

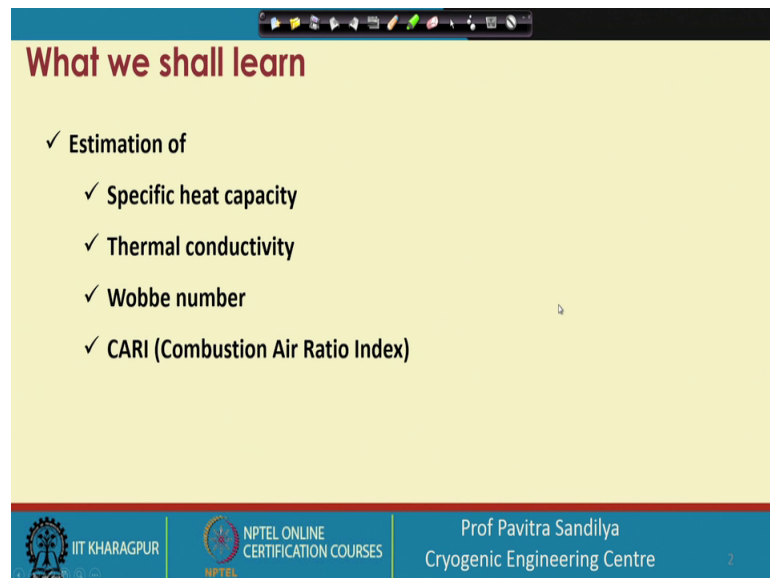
Upstream LNG Technology
Prof. Pavitra Sandilya
Department of Cryogenic Engineering Centre
Indian Institute of Technology, Kharagpur

Lecture – 20

Tutorial on the combustion and thermodynamic properties of natural gas

Welcome, after learning about the various estimation method for the thermo dynamic properties and the combustion properties, in this particular tutorial in this lecture we shall see some, Tutorial to use those methods to find out these properties. So, this particular lecture is on the estimation of the thermodynamic and combustion properties.

(Refer Slide Time: 00:41)



What we shall learn

- ✓ Estimation of
 - ✓ Specific heat capacity
 - ✓ Thermal conductivity
 - ✓ Wobbe number
 - ✓ CARI (Combustion Air Ratio Index)

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So, what we shall learn in this lecture are to estimate the specific heat capacity thermal conductivity Wobbe number and CARI that is the Combustion Air Ratio Index by with some specific example on a natural gas.

(Refer Slide Time: 01:01)

Problem statement

✓ A natural gas with the following composition is at 6000 psia and 150 °F.

Evaluate the

- Thermal Conductivity
- Specific heat
- Wobbe index and
- CARI

of the natural gas

Given: High heating value of the gas: 1050 Btu/ft³, and A/F ratio for complete combustion: 12.56.

[A/F : Air to fuel]

| Component | y _i |
|---|----------------|
| N ₂ | 0.0345 |
| CO ₂ | 0.0130 |
| H ₂ S | 0.0000 |
| CH ₄ | 0.8470 |
| C ₂ H ₆ | 0.0586 |
| C ₃ H ₈ | 0.0220 |
| <i>i</i> -C ₄ H ₁₀ | 0.0035 |
| <i>n</i> -C ₄ H ₁₀ | 0.0058 |
| <i>i</i> -C ₅ H ₁₂ | 0.0027 |
| <i>n</i> -C ₅ H ₁₂ | 0.0025 |
| <i>n</i> -C ₆ H ₁₄ | 0.0028 |
| <i>n</i> -C ₇ H ₁₆ | 0.0028 |
| <i>n</i> -C ₈ H ₁₈ | 0.0015 |
| <i>n</i> -C ₉ H ₂₀ | 0.0018 |
| <i>n</i> -C ₁₀ H ₂₂ | 0.0015 |

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Now, we see the statement of the problem it is like this, we have a natural gas with this particular composition at this pressure 6000 psia and 150 degree Fahrenheit. Now, this particular composition was also considered in the previous lecture where we were finding out the thermo physical properties of the natural gas. And we have kept the same composition because you will find that some properties will be taken from the earlier lecture in this problem too.

