enthalpy only for certain types of processors. Today we will look at a specific type of process where there is no phase change or reactions happening so we can actually have to calculate change in enthalpy for different steps during such assistant.

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Changes in P at Constant T

- Experiments show that $\hat{U} \neq f(P)$ for solids and liquids at fixed T, as is specific volume. If P of a solid or liquid changes at constant T, then
$$\Delta\hat{U} \approx 0 \text{ and } \Delta\hat{H} = \Delta\hat{U} + \Delta(P\hat{V}) \approx \hat{V}\Delta P$$
- Both \hat{U} and \hat{H} are independent of pressure for ideal gases
 - $\Delta\hat{U} \approx 0$ and $\Delta\hat{H} \approx 0$ for a gas undergoing an isothermal pressure change unless gases well below 0°C or well above 1 atm are involved unless tables of \hat{U} and \hat{H} as $f(T,P)$ are available
- If gases are far from ideal or undergo large ΔP , you must use property tables or sophisticated thermodynamic correlations

So the first type of the process would be where pressure changes at constant temperature now experiment have shown that specific internal energy is not a function of pressure for solids and liquids at a fixed temperature and this is also true for specific volume if pressure of a solid or a liquid changes at constant temperature then you can assume that the change internal energy for this process = 0.

And this approximately equal to 0 because it is also negligible and you also have the strange in specific enthalpy which is the summation of change in internal energy + delta of PV cap. So this can then be simplified to be V cap delta V so this value is usually very small because the V cap value for solids and liquids is small. So V cap being inverse density for solids and liquids we have high densities the value for V cap would be very small.

So the term would be of significant only when the pressure changes are very high so you can tend to ignore it even for solid and liquids for pressure changes which are very small. For ideal gases both U cap or H cap are independent of pressure so you can assume that change in specific internal energy and specific enthalpy would be 0 for ideal gases so if you have a gas which is undergoing an isothermal pressure change then you would assume this to be 0 even for real gases because it is almost negligible unless gases are at conditions well below 0 degree Celsius or above atmosphere.

Under these conditions what happens is ideality of the gases become questionable we cannot actually assume ideal gas behavior under condition where temperature is well below 0 and pressure is well above 1 atmosphere so because of this reason we would want to use these values for specific internal energy and specific enthalpy while performing energy balance calculations.

However there is no equation that can be used directly or this you would have to use it from tabulated values which are built on experimental data, So if gases are far from ideal behavior or even if the real gases are undergo huge changes in pressure then you must use property tables or other thermodynamic correlations which can be used to calculate the change specific internal energy and change in specific enthalpy.

So such thermodynamic correlations can be obtained from different thermodynamic books this is beyond the scope of thermodynamic course and we will not be discussing the thermodynamic correlations for this course most of the problem could have very small changes in pressure this is especially valid for biological system or even bio chemical reactions where you would usually not have that significant change in pressure.

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Changes in T

- Sensible heat – Amount of heat that needs to be transferred to raise or lower the temperature of a substance or a mixture
- Quantity of heat required to make a change in temperature

Closed system: $Q = \Delta U$ (or)

Open system: $\dot{Q} = \Delta \dot{H}$

- Sensible heat can be calculated from change in internal energy or enthalpy

The next type of process is where you have changes in temperature so for these processes when there is a constant pressure and temperature is changing we have to account for change in internal energy and change in enthalpy. Sensible heat is the term which is used to define the heat which is actually transferred to the system to raise or lower to the temperature of a substance of mixture.

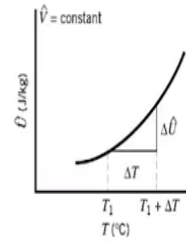
So when there is change in temperature there is actually sensible heat which is supplied to the system so this heat is absorbed by the system and the temperature actually increases because of this heat supplied. The quantity of heat which is required to make a change in temperature might have to be calculated when we perform energy balances and this is given as $Q = \Delta U$ for closed system and $\dot{Q} = \Delta \dot{H}$ for open systems.

So this equation itself comes from the generation energy balance equation assuming changing in kinetic energy potential energy and shaft work are negligible. Sensible heat can be calculated from change in internal energy or enthalpy and this value can be directly used for understanding how much energy is needed to be supplied or heat needs to be supplied to increase the temperature of the system to one point to another.

