Material and Energy Balances

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Module No # 01
Lecture No # 02
Process Parameters and Variables

Hello everybody welcome to the next lecture on material energy balances course today we will talk about process parameters and variables there are many parameters and variable which are used to define any process.

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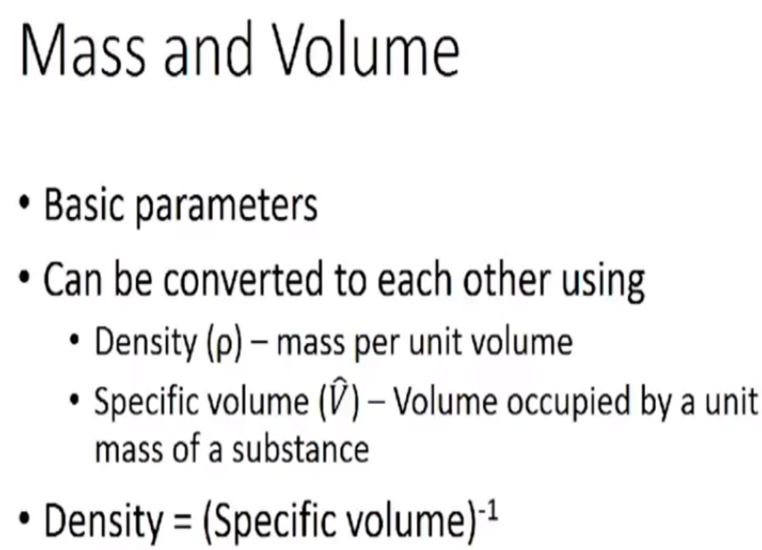

So the first and the most common one which is used are mass and volume this basically defines what assistance could be these can be converted from one to another using density and specific volume. Density is defined as the mass per unit volume and specific volume is defined as the volume occupied by a unit mass of the substance. Basically density is the inverse of the specific volume. So using density and specific volume we can actually convert mass to volume and the other way on.

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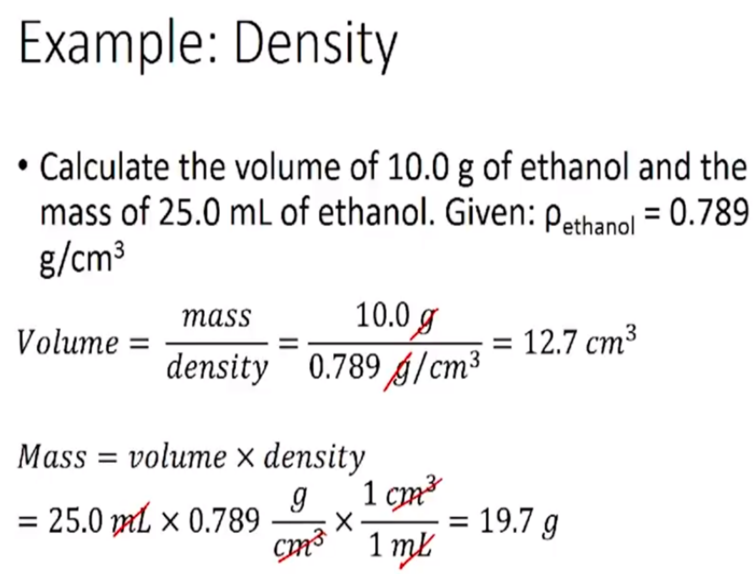

Here you have been asked to calculate the volume of 10 grams of ethanol and the mass of 25 ML of ethanol using the density of ethanol which is 0.789 grams per centimeter cube. So to calculate the volume of 10 grams of ethanol we would divide mass by density so what we do here is 10 grams divided by density which is 0.789 we end up volume of 12.7 centimeter cube.

If you look at the calculation when you look at the dimensional aspect of it the grams actually cancel each other of and the centimeter cube goes to the numerator there by giving you volume. When we calculate the mass of 25 ML of ethanol what we do here is volume times density which is 25 ML times density which is 0.789 grams per centimeter cube if you look at the third term I would have used 1 centimeter cube per ML.

Although numerically this conversion factor will not make a difference writing this is a good practice which ensures that you do not make mistakes while performing conversion. So the ML gets cancelled off and so does your centimeter cube there by you are left only to the grams which is the mass.