So, in this we have been given that a high heating value of the natural gas as 1050 Btu per cubic feet and the air to fuel ratio as 12.56 with these data, now we proceed to go for a solution.



(Refer Slide Time: 01:52)

Solution

Step I. Unit conversion


1 MPa = 145.037 psia
 $\Rightarrow 6000 \text{ psia} = \frac{6000}{145.0375} \text{ MPa} = 41.36 \text{ MPa}$

$T = 150 \text{ }^\circ\text{F} = (150 - 32) \times 5/9 \cong 65 \text{ }^\circ\text{C} = 338 \text{ K}$

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Now, before we go for the solution, we do some unit conversions because some of the units in the correlations are not in fps system, they may need the SI unit. So, we are putting or both the SI as well as the FPS units.

So, here we have that first we convert the psia into MPa from knowing this that 1 MPa is equal to 145 psia, and then we convert temperature in terms of Kelvin this is given in Fahrenheit and we make it in Kelvin.

(Refer Slide Time: 02:31)

Estimation of specific heat capacity

$$J = J_1 + J_2 y_{H_2S} + J_3 y_{CO_2} + J_4 y_{N_2} + J_7 \gamma_{gMIX} + J_8 \gamma_{gMIX}^2$$

$$K = K_1 + K_2 y_{H_2S} + K_3 y_{CO_2} + K_4 y_{N_2} + K_7 \gamma_{gMIX} + K_8 \gamma_{gMIX}^2$$

| | y_i | J_i | K_i | $J_i y_i$ | $K_i y_i$ |
|-------------------|--------|------------------------|--------|------------------------|-----------|
| - | - | 1.19×10^{-1} | 3.75 | 1.19×10^{-1} | 3.75 |
| H ₂ S | 0 | -2.87×10^{-1} | -3.404 | 0.0 | 0.0 |
| CO ₂ | 0.013 | -4.90×10^{-1} | -9.77 | -6.37×10^{-2} | -0.127 |
| N ₂ | 0.0345 | -2.36×10^{-1} | -9.47 | -8.16×10^{-2} | -0.3267 |
| γ_{gMIX} | 0.6872 | 7.30×10^{-1} | 19.7 | 5.02×10^{-1} | 13.517 |
| γ_{gMIX}^2 | 0.4722 | -1.18×10^{-1} | -2.99 | -5.57×10^{-2} | -1.412 |
| | | | | 5.51×10^{-1} | 15.4 |

$$P_{pc} = \frac{K^2}{J^2} \quad T_{pc} = \frac{K^2}{J}$$



$$P_{pc} = \frac{15.4^2}{(5.51 \times 10^{-1})^2} \quad T_{pc} = \frac{15.4^2}{5.51 \times 10^{-1}}$$

$P_{pc} = 782.41 \text{ MPa} \quad T_{pc} = 431 \text{ K}$

$$P_{pr} = \frac{P}{P_{pc}} \quad T_{pr} = \frac{T}{T_{pc}}$$

$$P_{pr} = \frac{41.36}{782.41} \quad T_{pr} = \frac{338}{431}$$

$P_{pr} = 0.05286 \quad T_{pr} = 0.7842$

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And after doing these unit conversions we go to the estimation of the specific heat capacity. We showed this particular expression earlier and in this expression we have some parameters J and K , again we find these parameters are given in terms of many other parameters J_1 up to J_8 and K_1 up to K_8 and when here we have the mole fractions of H_2S , carbon dioxide, nitrogen and the specific gravity of the mixture.

These specific gravity we found out in the earlier lecture for the same composition of the natural gas, that is why we kept the composition same. So, again we have another parameter K and which is in terms of K_1, K_2, K_3 etcetera which are associated with the mole fractions of the H_2S, CO_2 nitrogen etcetera. Now, these this is the table which gives us the value of this J_i and K_i and for this expression what we do write the mole fractions the J_i values and take these products of $J_i Y_i$ and $K_i Y_i$ and the gamma mix and is taken here from and then we find that this is the summation of the $J_i Y_i$ and the summation of the $K_i Y_i$.

