Mass, Momentum and Energy Balances in Engineering Analysis

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Lecture – 06
Balance Equations Preliminaries – II (Contd.)

Welcome back. After learning about the various types of constitutive relationship, now what we shall do that based on that lecture, we shall see some numerical problems about the various types of constitutive relationships which I alluded to in my previous lecture.

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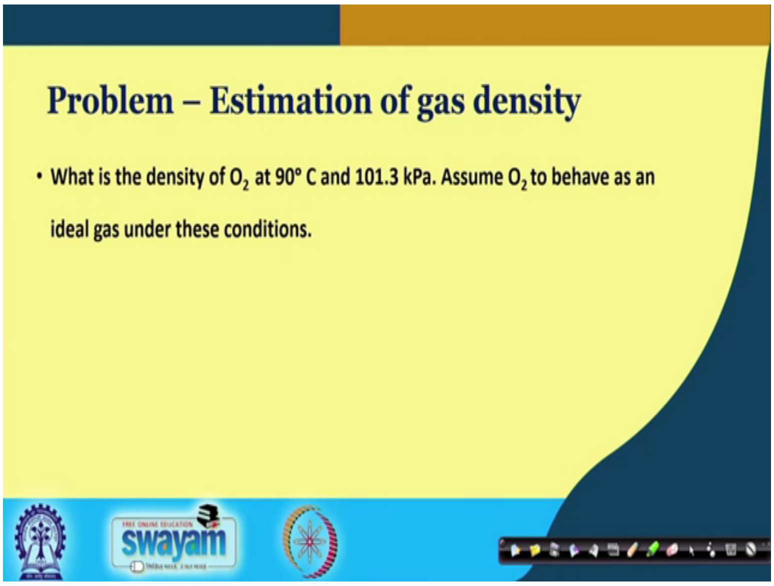

Problem – Estimation of gas density

- What is the density of O_2 at 90° C and 101.3 kPa. Assume O_2 to behave as an ideal gas under these conditions.

So, in this lecture we shall do some numericals, first is the problem on the Estimation of gas density. This is a very common problem you have done perhaps also many a times and you know that we use some kind of gas law, whether ideal gas or non ideal gas. So, first, we take a one problem that is to estimate the density of oxygen at 90 degree centigrade and 101.3 kilo Pascal that is about 1 atmosphere and because this pressure is low and the temperature is quite high; high means that how far is it from the critical temperature. So, it is quite higher than the critical temperature for oxygen and in this case the oxygen can be assumed to be behaving like an ideal gas. So, for this we need to find out the density.

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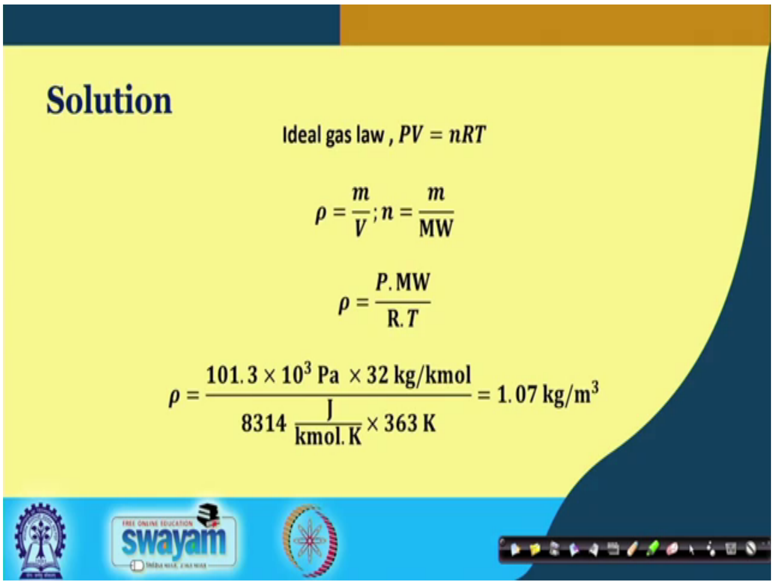

Solution

Ideal gas law, $PV = nRT$

$$\rho = \frac{m}{V}; n = \frac{m}{\mathrm{MW}}$$

$$\rho = \frac{P.\mathrm{MW}}{\mathrm{R}.T}$$

$$\rho = \frac{101.3 \times 10^3\ \mathrm{Pa} \times 32\ \mathrm{kg/kmol}}{8314\ \frac{\mathrm{J}}{\mathrm{kmol.K}} \times 363\ \mathrm{K}} = 1.07\ \mathrm{kg/m^3}$$

So, it is very straight forward and you can simply go to the ideal gas law that is the PV equal to nRT where n is the number of moles. Now, if you rearrange the equation what you get that you can take this V on this right hand side and you get n by V, n by V we will give you the mole per unit volume that is the molar density of oxygen. Now when we talk of density in general, we mean the mass density; that means, we need to convert the mole into mass and the conversion you know that the number of moles equal to the mass divided by the molecular weight.

So, that is what we have done here. So, this density is the mass by volume. So, this n number of moles is the mass divided by the molecular weight and this we substitute in this equation and we get this particular expression and from here, we can find how to find out the density. So, here we plug in the values of the various constants.

Now, whenever you are plugging in the values, I would suggest you that when you are starting, you please write the units of each of the components because if you falter in putting the right units you are going to have wrong answers. So, always make it a point initially when you are trying all the problems, you are putting the units of each of the dimensions, you are using and check the consistency of the dimensions and the units.

So, here we see that pressure, we are given in terms of the Pascal means; that means we are multiplying by 1000 to convert kilopascal to Pascal and then, we have the molecular weight of oxygen as 32 kg per kilo mole. Sometimes you also may use 32 gram per gram mole ok.

Now, here we are reporting everything in terms of the si units. So, we are putting in this kg per kilo mole and then the universal gas constant that is 8.314 joule per mole per Kelvin. So, here we are putting in terms of the 8314; that means, because we are putting in terms of kilo mole. So, we have multiplied the 8.314 in 2000 that is 8314 joule per kilo mole per Kelvin

Now, you see unless we put these units along, initially if you may not be able to understand that why we are taking these values or in what units we are taking the values and once you get used to this, then you may not write the units and this is the temperature in Kelvin. So, once you have ensured that everything is in consistent unit and perhaps you know that how the Julian Pascal are related. So, this Pascal is the force and joule is the work ok. So, this you know that force into the distance is the work. So, this is; that means, this joule is basically Pascal meter. So, this Pascal will get cancelled ok.

So, this with this now we compute the values and we find that this is the value of the density of oxygen at this 90 degree centigrade and this joule is a Newton per Newton meter and Pascal is Newton per meter square. So, Newton per meter square Newton meter; Newton Newton gets cancelled and you get meter cube in the denominator and that is how you get the density as kg per meter cube.

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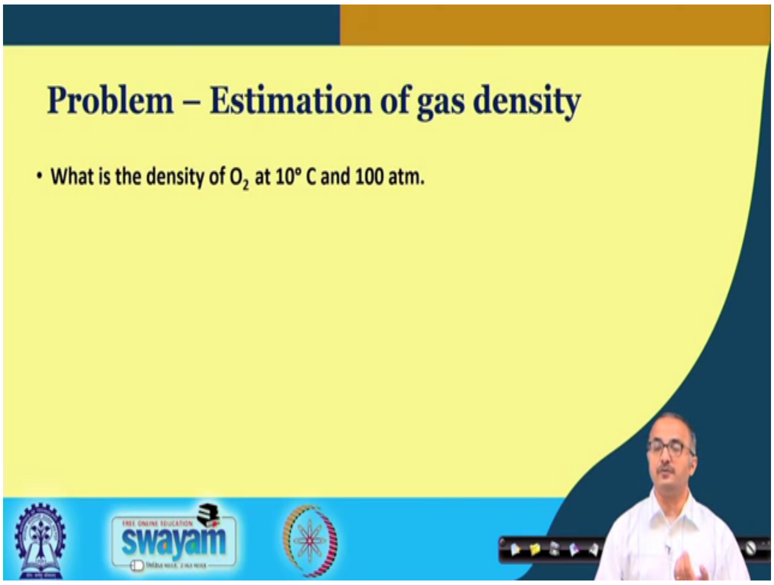

Problem – Estimation of gas density

- What is the density of O_2 at 10° C and 100 atm.

Now, we come to the density of the same oxygen at a bit lower temperature, but at a quite high pressure, now whenever this pressure is raising so much, we would say that we are not no more in the real gas domain sorry ideal gas domain. It will be the real gas domain. Now whenever we have real gas domain we cannot use the ideal equation equation of state, we have to go for real gas equation of state and for that we have this particular expression in terms of the compressibility factor.

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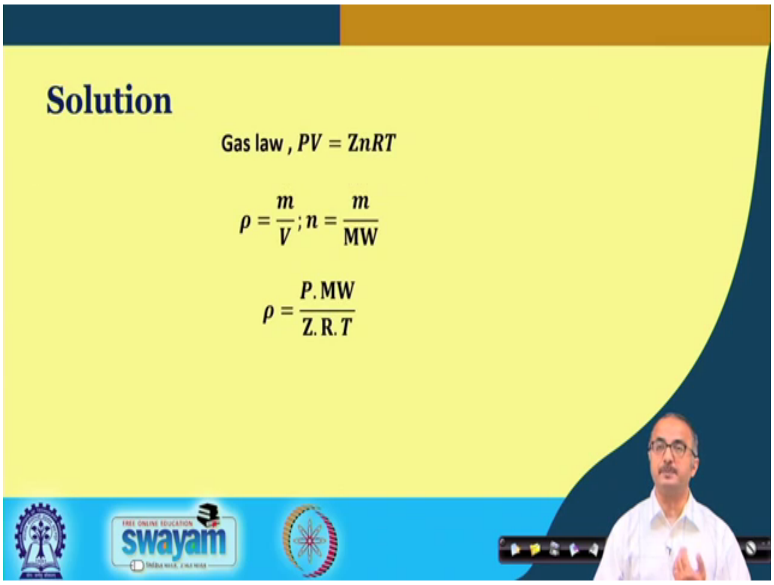

Solution

Gas law , $PV = ZnRT$

$$\rho = \frac{m}{V}; n = \frac{m}{\text{MW}}$$

$$\rho = \frac{P.\text{MW}}{Z.R.T}$$

Now, this value of the Z has to be obtained separately either from some kind of correlations or form from some kind of thermodynamic diagram. So, first again we what we do we see that the density is now put in terms of the Z; the additional thing what is happened and which is different from the ideal case is this the introduction of this Z and this Z if it is equal to 1, then we have the ideal gas equation of state.