So the final answer for these would be 19.7 gram please ensure that whenever you perform calculation simple or tedious write down the units along with the terms which you are using there by you can minimize any errors in calculation which could creep up.

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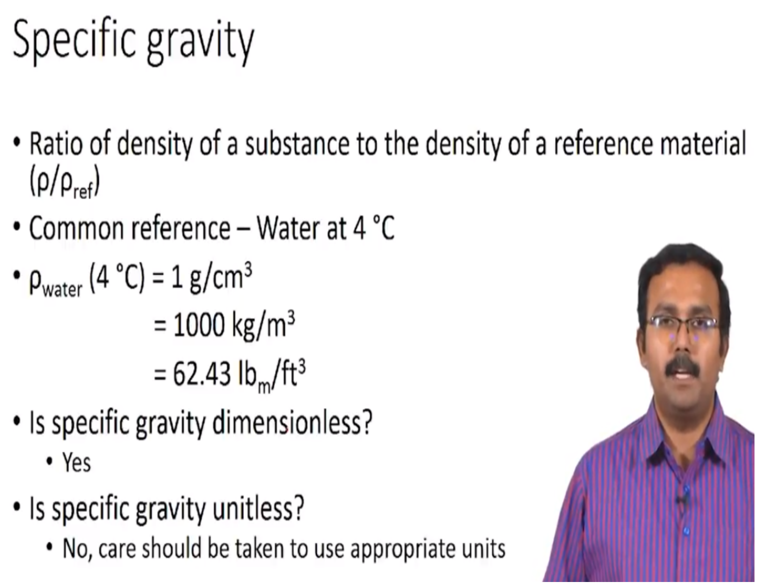

Specific gravity is defined as the ratio of density of the substance to the density of the reference material. The reference material which is commonly used is water at 4 degree Celsius this is because density of water at 4 degree Celsius is 1 gram per centimeter cube or 1000 kilograms per meter cube. So when we use SI units and CGI units these are round numbers which is easy to remember and apply.

However if you were American engineering units the number is a little more combustion which is 62.43 pound mass per feet cube. Now we looked at term which are dimension less and unit less in the last lecture will specific gravity be a dimensionless term yes because it is a ratio of two densities. Obviously the dimensions will get cancelled off and you will end up with the dimensionless terms the more interesting question is this a unit less term?

The answer is no this is not a unit less term you need to use the units appropriately to illustrate this let us try and example problem.

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Example: Specific gravity

- Specific gravity of nitric acid is given as $1.5129^{20\,°C}_{4\,°C}$. Water at 4 °C has been used as the reference. Calculate the density of nitric acid in g/cm³, kg/m³, and lb/ft³.

In lb/ft³ units, $SG_{HNO_3} = 1.5129\ \frac{lb\ HNO_3/ft^3}{lb\ H_2O/ft^3}$

As $\rho_{H_2O} = 62.4\ lb\ H_2O/ft^3$, $\rho_{HNO_3} = 1.5129\ \frac{lb\ HNO_3/ft^3}{lb\ H_2O/ft^3} \times 62.4\ lb\ H_2O/ft^3$

$\Rightarrow \rho_{HNO_3} = 94.4\ lb\ HNO_3/ft^3$

Specific gravity of nitric acid is given as 1.5129, 20 degree Celsius and 4 degree Celsius what are at 4 degree Celsius have been used as the reference calculate the density of nitric acid in grams per centimeter cube kilograms per meter cube and pound per feet cube so the pound used here is pound mass.

So the specific gravity which is given as written as 1.5129 20 degree Celsius and 4 degree Celsius this is the conventional way of writing specific gravity as ratio of density of the substance at 20 degree Celsius to the density of reference material at 4 degree Celsius here the substance is nitric acid and the reference is what. So if we were to find the density in terms of grams per centimeter cube then you should use appropriate units for the specific gravity of nitric acid.

In grams per centimeter cube especially gravity of nitric acid would be given as 1.5129 grams of nitric acid per centimeter cube divided by grams of water per centimeter cube. So when I multiply that density of water with the specific gravity I would end up with the density of nitric acid which is 1.5129 grams of nitric acid per centimeter cube. If I were to calculate the density in terms of kilograms per meter cube then the specific gravity for nitric acid to be written as 1.5129 kilograms of nitric acid per meter cube divided by kilograms of water per meter cube.