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Changes in T

- Specific internal energy – Strongly dependent on T
- If T changes and system volume remains a constant, \hat{U} depends on T as shown in figure
- The slope of this curve as $\Delta T \rightarrow 0$ is called the heat capacity at constant volume, C_v



$$C_v = \left\{ \lim_{\Delta T \rightarrow 0} \frac{\Delta \hat{U}}{\Delta T} \right\} = \left(\frac{\partial \hat{U}}{\partial T} \right)_v$$

Specific internal energy itself strongly dependent on temperature if temperature changes the system volume remains the constant then specific internal energy depends on the temperature as shown in the figure. So you can see that the specific internal energy increases in the exponential fashion as temperature changes. The slope of the curve is delta T tends to 0 is called as the heat capacity at volume or CV.

So we have already seen this term before and this slope which we have at that as a tangent for this curve would be the CV for the particular component at the given temperature. This CV is given as limit delta T tends to 0 delta U cap divided by delta T so which is we can also be written as Dou U cap Dou T at constant volume.

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Changes in T

- $\hat{U} = f(T)$ is not a straight line $\rightarrow C_v$ is dependent on T
- The change in \hat{U} for a temperature rise from T to T + dT at constant volume is

$$d\hat{U} = C_v(T)dT$$

$$\Delta\hat{U} = \int_{T_1}^{T_2} C_v(T)dT$$

- Exact for ideal gases
- Good approximation for solids and liquids
- Valid for non-ideal gases if V is constant



So specific internal energy is a function of temperature and as we saw you through the curve this particular function is not a straight line. Which means CV which is the slope of the tangent drawn to the curve will not be a constant for different temperature CV itself is actually dependent on temperature and it is given in terms of polynomial which can be obtained from textbooks and reference books.

The change in U cap for a temperature raise from T to T plus DT is at constant volume can be given as DU cap = CV which is a function of temperature DT. So delta U cap would be integral T1 to T2 CV DT where CV is actually a function of temperature So this correlation or CV can be different for different components and even for the same component which is in different phases you would have different series.

So water liquid versus water vapor would have CV values and you would have to use the appropriate CV value for the chemical component and also it is physical state. This equation is exact for ideal gases and it is very good approximation for solids and liquids while you perform calculations. It also for non ideal gases if volume is a constant.

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Changes in T

- Consider a process when both T and V changes
- Build a hypothetical path
 - Step 1 – V changes at constant T
 - Step 2 – T changes at constant V
- For step 1, $\Delta\hat{U} \approx 0$ for all substances except non-ideal gases
- For step 2, $\Delta\hat{U}$ is given by the integral equation just derived

So if you have a process where you have temperature and volume changing then what you would due to account for calculating the change in internal energy would be you assume a hypothetical path. The first step can be where volume changes at constant temperature and the second step would be where temperature changes at constant volume for the step one where there is volume change in no change in temperature ΔU cap would approximately be equal to 0 because it is negligible for all substances except non ideal gases where there is going to be huge changes in pressure or volume and so on.

For step 2 where ΔU cap it depends on the temperature you would have to calculate it using the integral equation that we just derived ΔU cap would be integral $CVdT$. So the summation of these two change in internal energy will give you total change in internal energy for the process.

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Changes in T

- Consider the change in enthalpy when a substance is heated at constant P
- Enthalpy – Strongly depends on T
- If $\Delta\hat{H}$ is the change in enthalpy for an increase in temperature for T to T + ΔT , then as $\Delta T \rightarrow 0$, the ratio $\Delta\hat{H}/\Delta T$ approaches a limiting value, called heat capacity at constant pressure

$$C_p = \left\{ \lim_{\Delta T \rightarrow 0} \frac{\Delta\hat{H}}{\Delta T} \right\} = \left(\frac{\partial\hat{H}}{\partial T} \right)_p$$

$$d\hat{H} = C_p(T)dT$$

$$\Delta\hat{H} = \int_{T_1}^{T_2} C_p(T)dT$$



Instead of a constant volume process if you were to have a constant pressure process when you would have to account for change in enthalpy when the substance is heated. So enthalpy also strongly depends on temperature and relationship is similar to what you saw with internal energy. So if ΔH_{cap} is the change in enthalpy for increase in temperature from T to T + ΔT then as ΔT tends to 0 the ratio of ΔH_{cap} by ΔT approaches the limiting value which is called as the heat capacity at constant pressure.