So, here we are going to find out the value of Z and this Z is a function of the pressure temperature and we will be showing you one of the ways of finding Z. This is one of the ways from the Thermodynamic diagram and there are many other ways of finding the Z and as an when we come to some specific problem, we shall see that what kind of expression or what kind of method we can adopt to determine the value of the Z.

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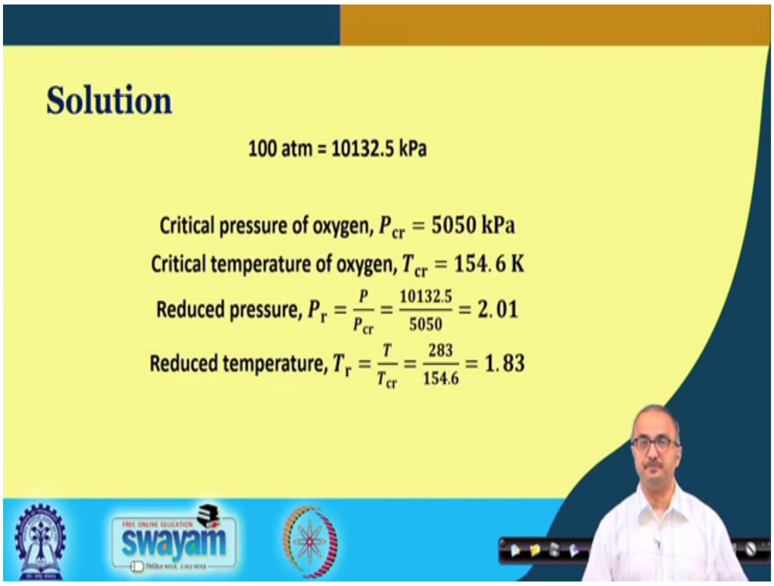

Solution

100 atm = 10132.5 kPa

Critical pressure of oxygen, $P_{cr} = 5050$ kPa

Critical temperature of oxygen, $T_{cr} = 154.6$ K

Reduced pressure, $P_r = \frac{P}{P_{cr}} = \frac{10132.5}{5050} = 2.01$

Reduced temperature, $T_r = \frac{T}{T_{cr}} = \frac{283}{154.6} = 1.83$

So, here you see to determine the value of Z, we need the reduced pressure reduced temperature. For first, for that we need to know the critical pressure and critical temperature of oxygen and here you see the values of this. This is the 5050 kilo Pascal and this is about 50 may bar ok. So, this is the critical pressure and this is the critical temperature of oxygen.

Now, in here you find the reduced pressure by dividing the actual value by the critical value. So, here we get the reduced pressure and we get the reduced temperature; please mind it the reduced values do not have any units.

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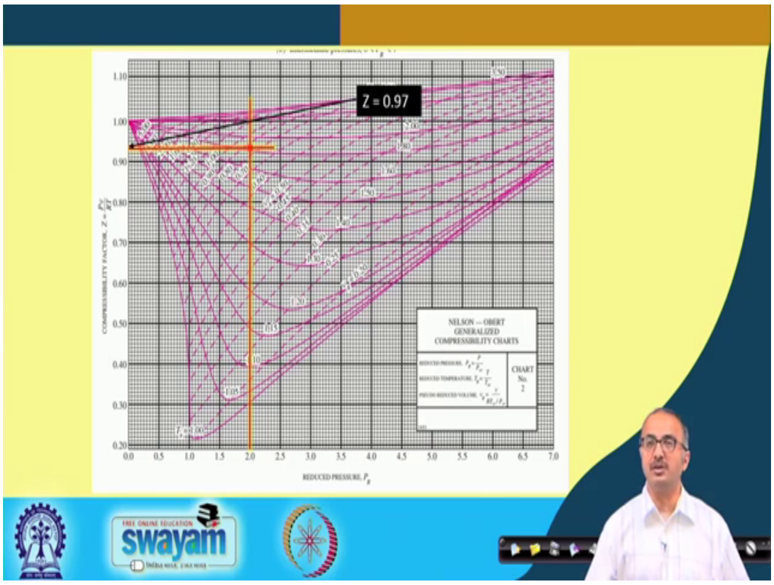

Now, based on this reduced value, we shall be now looking into some thermodynamic chart where it gives the compressibility factor in terms of the reduced pressure for different values of the reduced temperature. So, each of the curves belong to different reduced temperature.

Now, what you do now? What whatever reduced pressure you have found out you locate it on this x axis and from there you go vertically up and locate the reduced temperature on in this side. So, wherever you find you may also find that the reduced temperature may not be lying on any of these curves; it might be somewhere in between. So, you have to have proper knowledge of the interpolation methods so that you can locate the value of the T r in this thing. Once, you can locate T r and you find the intersection point and you make an horizontal and read from this y axis the value of the Z and here, you will see the value of Z is coming out about 0.97. This 0.97 indicates it is very near to the value 1 and 1 is for the ideal gas.

So, it shows that at this particular temperature pressure, there is not a very big difference from the ideality and that is happening because of the temperature not because of pressure; pressure is tending to make it non ideal, but temperature is also quite high with respect to the critical temperature. So, that is why you find that the value of the Z is not too much away from unity. So, the gas is almost like an ideal gas.

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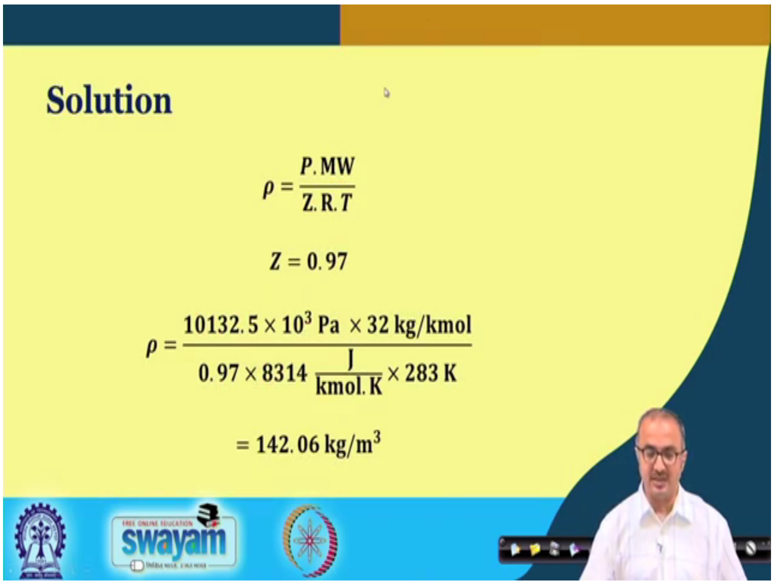

Solution

$$\rho = \frac{P.MW}{Z.R.T}$$

$$Z = 0.97$$

$$\rho = \frac{10132.5 \times 10^3\ \text{Pa} \times 32\ \text{kg/kmol}}{0.97 \times 8314\ \frac{\text{J}}{\text{kmol. K}} \times 283\ \text{K}}$$

$$= 142.06\ \text{kg/m}^3$$

But if you put this now value of the Z in this expression, you get the value of the density. So, you can see that how much will be the difference if you do consider Z or if you do not consider Z.

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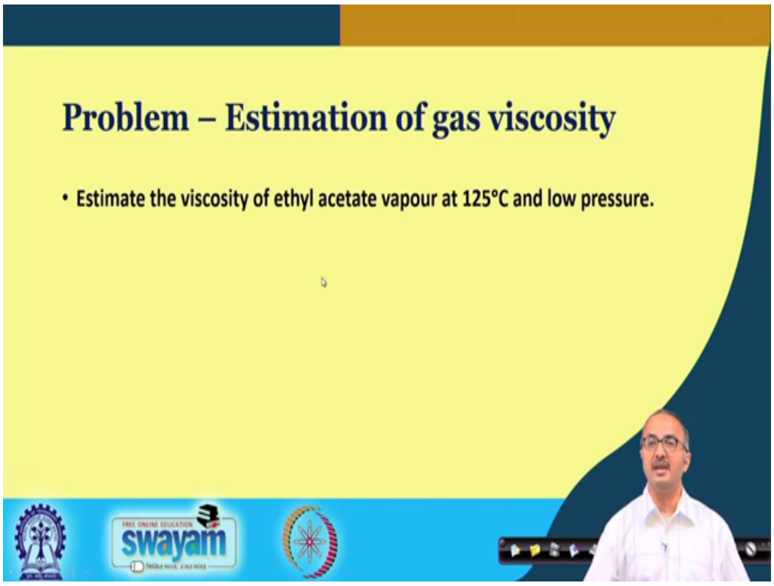

Problem – Estimation of gas viscosity

- Estimate the viscosity of ethyl acetate vapour at 125°C and low pressure.

Next, we come to another problem to estimate the gas viscosity and perhaps you know that gas viscosity and liquid viscosity, they depend on the pressure temperature. The variation in the viscosity with temperature is different in case of gases and liquid. For liquids, the viscosity decreases with increase in the temperature whereas, for the gases the viscosity increases with an increase in the temperature. So, these are some very fundamental knowledge you might be having from your high school science.

Now, we shall now look into the estimation way of the viscosity. Here in this problem, it is given for low pressure and 125 degree centigrade. Now, what is low pressure? Generally, low pressure we take it by thumb rule that it is a pressure between say 1 bar and 5 bar and by medium pressure we take between 5 bar and 10 bar and for high pressure anything beyond that is above 10 bar is taken to be high pressure. So, it is low pressure system. So, we are not really bothered about the pressure exact value of the pressure because you will find that for low pressure or this kind of medium pressure, we have some correlations which may be independent of the pressure. So, that is why the pressure has not been mentioned here.