Using the density of water as 1000 kilograms of water per meter cube I can calculate the density of nitric acid as 1.5129 times 10 power 3 kilograms of nitric acid per meter cube if want to calculate the density in terms of pound mass per feet cube when specific gravity should be written down as 1.5129 pounds of nitric acid per feet cube divided by pounds of water per feet cube.

Using the density of water as 62.4 pounds of water per feet cube I can calculate the density of nitric acid as 1.5129 times 62.4 giving a final value of 94.4 pounds of nitric acid per feet cube. The units of pounds of water per feet cube cancel of to finally give you the units of pounds =of nitric acid per feet cube which would be the units for the density of nitric acid. As you say based on the units which we have used for specific gravity we use the appropriate density for water to multiply.

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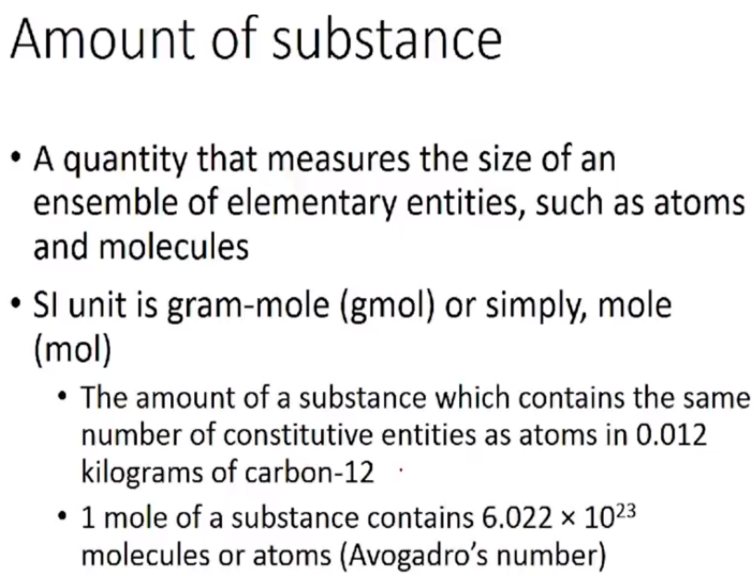

Thereby getting the density for nitric acid in the different units another important terms which is commonly used in addition to the mass and volume would be amount of substance. Any material which is coming in could be defined in terms of mass, volume or amount of substances. Amount of substance is quantity that measures the size of non-sample of elementary entities such as atoms or molecules.

SI unit for such amount of such amount of substance is gram moles or simply written as moles the amount of substance mole is defined as the amount of substance which contain contains the same number of constituent entities as atoms present in 0.012 kilograms of carbon 12. 1 mole of assumptions contains 6.022 times 10 power 23 molecules are atoms this is based on Avogadro's number.

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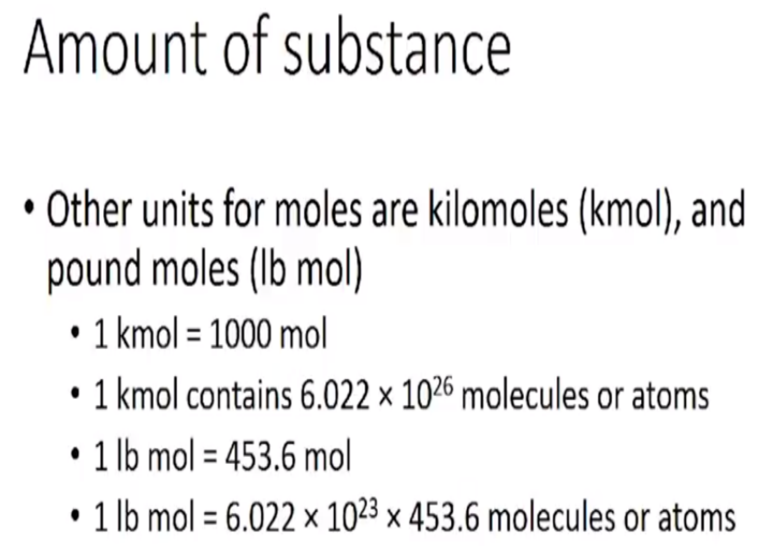

So in addition to gram moles you can also use units like kilo moles and pound moles it is important for you to understand what these represent. 1 kilo mole = 1000 moles this is something everybody remembers and understands because it is a simple conversion 1 kilo mole would then contain 6.022 times 10 power 26 molecules or atoms this is based on Avogadro's number again.