So this is similar to what we saw for the CV value here this is called CP which is the heat capacity at constant pressure. CP is given as limit ΔT tends to 0 ΔH_{cap} divided by ΔT which equals $\text{Dou } H_{cap} \text{ Dou } T$ at constant pressure. So from here we can calculate the value of ΔH_{cap} as integral $CPdT$ CP again is a function of temperature just like we had for CV.

As you saw the curve for ΔH_{cap} for internal energy changing with respect to temperature this is also not a straight line which means that the slope which would be drawn for the tangents would keep changing as the temperature changes. So there CP will also be function of temperature and we would have to calculate as integral $CPdT$.

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Changes in T

- Consider a process where both T and P changes
- Build a hypothetical path
 - Step 1 – P changes at constant T
 - Step 2 – T changes at constant P
- For step 1, $\Delta\hat{H} = 0$ for ideal gases and $\Delta\hat{H} = V\Delta P$ for solids and liquids
- For step 2, $\Delta\hat{H}$ is given by the integral equation just derived

So let us assume a process where both temperature and pressure changes here again will build a hypothetical path where the first step would be change in pressure and the second step would be the change in temperature. So for the first step ΔH_{cap} would be equal to 0 for ideal gases and it would be equal to $V \Delta P$ for solids and liquids.

So this $V \Delta P$ can be very very small the second step would be change in temperature so the ΔH_{cap} value for the second step would be calculating using the integral equation which we derived which is integral CPDT.

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Changes in T

- For ideal gases; and non ideal gases if ΔP is small

$$\Delta\hat{H} = \int_{T_1}^{T_2} C_p(T) dT$$

- For solids and liquids,

$$\Delta\hat{H} = \Delta\hat{H}_1 + \Delta\hat{H}_2 = \hat{V}\Delta P + \int_{T_1}^{T_2} C_p(T) dT$$

- Usually $\hat{V}\Delta P$ is negligible compared to the other term except for large changes in P

For the process that we described where both pressure and temperature changes for ideal gases and non-ideal gases with pressure changes that are small the equation for ΔH_{cap} which is the total change in enthalpy would be $\int CPDT$. So the first step were pressure changes would be 0 for ideal and it will be negligible for non-ideal gases. For solids and liquids the total change in enthalpy would be the summation of $\Delta H_{cap 1}$ and $\Delta H_{cap 2}$.

So this would be $V_{cap} \Delta P + \int CPDT$ $V_{cap} \Delta P$ is the enthalpy associated with the process where pressure changes at constant temperature usually $V_{cap} \Delta P$ is negligible compared to other term where because the other term would have a significant impact however if the pressure changes are very large then this term would also be accounted for because there could also have a significant magnitude.

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Heat Capacities

- C_p and C_v are tabulated in handbooks
- Amount of energy per unit amount per unit temperature interval (J/mol.K) or (BTU/lb_m.°F)
- Also called as specific heat
- Heat capacities are expressed as polynomials

$$C_p = a + bT + cT^2 + dT^3$$
- a, b, c and d can be obtained from textbooks and handbooks

To calculate the value for ΔH_{cap} and ΔU_{cap} we need to know the heat capacities these values which are C_p and C_v are tableted in hand books and text books. You would be able to get the difference C_p values and C_v values from different sources and usually it is a polynomial which is written in terms of amount of energy per unit amount per unit temperature integral.

So this would be joules per kilo Kelvin or BTU per pound mass per degree Fahrenheit so if you remember when we discuss temperature I talked about the difference between a unit change in temperature versus a unit of temperature itself. So here what we actually have is a temperature

interval. So what we look at as Kelvin or degree Celsius would be delta kelvin or degree del Celsius.

So we do not use that expressly so we just write it as Kelvin or degree Celsius this term is also called specific heat and the heat capacities are expressed as polynomials as I said which would take the form $CP = A + BT + CT^2 + DT^3$. So this particular polynomial represents how CP changes with respect to temperature. So this based on this equation we can calculate the delta H cap values by integrating with CP respect to temperature.