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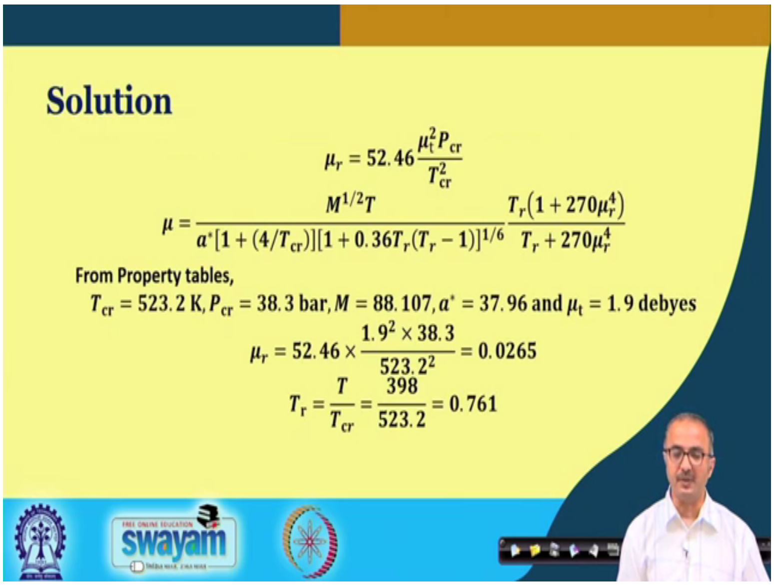

Solution

$$\mu_r = 52.46\frac{\mu_t^2 P_{cr}}{T_{cr}^2}$$

$$\mu = \frac{M^{1/2}T}{a^*[1+(4/T_{cr})][1+0.36T_r(T_r-1)]^{1/6}}\frac{T_r(1+270\mu_r^4)}{T_r+270\mu_r^4}$$

From Property tables,

$T_{cr} = 523.2\text{ K}, P_{cr} = 38.3\text{ bar}, M = 88.107, a^* = 37.96$ and $\mu_t = 1.9$ debyes

$$\mu_r = 52.46 \times \frac{1.9^2 \times 38.3}{523.2^2} = 0.0265$$

$$T_r = \frac{T}{T_{cr}} = \frac{398}{523.2} = 0.761$$

Now, you see this is the case here that we have an expression for the mu which is not having the pressure directory, but it is having temperature in terms of the reduced temperature and in terms of the actual temperature and the critical temperature. But there is no appearance of the pressure. So, that is why it is unimportant for us to know the pressure as long as we are in the low pressure domain and here you find that this particular mu r will be used in this particular expression of mu.

Now, to find this mu r we need the value of mu t and the critical values of pressure temperature and in this particular expression, we need the value of a star ok. Now all these things can be found out from some property tables and here we have the critical temperature, pressure, the molecular weight, the value of the a star and the mu t ok. And here now we find that if you plug in the values, we find this is the mu r value and once we mu r value we take here we find this is the value of the mu, we shall be having and this mu is coming in terms of micro poise.

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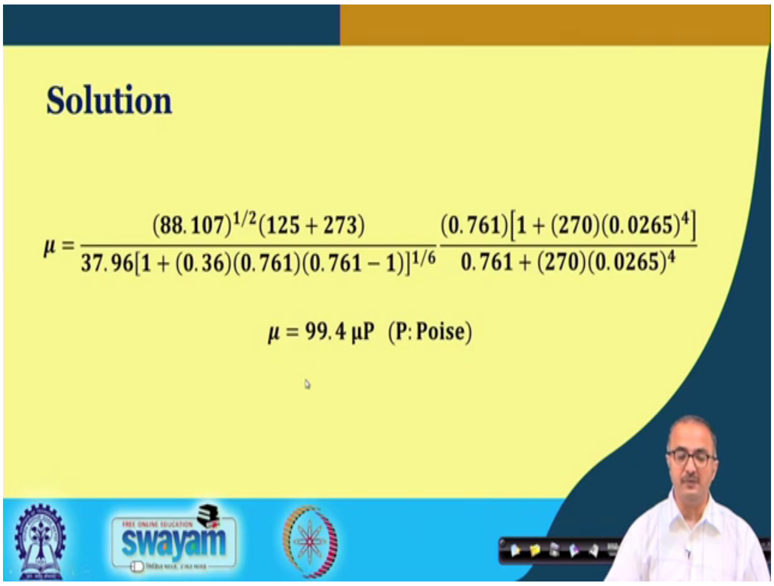

Solution

$$\mu = \frac{(88.107)^{1/2}(125+273)}{37.96[1+(0.36)(0.761)(0.761-1)]^{1/6}} \frac{(0.761)\left[1+(270)(0.0265)^4\right]}{0.761+(270)(0.0265)^4}$$

$$\mu = 99.4\ \mu\text{P} \quad (\text{P: Poise})$$

Now, what is this P stands for? Poise; actually Poise this you poise is used to find as a unit for viscosity in honor of the great scientist Poisely and perhaps you also know that there is something called Poisely flow which we are taught in the fluid mechanics. So, this poise comes from the scientist’s name.

So, here we find that we are having the viscosity of the gas to be this much micro poise. So, micro poise is very very small value and perhaps, you know that one Poises in terms of the mass the time and the length dimension; it is basically gram per centimeter per second. So, this is the Poise.

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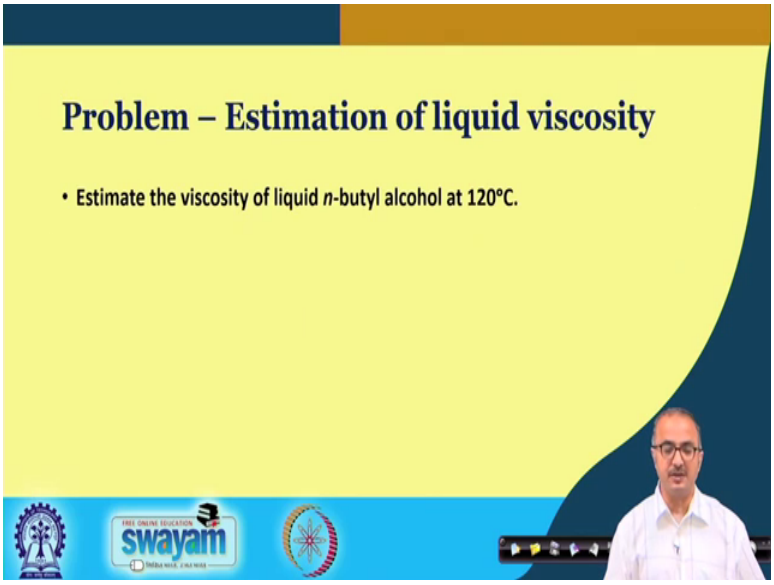

Problem – Estimation of liquid viscosity

- Estimate the viscosity of liquid *n*-butyl alcohol at 120°C.

Now, next we come to another problem on the liquid viscosity and here we have to find out the viscosity of liquid at this particular temperature. In this problem also you see that the pressure does not appear because the viscosity of liquid is not a very strong function of the pressure.

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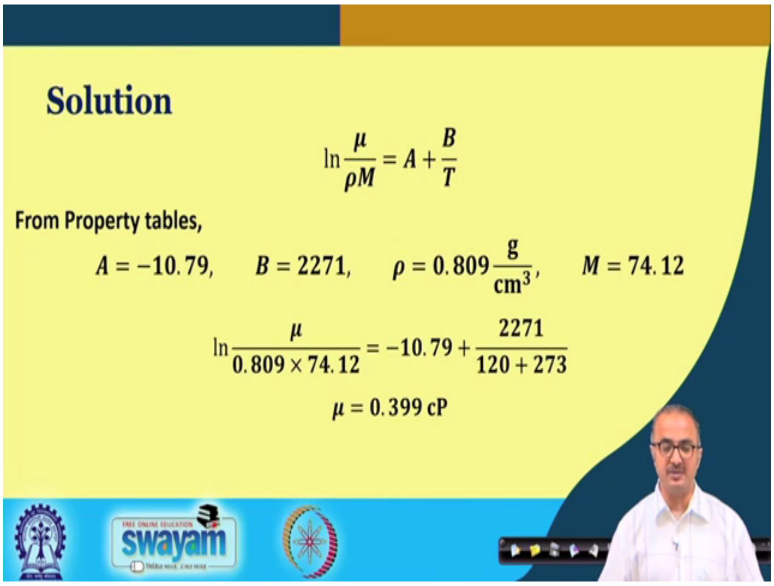

Solution

$$\ln \frac{\mu}{\rho M} = A + \frac{B}{T}$$

From Property tables,

$$A = -10.79, \quad B = 2271, \quad \rho = 0.809 \frac{\text{g}}{\text{cm}^3}, \quad M = 74.12$$

$$\ln \frac{\mu}{0.809 \times 74.12} = -10.79 + \frac{2271}{120 + 273}$$

$$\mu = 0.399 \text{ cP}$$

So, now when we see this particular expression, here you see that here it is coming in terms of density and temperature. So, you see that for liquids density is important which was not so in case of the gases at low pressure ok.

Now, here you see that we have these values of these specific constants from some data source and this is the density and this is the molecular weight. We simply plug in the values of all these in this expression and we get the values of the liquid viscosity, this is in terms of centipoise.

Now, centi and micro; centi means 10 to the power minus 2 and micro means 10 to the power minus 6. So, you can see now if you compare these values of the viscosities for the gas and the liquid; expectedly gases will have much less viscosity than liquid, but also what you find the kind of difference we have, we have about four orders of magnitude difference between the liquid viscosity and the gas viscosity. And that is why you find that many a times sometimes we ignore the viscosity effect in case of gases; that means, we say that viscosity basically give some result some resistance to flow over the surface ok.

So, this is the less the viscosity the less the resistance to flow and that we know from the fluid. The fluid mechanics, it is very important and we know that Reynolds number which gives us the type of the flow laminar flow turbulent flow and there we need viscosity. Now you can now see that because of the great difference in their values of the viscosity; why the Reynolds number becomes so different and ultimately, the nature of the flow also changes because of this change in the viscosity.