And here we find the pseudo critical temperature pressure and temperature by this formula. So, we take this K square value and this J square value from this tables, and we find out the, from this formula we find out the value of this; please understand that K_i and J_i they are the average values that is why we need to do this summation. So, their average K_i that is this and this is the average J_i that is this. So, we put this plug in the values to get out get the values of the pressure and temperature pseudo critical temperature to pseudo critical pressure, and with these are the units these are given in terms of megapascal and Kelvin.

So, we needed to convert the units of the given data to Kelvin and megapascal, and here we have the pseudo reduced pressure and pseudo reduced temperatures.

(Refer Slide Time: 04:51)

Estimation of specific heat capacity

$$A = 0.49694 \frac{\beta P_{pr}}{T_{pr}^2} = 5.68 \times 10^{-2}$$

$$B = 0.09012 \frac{P_{pr}}{T_{pr}} = 6.07 \times 10^{-3}$$

$$\beta = \beta_1 + \beta_2 \ln(P_{pr}) + \frac{\beta_3}{T_{pr}} + \beta_4 \ln^2(P_{pr}) + \frac{\beta_5}{T_{pr}^2} + \frac{\beta_5 \ln(P_{pr})}{T_{pr}} = 1.332$$

| | |
|-----------|------------------------|
| β_1 | 2.38×10^{-1} |
| β_2 | -3.51×10^{-2} |
| β_3 | 6.20×10^{-1} |
| β_4 | -5.74×10^{-3} |
| β_5 | -1.18×10^{-1} |

$$Z^3 - Z^2 + (A - B - B^2)Z - AB = 0$$

$$Z^3 - Z^2 + (0.0568 - 0.00607 - 0.00607^2)Z - 0.0568 \times 0.00607 = 0$$

Solving, we get

$$Z = 0.9461$$

$$R = 8.314 \frac{\text{J}}{\text{mol K}}$$

$$a = 0.49694 \frac{(RT_{pc})^2}{P_{pc}} = 8.15 \times 10^3$$

$$b = 0.09012 \frac{RT_{pc}}{P_{pc}} = 4.13 \times 10^{-1}$$

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Now, after knowing this we find the values of these parameters A and B, and in this we have these in this we have this beta given in this is given from this expression. And here we have the values of the various other parameters beta 1 beta 2 beta 3 beta 4 beta 5 from this table we plug in we get the value of beta and this beta is taken to find out the value of A.

So, now we come to the solution of this particular expression Z, we shall see we shall be using this value of the compressibility factor and when we put this value of A B etcetera and we find that we get this value of Z here. Now, please understand this is a cubic equation we have not shown the details of the solution of this cubic equation of state, but there are 3 solutions here and you will even if you do this calculation we will find that the 3 solutions become to real, now we take the maximum value of the Z for the vapor phase.

So, this is how we are getting the value of Z as 0.9461 by plugging in the values of this A and B in this expression. And after this we find this value of this small a and small B in terms of the pseudo critical pressure and temperature.

(Refer Slide Time: 06:25)

Estimation of specific heat capacity

$$\frac{d\beta}{dT} = -\frac{\beta_3 T_{pc}}{T^2} - \frac{2\beta_5 T_{pc}}{T^3} - \frac{\beta_6 \ln(P_{pr}) T_{pc}}{T^2}$$

$$\frac{d\beta}{dT} = -\frac{6.20 \times 10^{-1} \times 431}{338^2} - \frac{2 \times -1.18 \times 10^{-1} \times 782.41}{338^3} - \frac{8.18 \times 10^{-2} \times \ln(0.05286) \times 431}{338^2} = 1.8452 \times 10^{-4}$$

$$\frac{d^2\beta}{dT^2} = \frac{2\beta_3 T_{pc}}{T^3} + \frac{6\beta_5 T_{pc}}{T^4} + \frac{2\beta_6 \ln(P_{pr}) T_{pc}}{T^3}$$