In the table the value for A would be given as A times 10 power 3 equals some numerical values this means that you have A time 10 power 3 equals some value. So the actual value for A which you use in the polynomial would be the numerical value times 10 power -3. I will show you an example when we perform calculations but please understand that you need to look at the table carefully and use the values appropriately.

So simple logic you should use is the value for A would always be larger than the value for B and the value for B would be large then the value for C and the value for C would be larger than the value for D. Only then the impact of temperature would be accounted for correctly otherwise there would be an extremely high effect on temperature effect of temperature on CP that you are numerical values you arrive at would be completely half a circle.

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Heat Capacities and Specific Enthalpies

- Simple relationships exist under two conditions
 - $C_p \approx C_v$ for solids and liquids
 - $C_p = C_v + R$ for ideal gases
- For non-ideal gases, the relationship is complex
- If enthalpies have to be calculated frequently for species, build a table of \hat{H}
 - Steam tables
 - Species involved in combustion reactions
 - Reference states used are given



So you can get these values for A, B, C and D from any text book or hand book in many cases the text book or hand book would actually be list only CP values and you might have to calculate internal energy which means you would need CV values. So there are simple correlations which can help you calculate CP from CV so for solids and liquids CP is approximately equal to CV for ideal gases $CP = CV + R$.

So these are the simple correlation which you can use for calculating CP from CV or CV from CP. For non-ideal the relationships are very complex and you would have to use some kind of an empirical correlation which can actually be used so these you can get from other textbooks which would not be part of this course. If enthalpies have to be calculated very frequently then it is useful build a table which can be used and referred the commonly.

Example would be steam tables so the steam tables list the values for specific internal energies specific enthalpy and specific volume and because of this we can use it regularly and steam being a common in any chemical and biochemical process it is useful to have this kind of steam table. Similar tables has been built for combustion reaction gases so gases like carbon dioxide carbon monoxide and water vapor and so on which take part in the combustion reactions have also been tabulated.

So such tables are available in the text books described and also in other hand books so what you need to be careful about is whenever you are using such tables you need to use appropriate reference states. In the last lecture when we talked about objectives and procedures I also talked about identifying appropriate reference states. So identifying appropriate reference states would mean that when you are using tabulated data the reference state used should also be the reference state that is shown in the table.

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Example #1

- Assuming ideal gas behavior, calculate the heat that must be transferred in each of the following cases.
 - A stream of nitrogen flowing at a rate of 100 mol/min is heated from 20°C to 100°C
 - Nitrogen contained in a 5-liter flask at initial pressure of 3 bar is cooled from 90°C to 30°C

So here is the simple example problem which will help us understand how to calculate change in specific internal energy and specific enthalpy. Assuming ideal gas behavior calculate the heat that might be transferred in each of the following cases a stream of nitrogen flowing at a rate of 100 moles per minute is heated from 20 degrees Celsius to 100 degree Celsius.

Nitrogen contained at the second process is nitrogen contained a 5 liter flask at initial pressure of 3 bar being cooled form 90 degree Celsius to 30 degree Celsius. So the first process is where nitrogen is flowing and you are heating it from 20 to 100 degree Celsius the other one is in ahh close system where you have a 5 liter flask and there is a initial pressure of 3 bar given in the process is a cooling process from 90 to 30 Celsius.

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Example #1

- Heating 100 mol/min nitrogen from 20°C to 100°C

$$\begin{aligned} \dot{Q} &= \dot{\Delta H} \\ \Delta \hat{H} &= \dot{n} \int C_p dT \\ C_p &= 0.029 + 0.2199 \times 10^{-5} T + 0.5723 \times 10^{-8} T^2 - 2.871 \times 10^{-12} T^3 \\ \Delta \hat{H} &= \int_{20}^{100} C_p dT \\ \Delta \hat{H} &= 2.332 \text{ kJ/mol} \\ \dot{\Delta H} &= \dot{n} \Delta \hat{H} = 100 \times 2.332 = 233.2 \text{ kJ/min} \\ \dot{Q} &= 233.2 \text{ kJ/min} \end{aligned}$$

Let us see how to solve this problem for the first process where heating of 100 moles per minute of nitrogen is happening you have an open system the general energy balance equation would use enthalpy so you would have the general equation as \dot{Q} equals $\dot{\Delta H}$ so this is based on assumption that there is no change in internal energy, no change in kinetic energy or potential energy and there is no shaft work.