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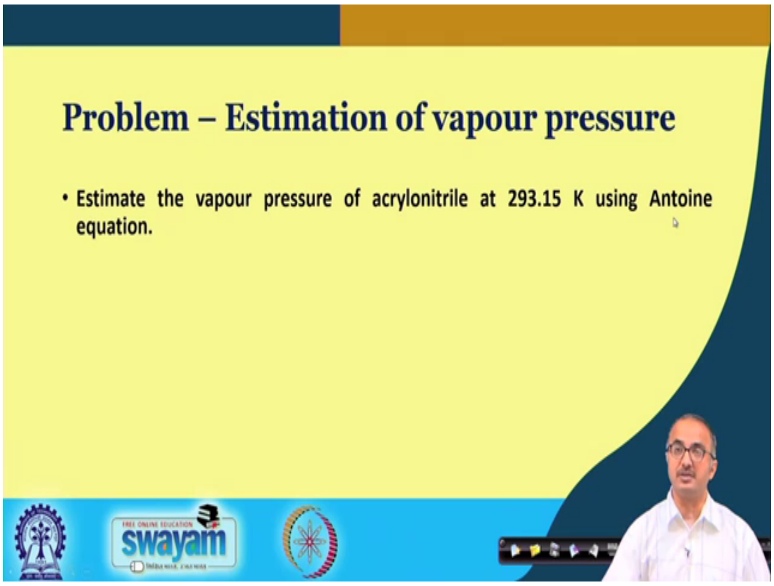

Problem – Estimation of vapour pressure

- Estimate the vapour pressure of acrylonitrile at 293.15 K using Antoine equation.

Now, next problem is on the estimation of vapor pressure of a liquid ok, liquid has paper pressure and this vapor pressure is a function of temperature. So, if you are given a temperature, you should be able to find out the vapor pressure and here in this x problem we are given that we have to use Antoine equation to find out the vapor pressure of acrylonitrile.

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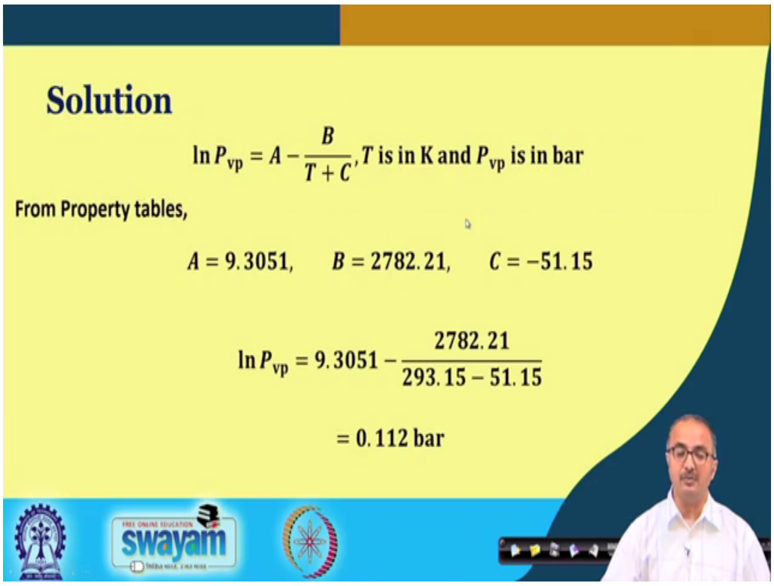

Solution

$$\ln P_{vp} = A - \frac{B}{T+C},\ T \text{ is in K and } P_{vp} \text{ is in bar}$$

From Property tables,

$$A = 9.3051, \quad B = 2782.21, \quad C = -51.15$$

$$\ln P_{vp} = 9.3051 - \frac{2782.21}{293.15 - 51.15}$$

$$= 0.112 \text{ bar}$$

Now, here is the Antoine equation and here you see this is the vapor pressure and these are the values of A B C and in this thing, the temperature is in Kelvin and the vapor pressure is in bar. So, you have to be careful whenever you are using any of the correlations about the units. So, if you are using this unit with the kind of values of this A B C because the values of A B C will change with the different unit systems ok. So, here with this we take from some data source, these values of this A B C.

Now, we just plug in the values over here with the temperature here and we find this is the logarithmic of the vapor pressure and to find out the vapor pressure, we have to take the exponential and we arrive at this particular value that is 0.112 bar. Now 0.112 bar, what does it signify to us? It signifies that you know that atmospheric pressure is one bar and this is 0.112 bar, it is much less than the atmospheric; that means, it is not a very highly volatile liquid. The more the vapor pressure, it will go means that it is the more volatile liquid.

So, that is what we get indicate from these values of the vapor pressure and you can also check that if you find the vapor pressure of different types of liquid at same temperature and you if you just compare them the you can see that whichever liquid has more volatility, will have more vapor pressure value ok. So, this homework you can also try out.

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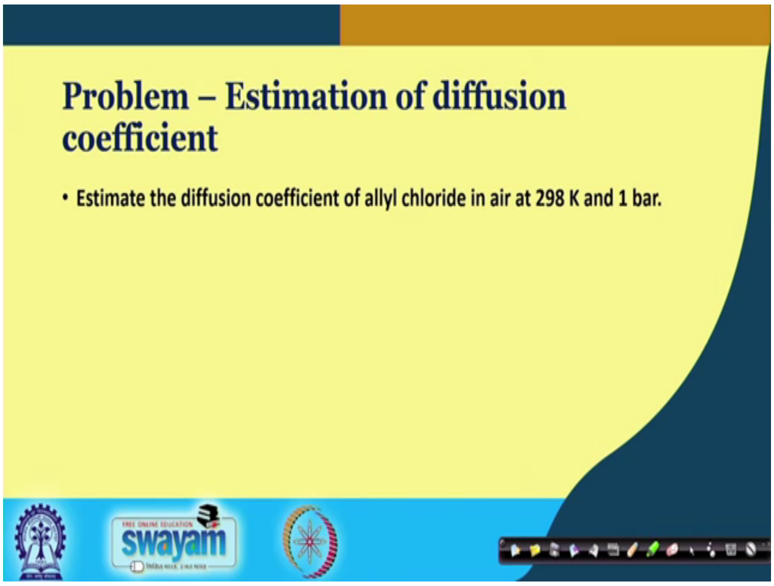

Problem – Estimation of diffusion coefficient

- Estimate the diffusion coefficient of allyl chloride in air at 298 K and 1 bar.

Next we come to another important parameter that is the diffusion coefficient and this is used in estimating the rate of mass transfer; for example, you are having some sugar which you want to dissolve in say milk or water. Now in this case what we will find? If you do not disturb the system, you simply put the sugar in the water or the milk you will find that it will take some time to get dissolved and this rate of the solution will be dictated by this diffusion coefficient ok.

So, this kind of system is also there for any other systems like liquid liquid system or liquid vapor system. So, whenever you are not disturbing the system you are keeping the system undisturbed. So, the mass transfer or the distribution of a component in another component will be occurring purely due to diffusion and whenever its diffusion you need diffusion coefficient or diffusivity and this diffusivity is a function of both temperature and pressure. So, it is important for us to mention the temperature and the pressure. So, this is for allyl chloride in air. So, you have to know which are the two components we are talking about, it is because diffusion cannot happen alone it has to be between at which a pair of components. So, these are the two components for which you have to find out the diffusion coefficient.

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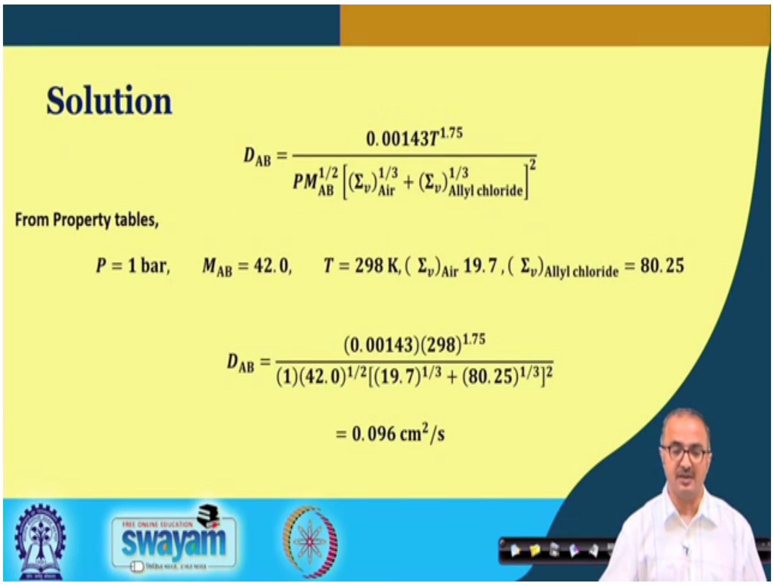

Solution

$$D_{AB} = \frac{0.00143T^{1.75}}{PM_{AB}^{1/2}\left[(\Sigma_v)_{Air}^{1/3} + (\Sigma_v)_{Allyl\ chloride}^{1/3}\right]^2}$$

From Property tables,

$P = 1$ bar, $M_{AB} = 42.0$, $T = 298$ K, $(\Sigma_v)_{Air}$ 19.7, $(\Sigma_v)_{Allyl\ chloride} = 80.25$

$$D_{AB} = \frac{(0.00143)(298)^{1.75}}{(1)(42.0)^{1/2}[(19.7)^{1/3} + (80.25)^{1/3}]^2}$$

$$= 0.096\ \text{cm}^2/\text{s}$$

So, here is one particular expression to estimate the diffusivity this A and B represent two components and here you see that how it is varies with temperature. It varies temperature to the power 1.75. That means, it is not a linear it is more than linear and with pressure, it is inversely proportional to the pressure; whereas, with the molecular weight this also a functional molecular weight because the heavier the molecule the more effort it will take to diffuse. So, low will be its diffusivity coefficient ok.