$$\frac{d^2\beta}{dT^2} = \frac{2 \times 6.20 \times 10^{-1} \times 431}{338^3} + \frac{6 \times -1.18 \times 10^{-1} \times 431}{338^4} + \frac{2 \times 8.18 \times 10^{-2} \times \ln(0.05286) \times 431}{338^3} = 4.6646 \times 10^{-3}$$

$$M = \frac{Z(Z+B)}{Z-B} = \frac{0.9461 \times (0.9461 + 6.07 \times 10^{-3})}{0.9461 - 6.07 \times 10^{-3}} = 0.9583$$

$$N = a \frac{B}{Rb} \frac{d\beta}{dT} = 8.15 \times 10^3 \times \frac{6.07 \times 10^{-3}}{8.314 \times 4.13 \times 10^{-1}} \times 1.8452 \times 10^{-4} = 2.6584 \times 10^{-3}$$

| | |
|-----------|------------------------|
| β_1 | 2.38×10^{-1} |
| β_2 | -3.51×10^{-2} |
| β_3 | 6.20×10^{-1} |
| β_4 | -5.74×10^{-3} |
| β_5 | -1.18×10^{-1} |
| β_6 | 8.18×10^{-2} |

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And here we have that this expression $d\beta$ by dT and this $d^2\beta$ by dT^2 is take given by this expression and we put this do you make use of this table given here, to find out the values of these various parameters β_3 β_5 β_6 etcetera and we get the value of the various derivatives of the β with respect to temperature as this. So, after getting these derivative values, we go to find out the value of 2 more parameters M and N in terms of this Z .

(Refer Slide Time: 07:06)

Estimation of specific heat capacity

$$C_{DL}^{corr} = B_1 + B_2 \ln(T_{pr}) + B_3 P_{pr} + B_4 \ln^2(T_{pr}) + B_5 P_{pr} \ln(T_{pr})$$

$$C_{DL}^{corr} = (5.57 \times 10^{-1}) + (6.348 \times 10^{-1} \times \ln(0.7842)) - (2.682 \times 10^{-2} \times 0.05286) + (7.838 \times 10^{-2} \times \ln^2(0.7842)) - (1.1171 \times 10^{-3} \times 0.05286 \times \ln(0.7842)) = 0.7145$$

$$C_p^0 = A_1 + A_2 T_{pr} + A_3 T_{pr}^2 + \frac{A_4}{y_{gMix}} + \frac{A_5}{y_{gMix}^2}$$

$$C_p^0 = 45.9 + (9.90 \times 0.7842) + (4.17 \times 10^{-1} \times 0.7842 \times 0.7842) + \left(\frac{7.095 \times 10^{-1}}{0.6872}\right) + \left(\frac{-9.02}{(0.6872)^2}\right)$$

$$C_p^0 = 35.84744$$

| | |
|-------|--------------------------|
| B_1 | 5.57×10^{-1} |
| B_2 | 6.348×10^{-1} |
| B_3 | -2.682×10^{-2} |
| B_4 | 7.838×10^{-2} |
| B_5 | -1.1171×10^{-3} |

| | |
|-------|------------------------|
| A_1 | 45.9 |
| A_2 | 9.90 |
| A_3 | 4.17×10^{-1} |
| A_4 | 7.095×10^{-1} |
| A_5 | -9.02 |

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And then we come to the expressions of the correction of correction factor this is given by this expression and in this expression we have this beta, B 1 B 2 B 3 etcetera which are taken from this particular table. And again in this when another C p naught, which the Cp naught is given in terms of the A 1 A 2 etcetera which is taken from this particular table, and then we get the value of the C p naught as this.

(Refer Slide Time: 07:37)