Similarly one pound mole would be 453.6 moles there by 1 pound mole would contain 6.022 times 23 sorry 6.022 times 10 power 23 times 453.6 molecules or atoms knowing this is crucial for understanding American engineering system and understand the concept of pound moles.

(Refer Slide Time: 08:33)

Converting moles to mass

- What information is needed to convert moles to mass?
- Molecular weight: mass of one mole of a substance

$$Molecular\ weight\ (MW) = \frac{Mass\ of\ the\ substance}{Number\ of\ moles}$$

  - E.g. – MW of O_2 is 16 g/mol
  - It can also be expressed as 16 kg/kmol or 16 lb/lb mol
- 1 mol of a substance weighs its MW in grams
- Similarly, 1 kmol of a substance weighs its MW in kilograms and 1 lb mol of a substance weighs its MW in pounds

Moles and mass can be converted between each other how would you do that what information do you need? You need to know the molecule weight of the substance molecular weight is basically the mass of 1 mole of substance so it is calculated as mass of substance divided by the number of moles. Mass molecular weight for oxygen is 16 grams per mole it is also expressed as 16 kilograms per kilo mole or 16 pound per pound mole.

So 1 mole of substance which is one gram mole of substance will weigh its molecular weight in grams and 1 kilo mole of substance will weigh its molecular weight in kilograms and one pound mole of substance will weigh its molecular weight in pounds.

(Refer Slide Time: 09:20)

Example: Conversion of moles to mass

- How many pounds would 10 mol, 10 kmol, and 10 lb mol of ethanol weigh? Given: MW of ethanol = 46.1 g/mol

10 mol weighs 10 mol × 46.1 g/mol = 461 g = 1.0163 lb

$$10\ kmol\ weighs\ 10\ kmol \times \frac{1000\ mol}{1\ kmol} \times 46.1\ \frac{g}{mol} \times \frac{1\ kg}{1000\ g}$$

$$= 461\ kg = 1016.3\ lb$$

$$10\ lb\ mol\ weighs\ 10\ lb\ mol \times \frac{453.6\ mol}{1\ lb\ mol} \times 46.1\ \frac{g}{mol} \times \frac{1\ lb}{453.6\ g}$$

$$= 461\ lb$$

To illustrate this let us and try and solve this example problem where we try to convert moles to masses you have been asked to calculate the number of pounds which should be present in 10 moles 10 kilo moles and 10 pound moles of ethanol given that the molecular weight of ethanol is 46.1 grams per mole. 10 moles of ethanol would weigh 10 moles times the molecular weight this is 46.1 grams per mole giving you 461 grams.

Converting this 461 grams into pounds we would 1.0163 pounds 10 kilo moles would weigh 1o kilo moles times 10000 moles divided by 1 kilo mole times 46.1 grams per mole times 1 kilo gram by 1000 grams giving you an answer of 461 kilograms or 1016.3 pounds so if you where to look at the calculation what you would observe I have converted this kilo moles to moles by multiplying with 1000 and converting the gram to kilo gram by divided it by 1000.

And the moles which is 10000 moles is cancelled of thereby you get the final answer in terms of kilo grams. So these kilo grams I have been converted to pounds similarly I can perform the calculation for pounds also. 10 pound moles would weigh 10 pound moles times 453 .6 moles divided by 1 pound mole times 46.1 grams per mole times 1 pound by 453.6 grams. So the pound moles cancel off so to the moles and so to the grams thereby giving you the final answer of in the units of pounds.

So the final answer you end up with this 461 pounds which is the mass of 10 pound moles of ethanol. So based on this we see that the molecular weight of each of these substances in terms of gram moles kilo grams sorry grams per mole kilo gram per kilo mole and pounds per pound mole can be used to convert them directly into masses.

(Refer Slide Time: 11:52)

Converting moles to mass

- Mass can be calculated as

$$\text{Mass in g} = (MW) \times (\text{mol})$$
$$\text{Mass in kg} = (MW) \times (\text{kmol})$$
$$\text{Mass in lb} = (MW) \times (\text{lb mol})$$

So you can calculate mass and grams as molecular weight express in terms as gram per mole times the moles and mass in kilograms can be calculated as molecular weight expressed in terms of kilo grams per kilo mole multiplied by the kilo moles. Mass in terms of pounds can be calculated as molecular weight in terms of pounds per pound mole times pound mole.