So, you see that it is inversely proportional to the square root of the molecular weight and these two expressions these things are representing the molecular volume and you can see that it is also inversely proportional to two-third of the molecular volume molecular volume raised to two-third. So, all these values this value of this these two things will be found in some data source and this value of the M AB can be found out by taking the sum average and this average is 1 by M A by 1 by M AB equal to 1 by 1 by M A plus 1 by M B ok. So, that is how you find the value of the M AB.

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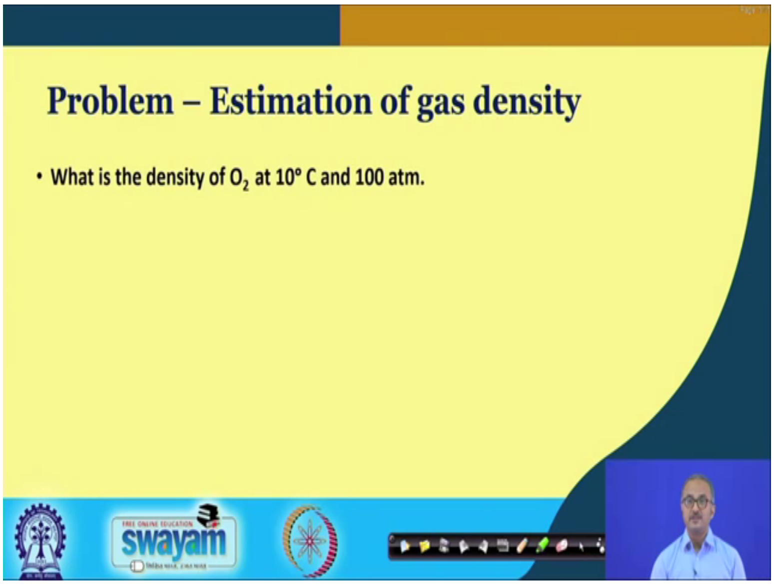

Problem – Estimation of gas density

- What is the density of O_2 at 10° C and 100 atm.

Next we shall take another problem here we are going to estimate the density of oxygen again, but now at some different temperature pressure. Now you see the temperature has been reduced to 10 degree centigrade, but which is still above the critical temperature of oxygen and this is the pressure and this pressure is much above the critical pressure of oxygen. So, we expect a bit of non ideality and let us see that how this non ideality can be taken into account.

Now, I have taught you in the theoretical class that there are many ways of accounting for the non ideality; we can use the various types of equation of state like Van der Waal system state or virial equation of state.

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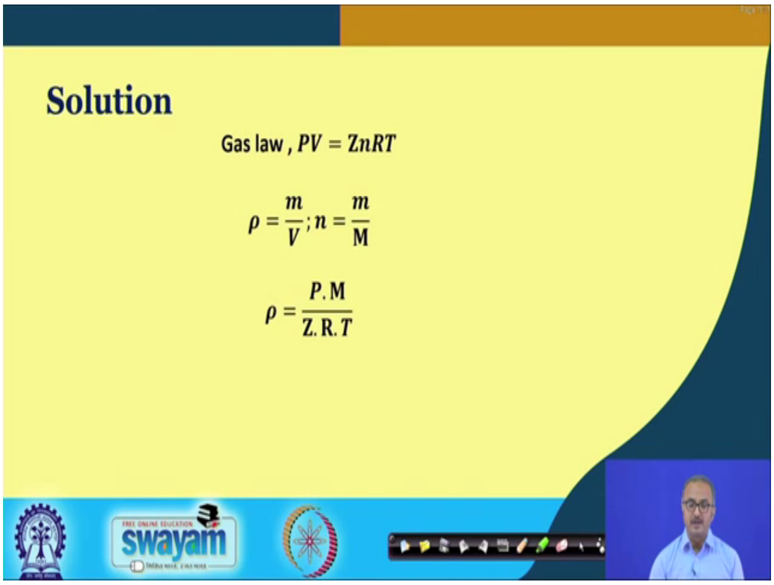

Solution

Gas law , $PV = ZnRT$

$$\rho = \frac{m}{V}; n = \frac{m}{\mathrm{M}}$$

$$\rho = \frac{P.\mathrm{M}}{Z.\mathrm{R}.T}$$

Another approach is to find out the compressibility factor Z. So, in this particular problem we shall be adopting this particular approach of Z. And we have to find out the value of Z from some thermodynamic chart.

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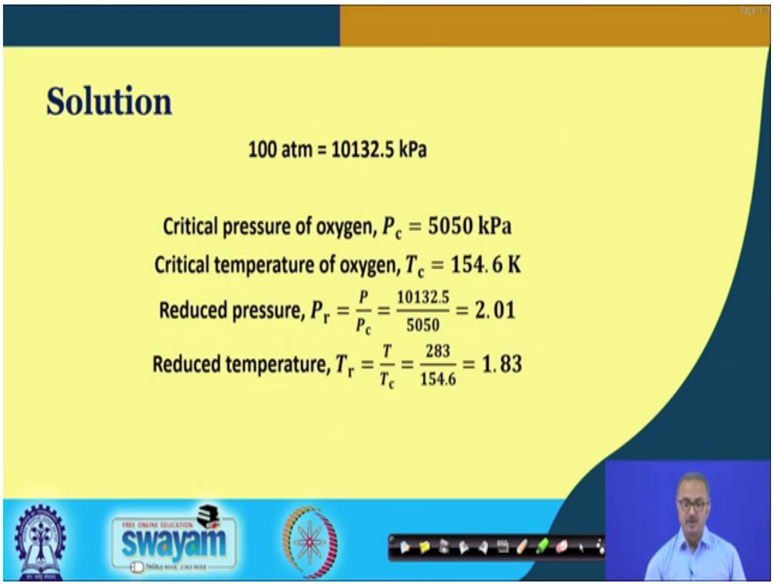

Solution

100 atm = 10132.5 kPa

Critical pressure of oxygen, $P_c = 5050$ kPa

Critical temperature of oxygen, $T_c = 154.6$ K

Reduced pressure, $P_r = \frac{P}{P_c} = \frac{10132.5}{5050} = 2.01$

Reduced temperature, $T_r = \frac{T}{T_c} = \frac{283}{154.6} = 1.83$

To find out the value of Z, what we need? We need the value of the reduced pressure and reduced temperature and to find out this reduced pressure reduced temperature, we need the critical pressure and critical temperature. So, here you see that we calculate the reduced pressure and the reduced temperature by taking the ratio of the actual pressure and the critical pressure actual temperature and the critical temperature and these are the two values we arrive at.

Now, with the help of this compressibility chart, what we try to do is this that on in this chart on the y axis the value of Z is given on the x axis the reduced pressure is plotted and on these various curves correspond to various reduced temperatures. Though, we first locate the reduced pressure on the x axis and then move vertically up and then we try to locate the reduced temperature to reduce to locate this reduced temperature point, please understand that you may have to interpolate between two curves.

So, you need to know the interpolation formula. Once you can interpolate it then you can find out the intersection of the T r and P r and from this point of intersection, we have to simply go horizontally to the left hand side to locate the value of the Z which is coming out to 0.97. Now this 0.97 is very near to the value of unity and that is what that; that means, that these gas is behaving almost like an ideal gas.

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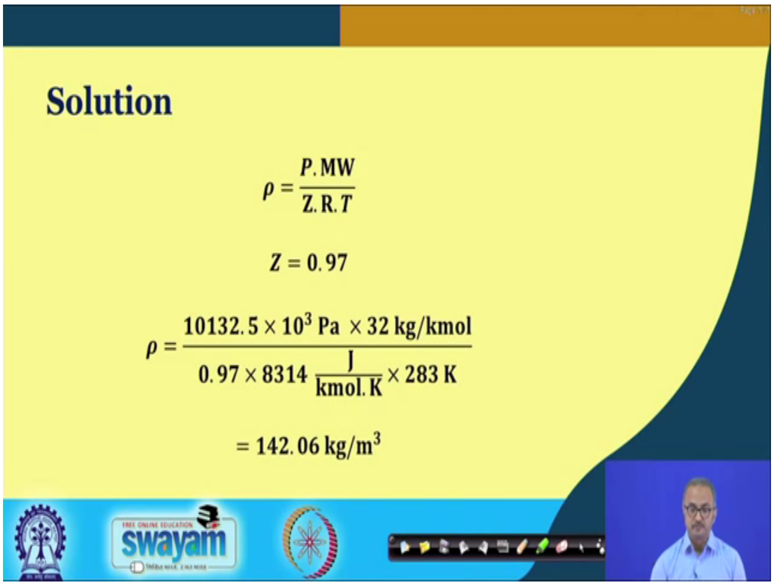

Solution

$$\rho = \frac{P.MW}{Z.R.T}$$

$$Z = 0.97$$

$$\rho = \frac{10132.5 \times 10^3\ \text{Pa} \times 32\ \text{kg/kmol}}{0.97 \times 8314\ \frac{\text{J}}{\text{kmol.K}} \times 283\ \text{K}}$$

$$= 142.06\ \text{kg/m}^3$$

Now, after knowing the value of Z, we plug in the values over in this particular formula and we find out this is M. So, we plug in the values and we find this is the density of the oxygen gas at the given temperature and pressure ok. So, it is quite a straight forward and what we have learned that how to look into the thermodynamic chart to find out the compressibility factor.

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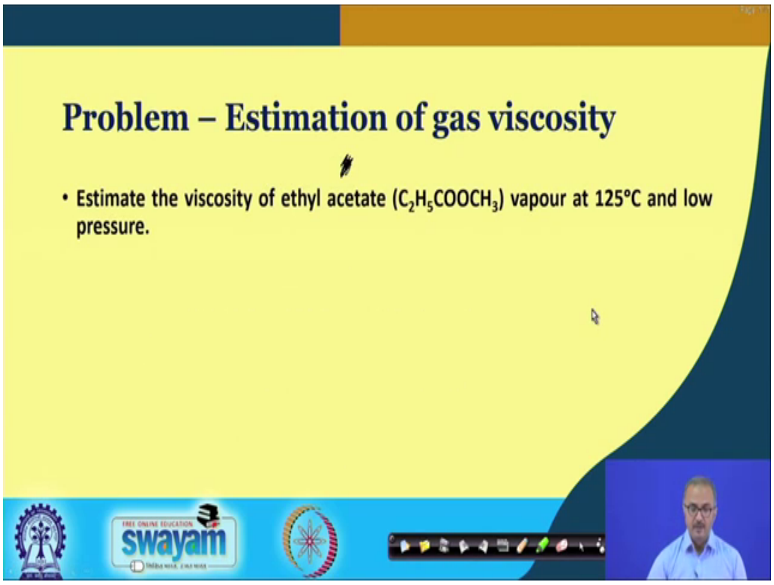

Problem – Estimation of gas viscosity

- Estimate the viscosity of ethyl acetate ($C_2H_5COOCH_3$) vapour at 125°C and low pressure.