Estimation of specific heat capacity

$$C_p = C_{p,DL}^{corr} \left[a \frac{T}{b} \left(\frac{d^2 \beta}{dT^2} \right) \ln \left(\frac{Z+B}{Z} \right) + \frac{R(M-N)^2}{M^2 - A(2Z+B)} - R \right] + C_p^\circ \left[\frac{J}{\text{mol K}} \right]$$

$$\left[a \frac{T}{b} \left(\frac{d^2 \beta}{dT^2} \right) \ln \left(\frac{Z+B}{Z} \right) + \frac{R(M-N)^2}{M^2 - A(2Z+B)} - R \right] =$$

$$\left[\left(8.15 \times 10^3 \times \frac{338}{4.13 \times 10^{-1}} (4.6646 \times 10^{-3}) \ln \left(\frac{0.9461 + 6.07 \times 10^{-3}}{0.9461} \right) \right) \right. \\ \left. + \frac{8.314 \times (0.9583 - 2.6584 \times 10^{-3})^2}{0.9583^2 - 5.68 \times 10^{-2} \times (2 \times 0.9461 + 6.07 \times 10^{-3})} - 8.314 \right] \approx 200$$

$$C_p = (0.7145 \times 200) + 35.84744 \approx 179 \frac{J}{\text{mol K}}$$

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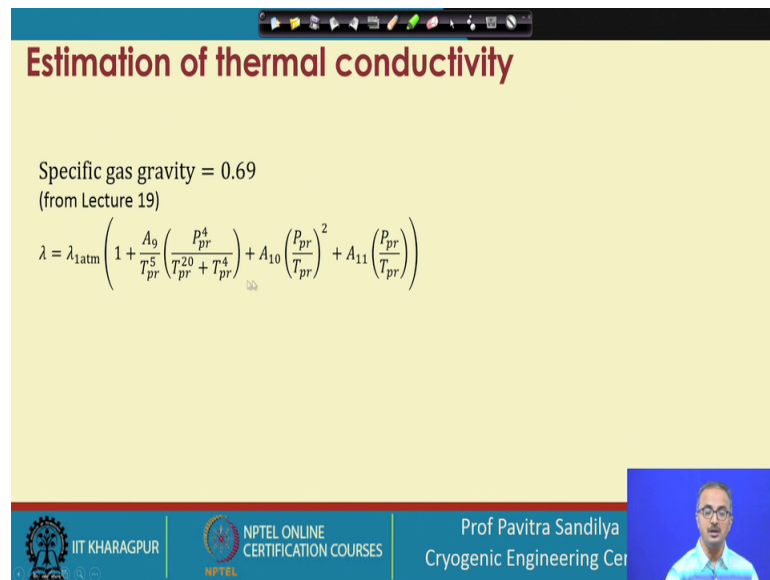
And ultimately we get the C p naught for the ideal gas and for the real gas we apply the correction factor through the ideal gas C p and we get this particular value as joule per mole per Kelvin by inputting the various parameter values.

Please understand that these expressions are to be taken from the literature and there is no need for memorizing these expressions, only thing is that we have to have the various parameter values available to us to calculate these various parameters and we find that all these parameters are depending on the temperature, pressure and the composition.

(Refer Slide Time: 08:23)

Estimation of thermal conductivity

Specific gas gravity = 0.69
(from Lecture 19)

$$\lambda = \lambda_{1\text{atm}} \left(1 + \frac{A_9}{T_{pr}^5} \left(\frac{P_{pr}^4}{T_{pr}^{20} + T_{pr}^4} \right) + A_{10} \left(\frac{P_{pr}}{T_{pr}} \right)^2 + A_{11} \left(\frac{P_{pr}}{T_{pr}} \right) \right)$$


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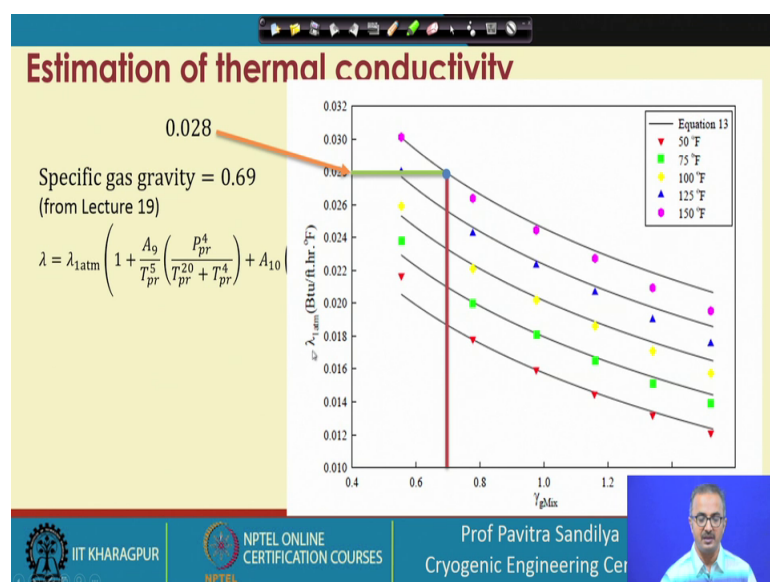
Now, after this we come to the estimation of thermal conductivity, this is an expression given and in this we find that this thermal conductivity depends on the thermal conductivity at one atmosphere. So, first we shall see how to estimate this conductivity at one atmosphere to which we put some correction factor to get the actual thermal conductivity.