(Refer Slide Time: 12:17)

Composition of a mixture

- Mass fraction (x) – ratio of mass of a substance to the total mass of the system

$$x = \frac{mass\ of\ a\ substance}{total\ mass}$$

- Mole fraction (y) – ratio of number of moles of a substance to the total number of moles of the system

$$y = \frac{moles\ of\ a\ substance}{total\ moles}$$

- Mass percentage = 100x
- Mole percentage = 100y

Another parameter which we need to know about when we talk about any process is the composition of mixture so we initially looked at mass, volume and mole are the amount of substance which are all the measures of the magnitude. We also need to know the composition of the stream which are entering and leaving the system. For this we use two most common terms the first one is mass fraction it is the ratio of mass of the substance to total mass of the system.

So this is conventionally written as X you also have mole fraction which is conventionally written as Y as the ratio of the number of moles of the substance to the total number of moles of the system. These mole fractions and mass fraction can also be written as mass percentages and mole percentages by multiplying these values by 100.

(Refer Slide Time: 13:14)

Example: Mass and mole fractions

- If 10.0 kg of acetic acid is mixed with 90.0 kg of water to prepare vinegar, what are the mass and mole fractions of acetic acid and water in this mixture? Given: MW of acetic acid is 60.1 kg/kmol and MW of water is 18.0 kg/kmol.

Component	Mass (kg)	Mass fraction	MW (kg/kmol)	Moles (kmol)	Mole fraction
CH_3COOH	10.0	$\frac{10.0}{100.0} = 0.100$	60.1	$\frac{10.0}{60.1} = 0.166$	$\frac{0.166}{5.166} = 0.032$
H_2O	90.0	$\frac{90.0}{100.0} = 0.900$	18.0	$\frac{90.0}{18.0} = 5.000$	$\frac{5}{5.166} = 0.968$
Total	100.0	1.000		5.166	1.000

Here is an example problem where we can try to calculate the mass fraction and mole fraction for a mixture which is given. If 10 kilograms of acetic acid is mixed with 90 kilograms of water to prepare vinegar what are the mass and mole fraction of acetic acid and water in this mixture. You are given that molecular weight of acetic acid is 60.1 kilogram per kilo mole and molecular weight of water is 18 kilo grams per kilo mole.

To make our calculation easier we will construct the table the first column contains the components and the second columns gives us the information of the masses which have been provided to us and based on these massed we can then calculate the fraction. The fourth columns is the molecular weight which has been provided to us based weight and the mass calculate the number of moles and based on these you would be able to calculate the mole fraction.

So the problem statement gives us that 90 kilograms of water and 10 kilograms of acetic acid are mixed so these term would be 10.0 and this would be 90.0 giving us the total mass of 100 kilogram. So the mass fraction of acetic fraction would be 10 / 100 giving you 0.000. Similarly the mass fraction of water can be calculated as 90.0 / 100 .0 giving you 0.900 the summation of these two mass fraction would give you unity which is 1.000.

The molecular weight for acetic acid is given as 60.1 kilograms per kilo mole and 18.0 kilogram per kilo mole based on this we can calculate the number of moles of acetic acid as mass which is 10.0 mass which is 10.0 divided by 60.1 giving you a value of 0.166 and mass which is 90 kilo grams divided by the molecular weight giving you a total number moles of 5 moles. So you are left with a final answer which is the total number of moles as 5.166.

So using this you can calculate the mole fraction as 0.166 divided by 51.66 which should be equal to 0.032 and the mole fraction of water would be 5 divided by 5.166 so that the numerical value should be 0.968 the summation of these two would give you unity again. So this how you would go about calculating your mass fraction and mole fraction.

In case you have not been given the masses and only the mass fraction has been given what you can do is you can assume that the total mass of the mixture is 1 grams or 100 kilograms and use the mass fraction to calculate the mass of these mixtures mass of these components in mixtures and then convert those masses to moles and still calculate the moles fraction because mole fractions or ratios the final answer you get will still be applicable will based on it does not depend on any value you are presume for total mass of the mixture.