Next, we come to a problem to estimate the viscosity. Now, in this case we are going for the gas viscosity and the gas is ethyl acetate and perhaps you know the formula is C 2 H 5 COOCH 3 and this is in vapor state and the temperature is at 125 degree centigrade and the pressure has not been mentioned it is a low pressure. And you see that the viscosity correlations are given for various types of pressure ranges and what we understand by low is this; if the pressure is between 1 atmosphere and 5 atmosphere, we take it to be low pressure region. If the pressure is between 5 atmosphere and about 10 atmosphere we take it to be moderate pressure and then more than 10 atmosphere is taken to be high pressure.

So, here and accordingly where we are in these three pressure zones the correlations may differ. So, in this particular case we have been asked to find out the viscosity at low pressure zone and you will find that the value of the pressure is not necessary to compute the viscosity that is why the pressure value has not been mentioned in this particular problem.

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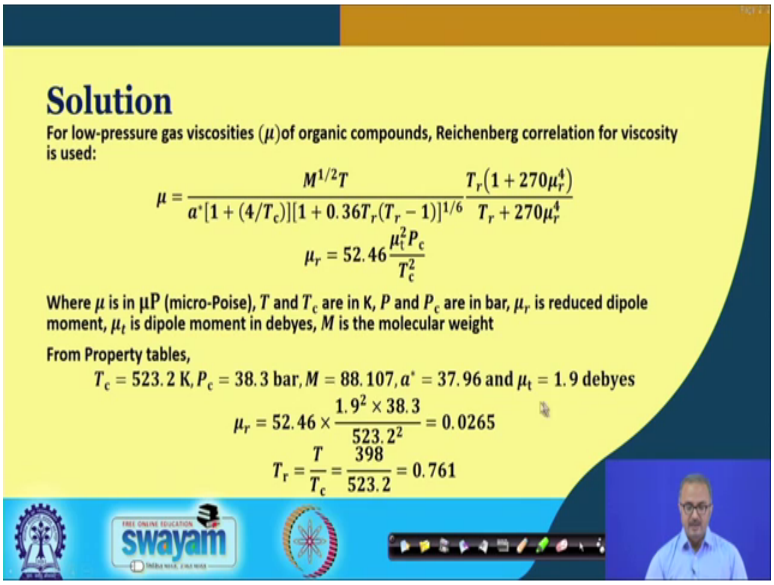

Solution

For low-pressure gas viscosities (μ) of organic compounds, Reichenberg correlation for viscosity is used:

$$\mu = \frac{M^{1/2}T}{a^{*}[1+(4/T_c)][1+0.36T_r(T_r-1)]^{1/6}}\frac{T_r(1+270\mu_r^4)}{T_r+270\mu_r^4}$$

$$\mu_r = 52.46\frac{\mu_t^2 P_c}{T_c^2}$$

Where μ is in μP (micro-Poise), T and T_c are in K, P and P_c are in bar, μ_r is reduced dipole moment, μ_t is dipole moment in debyes, M is the molecular weight

From Property tables,

$$T_c = 523.2 \text{ K}, P_c = 38.3 \text{ bar}, M = 88.107, a^{*} = 37.96 \text{ and } \mu_t = 1.9 \text{ debyes}$$

$$\mu_r = 52.46 \times \frac{1.9^2 \times 38.3}{523.2^2} = 0.0265$$

$$T_r = \frac{T}{T_c} = \frac{398}{523.2} = 0.761$$

Now, going to the solution first we see that we have to a fine from the appropriate source data and I have given you the names of the books from which we have collected these correlations to find that this is one correlation for the viscosity and this correlation was proposed by Reichenberg.

So, we are using this correlation to find out the viscosity of the gas and here you see that in this correlation, we need the value of the critical temperature the reduced temperature has to be calculated based on the critical temperature and the actual temperature and then, we have two parameters mu r and mu t mu r is the reduced dipole moment and mu t is the dipole moment in debyes. And M is the molecular weight which is coming here and the correlation says that the viscosity we obtain will be in micro poise ok. So, you have to and here the temperatures have to be in Kelvin and pressures if is there it is there it is the pressure is in bar.

Now, we look into the property tables from those sources and we get all these values for the particular component and now it is now a simple job once you find these values you simply plug in the values in these particular equations and you will get the values of the mu r and the value of the T r please note mu r and T r do not have any units.

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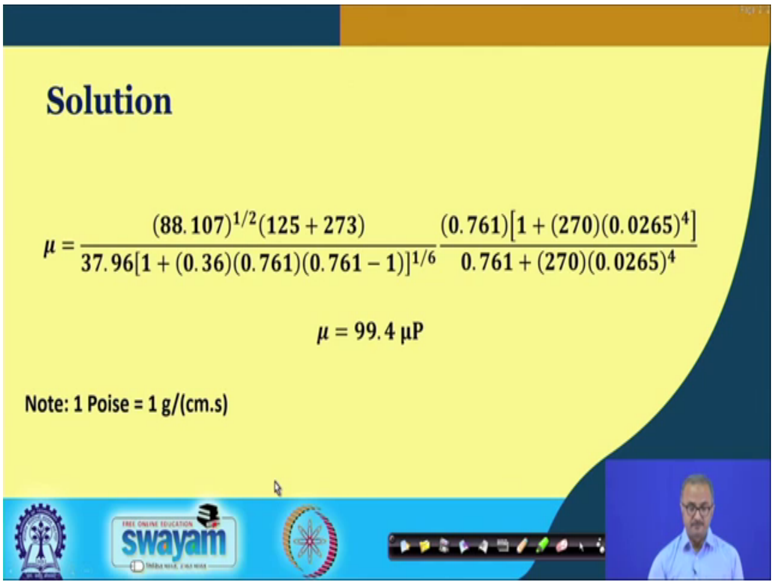

Solution

$$\mu = \frac{(88.107)^{1/2}(125+273)}{37.96[1+(0.36)(0.761)(0.761-1)]^{1/6}} \frac{(0.761)\left[1+(270)(0.0265)^4\right]}{0.761+(270)(0.0265)^4}$$

$$\mu = 99.4\ \mu\text{P}$$

Note: 1 Poise = 1 g/(cm.s)

Now, what you do you simply put these values of mu r and T r in this correlation of viscosity and you obtain the viscosity value like 99.4 micro poise. Now please see this one poise is one gram per centimeter per second and the poise is an abbreviation of Poisely the famous scientist ah. So, this is how we are able to find out the viscosity of a fluid.

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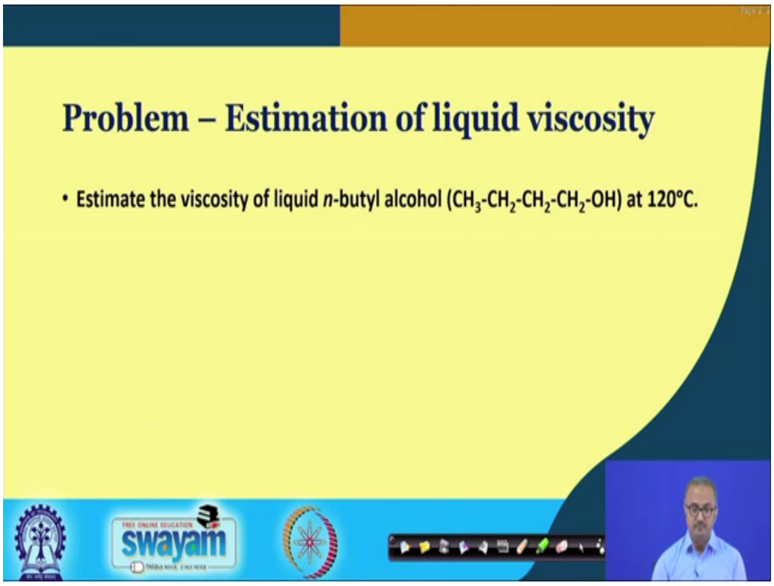

Problem – Estimation of liquid viscosity

- Estimate the viscosity of liquid *n*-butyl alcohol (CH_3-CH_2-CH_2-CH_2-OH) at 120°C.

Now, we come to another problem in this case it is a liquid viscosity and here which is the liquid is n butyl alcohol and this ensures the slit straight chain. So, the straight chain alcohol, this is the formula and the viscosity has to be found out at 120 degree centigrade.