So here this system does not have any moving parts and you also have that there is no change in velocity or change in position given. So we can assume these things and we would end up with \dot{Q} equals $\dot{\Delta H}$. So what we need to do is calculate $\dot{\Delta H}$ so $\dot{\Delta H}$ would be equal to \dot{n} times integral $C_p dT$. So we now need to identify the C_p values which are given in the text books.

So the C_p value given for nitrogen is $0.029 + 0.2199 \times 10^{-5} T + 0.5723 \times 10^{-8} T^2 - 2.871 \times 10^{-12} T^3$. So integrating these equations we can actually get $\Delta \hat{H}$ so $\Delta \hat{H}$ would be integral $C_p dT$ so integrating with respect to the temperature given from heating from 20 degree Celsius to 100 degree Celsius we would be able to get the value for $\Delta \hat{H}$.

So when we do this we get $\Delta \hat{H} = 2.332$ kilojoules per mole so now we need to calculate $\dot{\Delta H}$ which is equal to \dot{n} times $\Delta \hat{H}$ which is 100 times 2.332 giving you 233.2

kilojoules per minute. Now this is the heat which we need to be transferred also \dot{Q} equals $\dot{\Delta U}$ equals 233.2 kilojoules per minute.

So this is simple calculation that needs to be done to calculate the amount of heat that needs to be transferred for this process where nitrogen is being heated from 20 degree Celsius to 100 degree Celsius.

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Example #1

- 5-liter nitrogen flask at initial pressure of 3 bar cooled from 90°C to 30°C

$$Q = \Delta U \quad C_v = C_p - R$$

$$\Delta U = n \Delta \hat{U}$$

$$\Delta \hat{U} = \int_{T_1}^{T_2} C_v dT \quad C_v = \left(0.02900 + 0.2199 \times 10^{-5} T + 0.5723 \times 10^{-8} T^2 - 2.871 \times 10^{-12} T^3 \right) - R$$

$$\Delta \hat{U} = -1.25 \text{ kJ/mol} = 0.02069 + 0.2199 \times 10^{-5} T + 0.5723 \times 10^{-8} T^2 - 2.871 \times 10^{-12} T^3$$

$$n = \frac{PV}{RT} = \frac{(3 \text{ bar}) \times (5 \text{ L})}{(0.008314 \frac{\text{kJ}}{\text{mol}\cdot\text{K}}) (363 \text{ K})} = 0.497 \text{ mol}$$

$$Q = \Delta U = n \Delta \hat{U} = -0.621 \text{ kJ}$$

So the next process is a 5 liter nitrogen flask at an initial pressure of 3 bar is cooled from 90 degree Celsius to 30 degree Celsius. So this would be a close system and it is a constant volume system so you have $Q = \Delta U$ so now you have to calculate ΔU ΔU would be equal to $N \Delta U_{cap}$. So we need to know the values for N and ΔU_{cap} .

So ΔU_{cap} can be calculated as integral $C_v dT$ so C_v can be calculated from this C_p value which we had C_v would be equal to $C_p - R$ because we know the correlation for C_p and C_v for an ideal gas. So now we can from this we can calculate the values for C_v as SP which is $0.02900 + 0.2199 \times 10^{-5} T + 0.5723 \times 10^{-8} T^2 - 2.871 \times 10^{-12} T^3 - R$.

So using the R with the appropriate units you would have R value as 0.008314 So which is kilojoules per mole degree Celsius that is the units for C_v used so we would have to use the same units and we would be having this value as $0.02069 + 0.2199 \times 10^{-5} T + 0.5723$

times $10^{-8} T^2 - 2.871 \times 10^{-12} T^3$. So performing integral CPDT we can get ΔU_{cap} as -1.25 kilojoules per mole.

So the initial temperature is 90°C and the final temperature is 30°C so within this limits we have integrated it to get -1.25 kilojoules per mole as the process is cooling process the change in internal energy is negative. Now we need to know the value for N , N is the number of moles so using ideal gas law we can calculate N as PV / RT so which would be 3 bar times 5 liters.