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Concentration

- Mass concentration – mass of a substance per unit volume of the mixture
- Molar concentration– number of moles of a substance per unit volume of the mixture
- Molarity of a solution – molar concentration of solute expressed as moles of solute per liter of solution
- Molality – number of moles of a solute per kg of the solvent
- Parts per million (ppm) and part per billion (ppb)
    - Discouraged, but widely used in some domains
    - Traditionally, billion is 10^9 in US and 10^{12} in Britain
    - Although the convention in the UK has changed recently, it can still bring in confusion

In addition to composition of the being defined as mass concentration and mole concentration you can also have concentrations. Concentrations are basically mass or moles of substance per unit volume so it is written as mass concentration which is mass of the substance as units volume and mole concentration which is moles of a substance per unit volume.

Another term which is used for defining concentration is molarity of solution is defined as the molar concentration of a solute express in terms of mole of solute per liter of solution. So this is mole of solute per liter of solution you also have molality which is number of moles per solute per kilogram of the solvent. So please understand that molality uses number of moles solute in the numerator and kilo grams of the solvent not the solution but the solvent in the denominator.

You also have the parts per million and parts per billion which are also used these are discouraged by scientific community but it is still widely used in many domain. Traditionally billion in US is 10 power 9 and billion in UK is 10 power 12 this can cause confusion and it is better to avoid PPM and PPB terms as much as possible

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Flow rate

- Rate at which a material flows
- Mass flow rate ($\dot{m}$) – mass flowing per unit time
- Volumetric flow rate (F) – volume flowing per unit time
- Molar flow rate ($\dot{n}$) – moles flowing per unit time
- Mass flow rate = Density × Volumetric flow rate
- Molar flow rate = Mass flow rate/Molecular weight
- Linear speed = Volumetric flow rate/cross sectional area
- Exercise: Perform dimensional analysis to verify these equations

Flow rate is a terms which is used for defining the flows which are entering and leaving the system. So you have the rate at which material flows which can be express as mass flow rate which is mass flowing per time or volumetric flow rate which is volume flowing per unit time or molar flow which is more flowing per unit time.

Just like how you convert mass and volume between each you can convert mass flow rate to volumetric flow rate using density. So mass flow rate = density times volumetric flow rate you can also convert molar flow rate and mass rate flow between using molecular weight. Molar flow rate would be equal to mass flow rate divided by molecular weight you need to understand that this can be used only when the molecular weight of the substance is known.

And in case you have a mixture it might not be appropriate to use this directly unless you have average molecular weight of the mixture. Linear speed can be calculated as volumetric flow rate divided by sectional area. So when you have any material flowing through a pipe or through any stream then the cross sectional area of flow can be used in the dominator and you multiply it with the volumetric flow rate.

So basically you do volumetric flow rate divided by cross sectional area to obtain linear speed as an exercise I would for you to perform dimensional analysis to verify if these three equations are dimensional correct. So check whether mass flow rate can be written as density times volumetric flow rate molar flow rate can be written as mass flow rate time molecule divided by molecular weight and linear speed can be written as volumetric flow rate divided by cross sectional area.

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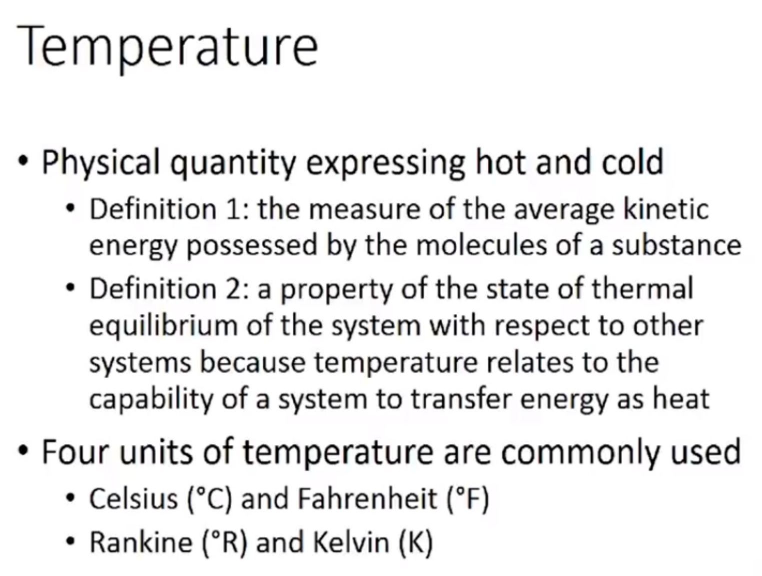

Now that we have looked at all the parameter which defined the amounts and flow rates and so on. The condition of process can be defined based on two major things which are temperature and pressure let us push look at what temperature is. Temperature is the physical quantity which expresses hot and the cold condition of the system it is defined as the measure of the average kinetic energy processed by the molecule of the substance.