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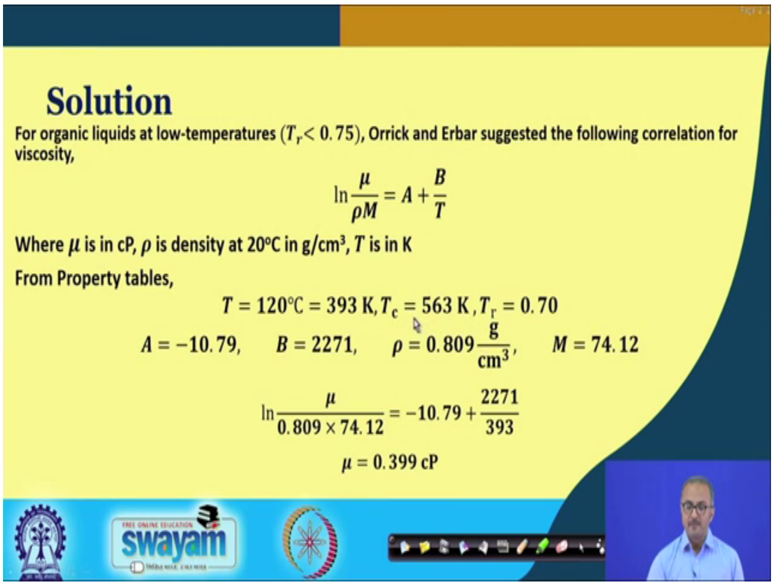

Solution

For organic liquids at low-temperatures ($T_r < 0.75$), Orrick and Erbar suggested the following correlation for viscosity,

$$\ln\frac{\mu}{\rho M} = A + \frac{B}{T}$$

Where μ is in cP, ρ is density at 20°C in g/cm³, T is in K

From Property tables,

$$T = 120^\circ\text{C} = 393\ \text{K}, T_c = 563\ \text{K}, T_r = 0.70$$

$$A = -10.79, \quad B = 2271, \quad \rho = 0.809\frac{\text{g}}{\text{cm}^3}, \quad M = 74.12$$

$$\ln\frac{\mu}{0.809 \times 74.12} = -10.79 + \frac{2271}{393}$$

$$\mu = 0.399\ \text{cP}$$

Now here you see that at low temperatures for organic liquids, this particular formula or the correlation has been proposed by Orrick and Erbar. Now you see that these conditions have to be very clearly noted because unless you are noting the particular conditions under which a particular correlations valid, you again will land up with wrong results. So, when whenever you are using any correlation please make sure the validity of the particular correlation in terms of temperature, pressure and other parameters.

So, here the viscosity will be obtained in centipoise and the rho is the density of the particular liquid at 20 degree centigrade in gram per centimeter cube and the temperature is in Kelvin. So, with this now we again get these values of the various parameters from the source book and we find that as per this T c and the given temperature that is 120 degree centigrade we are getting the value of T r like this.

Now, please note that whenever you are finding the value of the reduced temperature, always convert the centigrade into Kelvin otherwise you are again going to land up with wrong result. So, you convert it to the Kelvin 393 K and then divide by the critical temperature. Once you obtain the T r value you get the values of A B from again the source book and the rho is also given there and this is a molecular weight and plug in the values in this particular correlation A B rho m mu and now you are able to get the value of mu in centipoises.

So, you can see that at least that this is coming in centipoise and for the vapor, it was coming in micro poise ah, even though the two compounds are different, but the order of magnitude of the viscosities almost remain similar in case of vapor and in case of liquid. And we find that the viscosity of liquid is much higher about 3 order of magnitude higher than the viscosity of the gas. So, what it means? It means that whenever there is a flow the liquid will experience more resistance due to drag on the particular surface than a gas and this drag force decides the type of the flow we have like; whether it will be laminar or whether it will be turbulent that will depend on this viscosity value.

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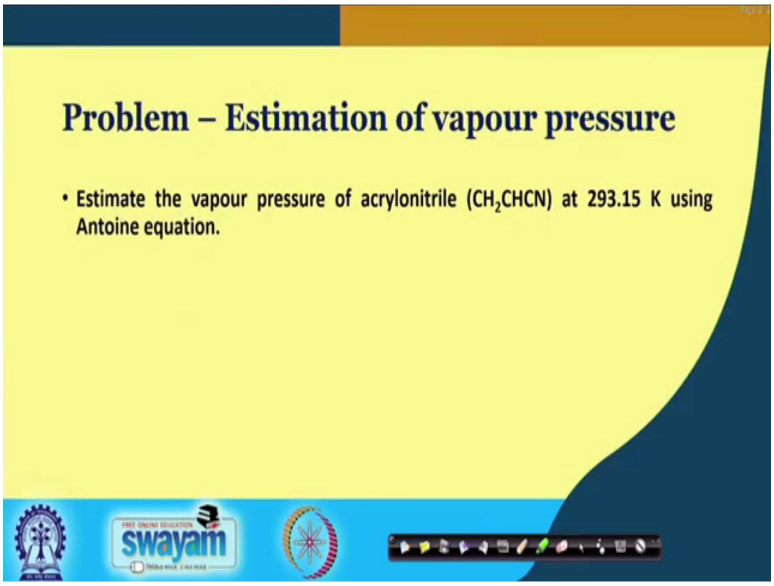

Problem – Estimation of vapour pressure

- Estimate the vapour pressure of acrylonitrile (CH_2CHCN) at 293.15 K using Antoine equation.

Next we come to another important parameter that is the vapor pressure of a liquid and you know that vapor pressure decides that how easy or difficult for will it be for a liquid to vaporize. So, here we have a liquid that is acrylonitrile with this is the formula and for which we have to find out the vapor pressure at this particular temperature and you know that vapor pressure is a function of temperature.

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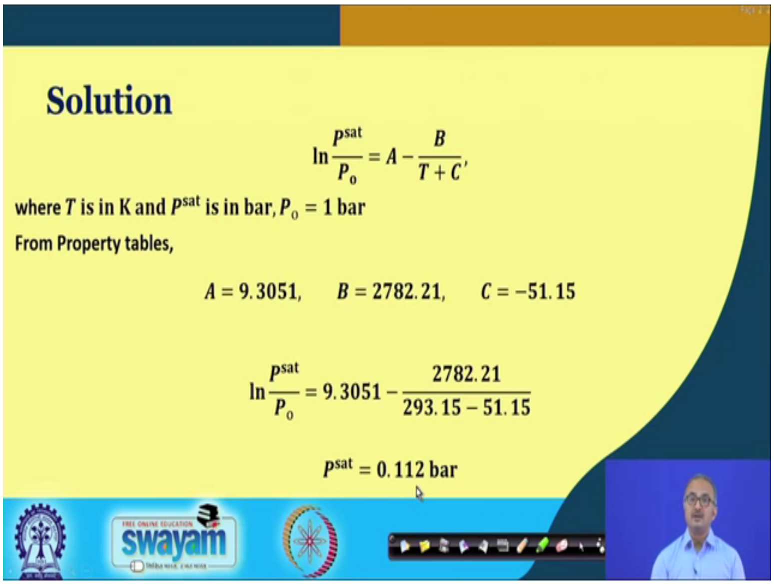

Solution

$$\ln\frac{P^{sat}}{P_0} = A - \frac{B}{T+C},$$

where T is in K and P^{sat} is in bar, $P_0 = 1$ bar

From Property tables,

$$A = 9.3051, \quad B = 2782.21, \quad C = -51.15$$

$$\ln\frac{P^{sat}}{P_0} = 9.3051 - \frac{2782.21}{293.15 - 51.15}$$

$$P^{sat} = 0.112 \text{ bar}$$

So, we have been asked to use the Antoine equation and in the lecture we saw the form of the Antoine equation. So, these are form of Antoine equation and here what we have to do is this, we have to find out the value of this A B C corresponding to the given liquid from the literature.

Now, here it has been mentioned the T should be in Kelvin and P sat will be in bar and this P 0 is some reference pressure and that is 1 bar. So, from the property tables you obtain these A B C values and the plug in the values in this particular formula and you get the p sat value as this. That means, you see that the vapor pressure is much much lower than the atmospheric pressure that is 1 bar. What it signifies? It tells us that it because it has such a low vapor pressure. So, this particular liquid will have very low tendency to go to the vapor phase and especially under the atmospheric condition even at that temperature you find that it is not going to evaporate much or it will be evaporating very very slowly.

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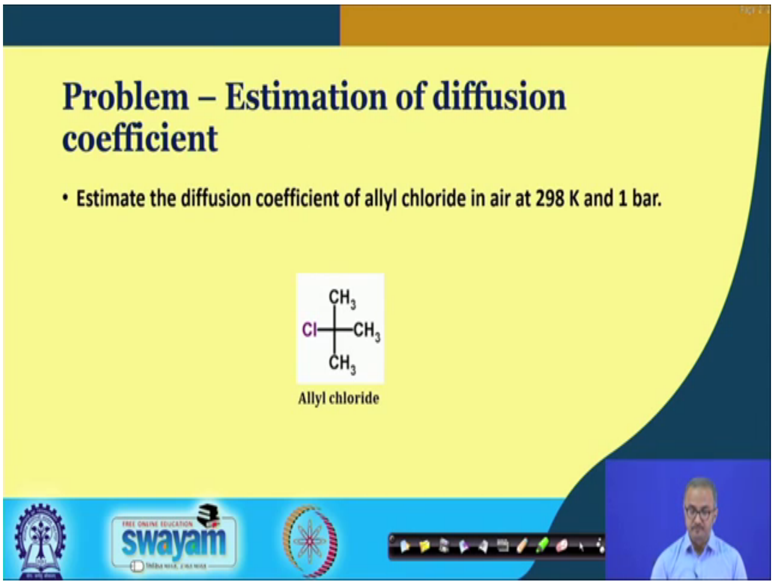

Problem – Estimation of diffusion coefficient

- Estimate the diffusion coefficient of allyl chloride in air at 298 K and 1 bar.

Allyl chloride

Next we come to another important problem that is the diffusion coefficient and you know diffusion coefficient tells us that how a particular molecule will be able to distribute itself in another type of molecule. So, here we are asked to find out the diffusion coefficient of allyl chloride in air, at this particular temperature and pressure and this is the formula of allyl chloride. Here you see there are 3 methyl group and 1 chlorine group.