So this divided by temperature which is 363 Kelvin which is the initial temperature of 90°C and the R value with in terms of bar and liters and Kelvin would be 0.08314 and the units could be liter bar divided by mole kelvin so cancelling out the appropriate units you would get the number of moles as 0.497 moles so from here we can calculate ΔU or Q .

Q would be equal to ΔU which is equal to $N \Delta U_{cap}$ which is equal to -0.621 kilojoules so this is the amount of heat that needs to be removed to cool in a 5 liter flask at a initial pressure of 3 bar from 90°C to 30°C with this we have looked at 2 simple processes where we have calculated change in enthalpy change in internal energy using C_P and C_V values.

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Estimation of Heat Capacities

- Polynomial expression is based on experimental data
- If tabulated formulas don't exist, approximation techniques can be used
- Kopp's rule
 - Simple empirical method for estimating heat capacity of a solid or liquid at or near 20°C
- More accurate techniques are also available in other thermodynamics books and handbooks



In both these processes we had the luxury of having the value for CP given to us in some cases CP values or CV values are not readily available this is especially true in biochemical processes or biochemical processes where the components which are which we are using are unique and we might not actually have the exact value of CP which is measured. So this polynomial expression which is actually based on experimental data and this cannot be exhaustive for all the possible compound and elements which are present in the nature.

So if tabulated formula does not exist we need to look at some approximation technique which would help us estimate the CP or CV values and we can use them appropriately for performing calculations. Once such method is cop rule this the simple experimental sorry simple empirical method which is used for estimating heat capacity of solids and liquids at around 20 degree Celsius.

So the logic here is each element in the compound has an particular compounds toward the CP value and depending upon the number of atoms of the element. We multiply it with the individual contributions and the summation of all the contribution by individual elements gives us a approximate CP value so this approximation is a very simplistic approach there are much more accurate techniques that are available which are which can be seen in thermodynamic text books and hand books.

So we will not go into to greater detail of how to use these so the cop rule is very handy to use and a very simple thing to use that is the very only reason we introduce to it. You can actually look up a text books to find what would be contributions for the individual elements which are involved in the compound.

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Heat Capacity of Mixtures

- Rule 1 – For a mixture of gases or liquids, calculate the total enthalpy change as the sum of the enthalpy changes for the pure mixture components
 - Ignoring enthalpies associated with mixing
 - Good approximation for gases and similar liquids
 - Poor one for dissimilar liquids
 - $(C_p)_{mix}(T) = \sum y_i C_{pi}(T)$
 - $\Delta \hat{H} = \int_{T_1}^{T_2} (C_p)_{mix} dT$
- Rule 2 – For highly dilute solutions of solids or gases in liquids, neglect the enthalpy change of the solute



In addition to this we might also have mixtures so where we might have to calculate the heat capacity of mixtures the rule 1 for the gases and liquids this you can calculate the total enthalpy change as the summation of the enthalpy changes of the pure mixture components. So this means that you are ignoring the enthalpy associated with mixing that this is a good approximation for gases and for similar liquid for example ethanol and methanol being mixed.

These are similar liquids so it does not matter we do not have to account for the heat associated with or mixing if it is a process like mixing of water and sulfuric acid these are very dissimilar liquids. In that case we would have to account for the heat of mixing or enthalpy of mixing. So that is when it becomes a pure approximation to use. So when you do this kind of approximation where you are thinking where you calculating the total change in enthalpy as the summation of the enthalpies associated with individual components in the mixture.

You are basically in implicitly calculating the CP of the mixture so this CPE of the mixture would actually be equal to the mole fraction of the particular component times the CPU of the component and a summation of all the terms which we exist in this system. So delta H cap would be equal to integral CP mixture DT so this is what we do implicitly we could also explicitly calculate the value for CP of the mixture and still perform these calculations.

For highly dilute solutions or gases solutions of solids or gases you can actually neglect the effect of the solute which is dispersed in the liquid and we can use the CP and CV of the liquid itself and this is a very good approximation only for very very dilute solutions.