It can also be defined as a property of the state of thermal equilibrium of the system with respect to other systems because temperature relates to the capability of the system transfer energy as heat. These two definitions are actually different and where we solve the energy solving balance you would be able to understand and appreciate how these two definitions are actually unique different.

There are four units for temperature which are commonly used you can have Celsius and degrees Fahrenheit you also have the Rankine and Kelvin which are commonly used for measuring temperature.

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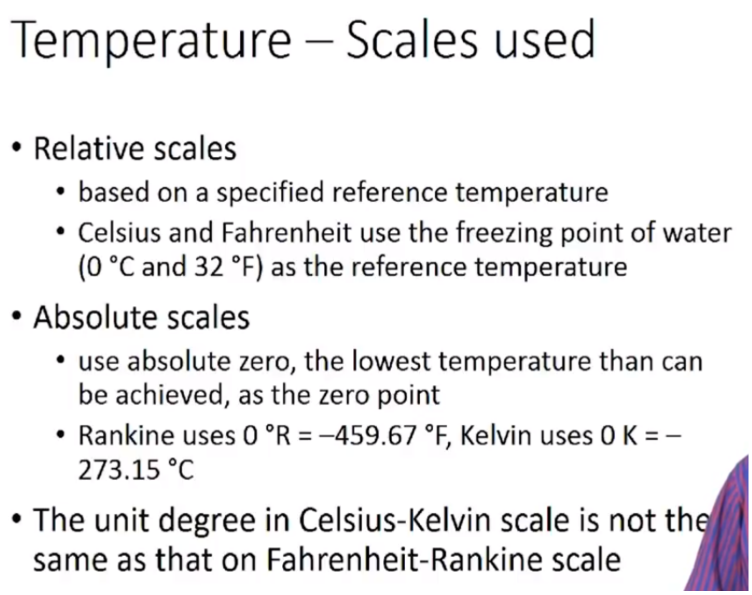

You have the relative scales which are the cellists and degree Fahrenheit which are based on specified reference temperatures. So the reference temperatures which are used Celsius and Fahrenheit are based on the freezing point of the water which is 0 degree Celsius and 23 degree Fahrenheit. You also have obsolete scales which are based on the obsolete 0 which is the lowest temperature can be achieved as the 0 point.

So degree Rankine and kelvin use obsolete 0 as the 0 point degree Rankine uses degree Rankine which is -459.67 degree Fahrenheit and Kelvin uses 0 kelvin which is -273.15 degree Celsius for ease of use these two values are rounded off to – 460 degree Fahrenheit and -273.15 degree Celsius which performing convictions. We need to also understand that the term degree which is 1 unit degree in a Celsius and Kelvin scale is not the same as the degree which is referred to in Fahrenheit and Rankin Scale.

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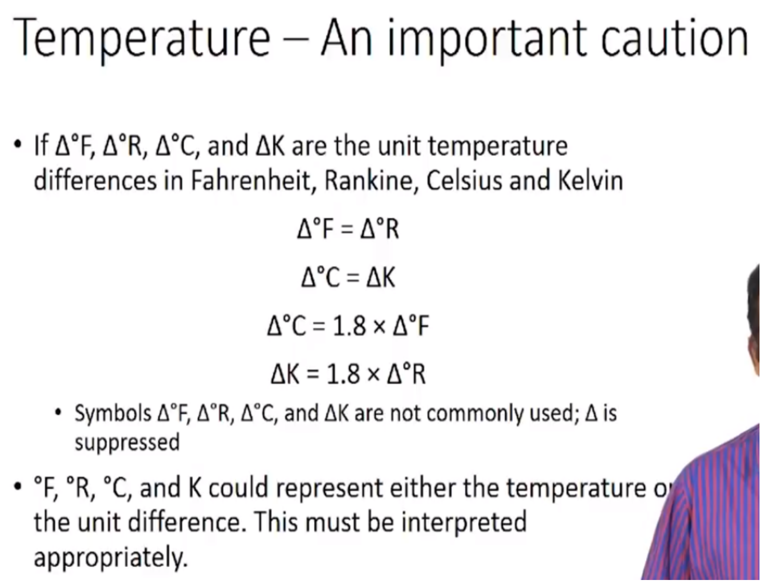

If you were to use delta degree Fahrenheit and delta degree rankine delta degree Celsius and delta kelvin as the unit temperature differences in Fahrenheit rankine Celsius and kelvin then what would you have is delta degree Fahrenheit will be equal to delta degree rankine delta degree Celsius will be equal to delta kelvin but delta degree Celsius will be equal to 1.8 times delta degree Fahrenheit and delta kelvin will be equal to 1.8 times delta degree rankine.