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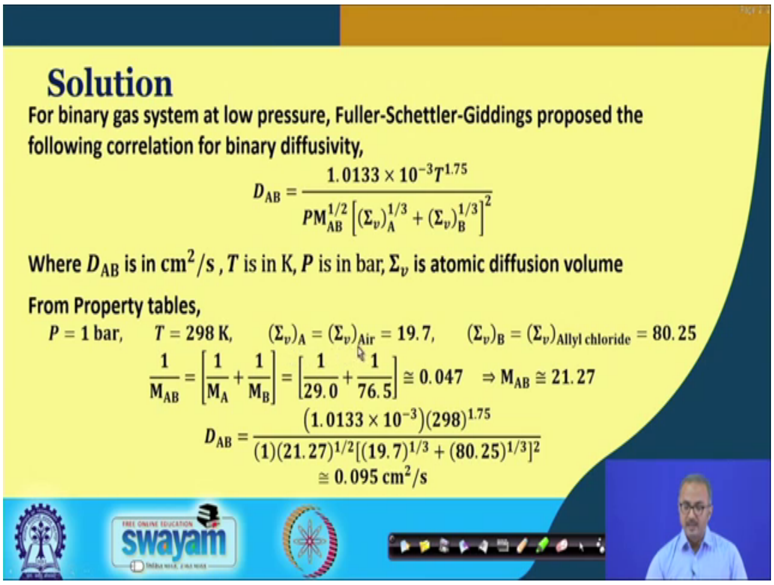

Solution

For binary gas system at low pressure, Fuller-Schettler-Giddings proposed the following correlation for binary diffusivity,

$$D_{AB} = \frac{1.0133 \times 10^{-3} T^{1.75}}{P M_{AB}^{1/2} \left[(\Sigma_v)_A^{1/3} + (\Sigma_v)_B^{1/3} \right]^2}$$

Where D_{AB} is in cm^2/s, T is in K, P is in bar, Σ_v is atomic diffusion volume

From Property tables,

$$P = 1 \text{ bar}, \quad T = 298 \text{ K}, \quad (\Sigma_v)_A = (\Sigma_v)_{Air} = 19.7, \quad (\Sigma_v)_B = (\Sigma_v)_{\text{Allyl chloride}} = 80.25$$

$$\frac{1}{M_{AB}} = \left[\frac{1}{M_A} + \frac{1}{M_B} \right] = \left[\frac{1}{29.0} + \frac{1}{76.5} \right] \cong 0.047 \quad \Rightarrow M_{AB} \cong 21.27$$

$$D_{AB} = \frac{(1.0133 \times 10^{-3})(298)^{1.75}}{(1)(21.27)^{1/2}[(19.7)^{1/3} + (80.25)^{1/3}]^2}$$

$$\cong 0.095 \; cm^2/s$$

Now, for the low pressure zone, these Fuller-Schettler Giddings proposed this particular correlation for binary diffusivity means for two component system, this is the diffusivity and here you can see that the time it is this diffusivity this D AB is varying with the temperature raised to 1.75. That is not linearly more than linear and with pressure as inverse of pressure and square root of some average molecular weight here in this case A and B represent the two different species and in this correlation D AB will be in centimeter square per second, T will be in Kelvin, P will be in bar and this sigma V is the atomic diffusion volume.

So, now again from the property table, what we do that we can get this value of this sigma V for air and for allyl chloride and we find the value of the M AB by from this particular formula. And then, the job is now simple, that you simply put the values in this particular correlation and compute the diffusivity and this is coming out to be 0.095 centimeter square per second.

Now, this is for this allyl chloride to into air. Now you see this diffusivity value will again will be differing for different types of systems, now gases will be have the highest diffusivity then liquid and least will be the solid. So, depending on the type of the species and its phase the diffusivity value will keep changing.

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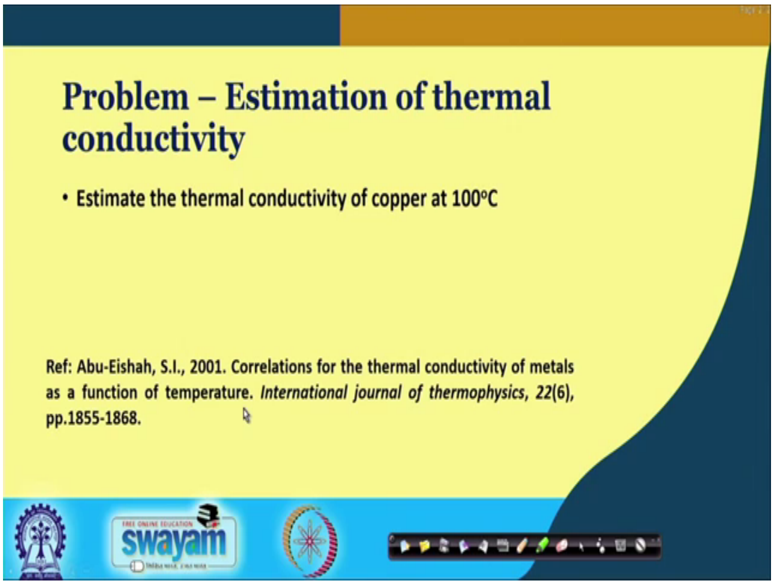

Problem – Estimation of thermal conductivity

- Estimate the thermal conductivity of copper at 100°C

Ref: Abu-Eishah, S.I., 2001. Correlations for the thermal conductivity of metals as a function of temperature. *International journal of thermophysics*, 22(6), pp.1855-1868.

Next we come to another important property that is thermal conductivity in this we have to find out the thermal conductivity of copper at 100 degree centigrade. Now please understand that thermal conductivity is again dependent on the pressure and temperature not much so much on pressure for the solids, but temperature yes it is and so, we need to know the particular correlation to find out the thermal conductivity.

Now, what happens is this correlations are again based on some kind of experimental data. So, first which has we shall see that how this correlation is giving the value and here is one reference we have taken to obtain the correlation for thermal conductivity.

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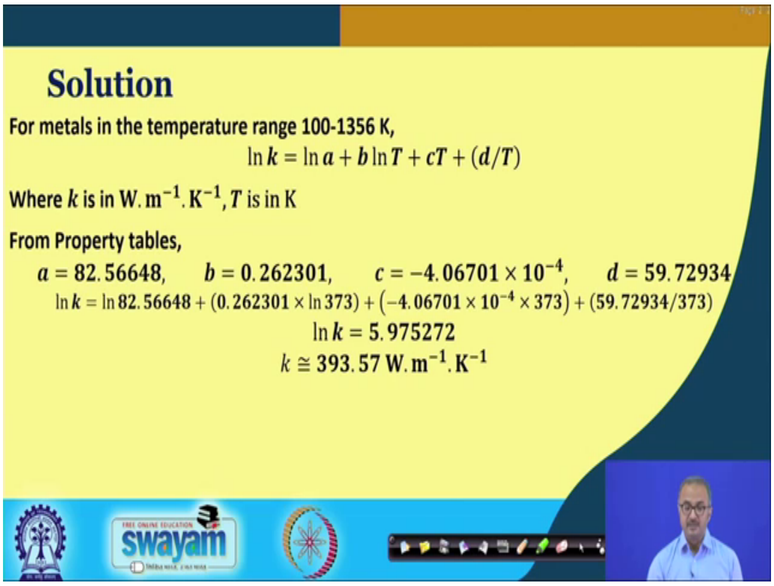

Solution

For metals in the temperature range 100-1356 K,

$$\ln k = \ln a + b \ln T + cT + (d/T)$$

Where k is in $\mathrm{W.m^{-1}.K^{-1}}$, T is in K

From Property tables,

$$a = 82.56648, \quad b = 0.262301, \quad c = -4.06701 \times 10^{-4}, \quad d = 59.72934$$

$$\ln k = \ln 82.56648 + (0.262301 \times \ln 373) + \left(-4.06701 \times 10^{-4} \times 373\right) + (59.72934/373)$$

$$\ln k = 5.975272$$

$$k \cong 393.57\ \mathrm{W.m^{-1}.K^{-1}}$$

So, this is the correlation for thermal conductivity and this you can see that it is not particularly polynomial, but it has some logarithmic term in this and in this is the conductivity will be in watt per meter per Kelvin and the T has to be in Kelvin.

Now, what we do? Again, from that particular reference given to you can find the value of this a b c d and then, you plug in the values of a b c d here and temperature you get the value of the conductivity like this 393 about 394 watt per meter per Kelvin.

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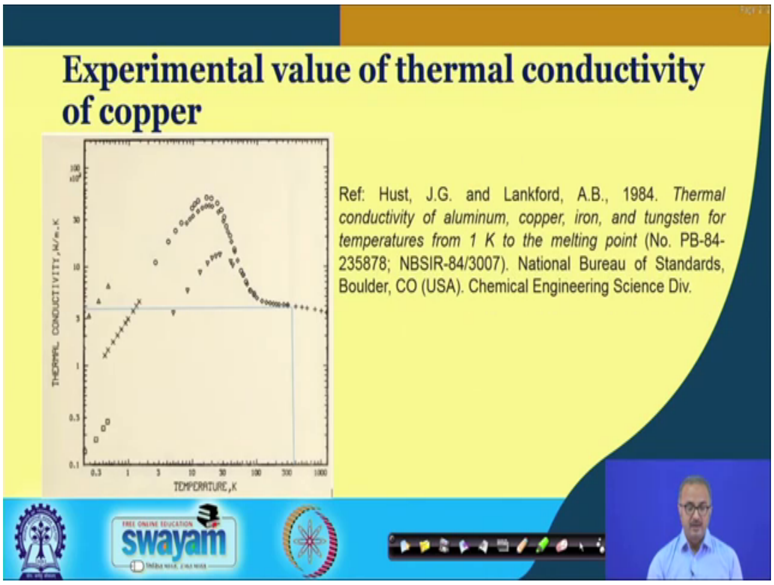

Experimental value of thermal conductivity of copper

Ref: Hust, J.G. and Lankford, A.B., 1984. *Thermal conductivity of aluminum, copper, iron, and tungsten for temperatures from 1 K to the melting point* (No. PB-84-235878; NBSIR-84/3007). National Bureau of Standards, Boulder, CO (USA). Chemical Engineering Science Div.

Now, to check that whether this value is right or not or how good is this estimation what we can do is this, we can look into the actual experimental data of this thermal conductivity and here we have this particular chart given in this particular source. So, from this chart you can again figure out the thermal conductivity of copper as a function of temperature and I have shown you here the how to locate the thermal conductivity for the given conditions in this problem. And here you can read out the values of thermal conductivity by locating the temperature and you can see that this value is coming nearly same of the value we have computed from the given correlation.

So, in this lecture we have seen that how to estimate the various types of properties of vapor liquid and solid which come under the constitutive relationships. More such properties are there as and when we encounter them we shall see how to estimate those properties.

Thank you.