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Example #2

- Calculate the heat required to bring 150 mol/h of a stream containing 60% C₂H₆ and 40% C₃H₈ from 0°C to 400°C. Determine a heat capacity for the mixture as part of the problem solution.

$$(C_p)_{C_2H_6} = 0.04937 + 13.92 \times 10^{-5} T - 5.816 \times 10^{-8} T^2 + 7.280 \times 10^{-12} T^3$$

$$(C_p)_{C_3H_8} = 0.06803 + 22.59 \times 10^{-5} T - 13.11 \times 10^{-8} T^2 + 31.71 \times 10^{-12} T^3$$

$$(C_p)_{\text{mix}} = Y_{C_2H_6} (C_p)_{C_2H_6} + Y_{C_3H_8} (C_p)_{C_3H_8}$$

Here is another simple problems which helps us understand how we inherently calculate CP of the mixture and how we could actually explicitly do that as well. We are asked to calculate the heat required to bring 150 moles per hour of a steam containing 60% ethane and 40% propane from 0 degree Celsius to 400 degree Celsius. Determine a heat capacity for mixture as part of the problem solution.

So what we should usually do is we would calculate the change in enthalpy for ethane and calculate the change in enthalpy for an propane and add these two values to calculate the total change in enthalpy of the mixture. So instead we could also calculate the CP of the mixture using the mole fraction given and use that CP of the mixture to get the final value for enthalpy.

So I will only solve the technique where we calculate the CP of the mixture I suggest you perform the calculations for individual enthalpy changes and summation and compare it against the numerical values which I will be arriving at. To calculate CP of the mixture we first need to know the CP of ethane and propane. So CP of ethane C₂H₆ is given as 0.04937 + 13.92 times 10 power 5 T – 5.816 times 10 power -8 T squared + 7.280 times 10 power 12 T cube.

CP of propane is $0.06803 + 22.59 \times 10^{-5} T - 13.11 \times 10^{-8} T^2 + 31.71 \times 10^{-12} T^3$. So these values I have taken from your textbook you could also get these from other hand books so now that we have these two CP values you can calculate the CP of the mixture. The CP of the mixture would basically be the moles fraction of C₂H₆ times CP of C₂H₆ + mole fraction of C₃H₈ times the CP value of C₃H₈.

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Example #2

$$(C_p)_{\text{min}} = 0.6(C_p)_{\text{C}_2\text{H}_6} + 0.4(C_p)_{\text{C}_3\text{H}_8}$$

$$(C_p)_{\text{min}} = 0.05683 + 17.39 \times 10^{-5} T - 8.734 \times 10^{-8} T^2 + 17.05 \times 10^{-12} T^3$$

$$\Delta \hat{H} = \int_0^{400} (C_p)_{\text{min}} dT$$

$$\Delta \hat{H} = 34.89 \text{ kJ/mol}$$

$$\dot{Q} = \dot{\Delta H} = \dot{n} \Delta \hat{H} = 150 \times 34.89$$

$$\dot{Q} = 5230 \text{ kJ/h}$$

So this would be CP of mixture = 0.6 times CP of C₂H₆ + 0.4 times CP of C₃H₈. So calculating this we can get CP of mixture as $0.05683 + 17.39 \times 10^{-5} T - 8.734 \times 10^{-8} T^2 + 17.05 \times 10^{-12} T^3$. now that we have the CP of the mixture the delta H Cap value can be calculated as integral CP of the mixture DT and the change in temperature is from 0 degree Celsius from 400 degree Celsius.

So delta H cap after the integration would be 34.89 kilojoules per mole so one thing you should be careful about the temperature you use is the temperature you use should be in the same units as the temperature is given temperature units of the CP term because you have higher degree polynomials the integration would lead to an error if you use Celsius instead of kelvin and kelvin instead of Celsius.

So from the equation of open system we would have $\dot{Q} = \dot{\Delta H}$ which is equal to $\dot{n} \Delta \hat{H}$. So \dot{n} here is 150 so which would be 150 times 34.89 giving $\dot{Q} = 5230$ kilojoules per hour. So this would be the heat required for the process. So with this we have

looked at some of the fundamentals required for performing energy balance calculations in systems where there is no phase change or reaction.

So we will look at real processes where we will have such energy balances and we will perform more calculations we will look at how to perform this calculations in the next class until then thank you.