However the symbols delta degree Fahrenheit delta degree Rankine delta degree Celsius and delta kelvin are not commonly used. The delta is suppressed so this means degree Fahrenheit degree Rankine degree Celsius and Kelvin which are used in units could either represent the actual temperature or the unit difference in temperature. And this must be interpreted appropriately if you want an example the best thing can look at is the units for specific heat.

Specific heat capacity can be given in term of per kelvin or per degree Celsius where it is actually temperature difference is being looked at and no the actual temperature written.

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Temperature – Unit coversion

$$T\ (in\ {}^\circ R) = T\ (in\ {}^\circ F)\frac{(1\ \Delta{}^\circ R)}{(1\ \Delta{}^\circ F)} + 460\ {}^\circ R$$

$$T\ (in\ K) = T\ (in\ {}^\circ C)\frac{(1\ \Delta K)}{(1\ \Delta{}^\circ C)} + 273\ K$$

$$T\ (in\ {}^\circ F) - 32\ {}^\circ\mathrm{F} = T\ (in\ {}^\circ C)\left(\frac{1.8\ \Delta{}^\circ\mathrm{F}}{1\ \Delta{}^\circ\mathrm{C}}\right)$$

These temperature units can be converted among each other using these formula if you are already familiar with them the great not please go through that try to convert these numbers between each other and have a feel for how temperatures can be converted form one unit to another.

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Pressure

- Ratio of a perpendicular force to the area
- SI unit is pascal (Pa)
- Other commonly used units of pressure
  - Atmospheres (1 atm = 1.01325×10^5 Pa)
  - Bars (1 bar = 100 kPa)
  - Torr (1 atm = 760 Torr)
  - mm Hg (1 atm = 760 mm Hg)
  - pound-force per square inch (psi)

Pressure which is the other parameter which can be defined for the system is the ratio of perpendicular force to the area. SI unit for pressure is Pascal there are many other units which are commonly used atmospheres Bars, Torr, MMHG and pound force per square inch are all common terms for common units for pressure. So here I have given you a conversion which can be used directly for converting these common terms to SI units and other units.

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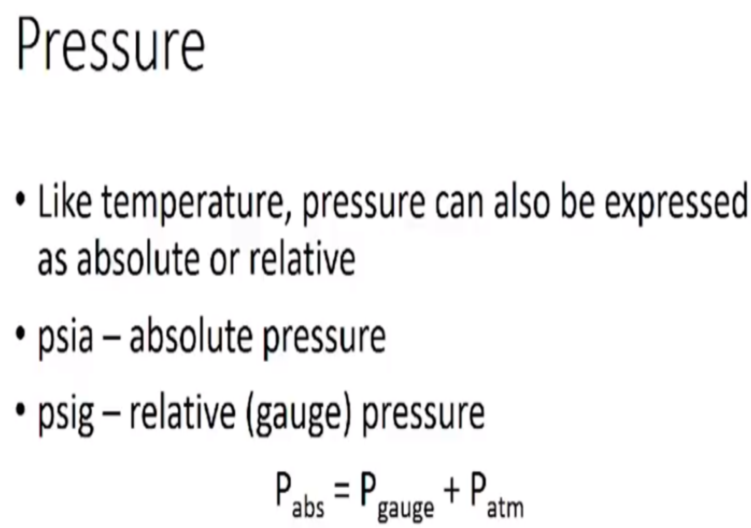

Like temperature pressure can be also expressed in terms of obsolete or relative pressure and obsolete pressure is usually given as PSIA and relative pressure is given as the PSIG is the gauge pressure. Obsolete pressure is nothing but the sum of gauge pressure and atmosphere pressure so this gives you all the fundamental you need to understand the process parameter and variables which are used to define or describe any chemical process.

In the next lecture we will look on what we can do to perform material balance and what are the fundamental which we need to understand to perform such material balance calculations thank you.