(Refer Slide Time: 08:45)

Estimation of thermal conductivity

0.028

Specific gas gravity = 0.69
(from Lecture 19)

$$\lambda = \lambda_{1\text{atm}} \left(1 + \frac{A_9}{T_{pr}^5} \left(\frac{P_{pr}^4}{T_{pr}^{20} + T_{pr}^4} \right) + A_{10} \right)$$


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So, here we have the a chart, in this chart we have this value of the gamma and this value is 0.69, and then we go to the this is the pressure given the temperature given to us 150

degree Fahrenheit. So, at this temperature for this particular gamma, we read out the value as about 0.028 for this lambda 1 atmosphere.

(Refer Slide Time: 09:18)

Estimation of thermal conductivity

Specific gas gravity = 0.69
(from Lecture 19)



$$\lambda = \lambda_{1\text{atm}} \left(1 + \frac{A_9}{T_{pr}^5} \left(\frac{p_{pr}^4}{T_{pr}^{20} + T_{pr}^4} \right) + A_{10} \left(\frac{p_{pr}}{T_{pr}} \right)^2 + A_{11} \left(\frac{p_{pr}}{T_{pr}} \right) \right)$$

$$\lambda = 0.028 \left(1 + \frac{1.85}{0.7842^5} \left(\frac{0.05286^4}{0.7842^{20} + 0.7842^4} \right) - \right)$$

$$1.2757 \times 10^{-3} \times \left(\frac{0.05286}{0.7842} \right)^2 + 1.925 \times \left(\frac{0.05286}{0.7842} \right)$$

$$\lambda \cong 1.13 \frac{\text{Btu}}{\text{ft. hr. F}}$$

| Coefficient | Tuned coefficient |
|-----------------|-------------------------------------|
| A ₁ | 3.095251494612 × 10 ⁻⁰⁵ |
| A ₂ | -3.054731613002 × 10 ⁻⁰¹ |
| A ₃ | 1.205296187262 × 10 ⁻⁰² |
| A ₄ | -2.155542603544 × 10 ⁻⁰² |
| A ₅ | 1.695938319680 × 10 ⁻⁰² |
| A ₆ | 1.983908703280 × 10 ⁻⁰³ |
| A ₇ | 1.469572516483 × 10 ⁻⁰² |
| A ₈ | 7.570807856000 × 10 ⁻⁰⁴ |
| A ₉ | 1.854452341597 × 10 ⁻⁰⁰ |
| A ₁₀ | -1.275798197236 × 10 ⁻⁰³ |
| A ₁₁ | 1.925784814025 × 10 ⁻⁰¹ |



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So, we put in these values in this particular expression and then we have been given this particular chart, and in this chart we get the value of the A 9 A 10 A 11 and these we plug in to get the value of the thermal conductivity as 1.13 Btu per feet per hour per Fahrenheit this is as per the correlation.



(Refer Slide Time: 09:39)

Estimation of Wobbe number of natural gas

$$WB = \frac{HHV}{\sqrt{\frac{\rho_g}{\rho_{air}}}}$$

$$\rho_g = 333 \frac{\text{kg}}{\text{m}^3} \quad \rho_{air} = 425 \frac{\text{kg}}{\text{m}^3} \quad HHV = 1050 \frac{\text{Btu}}{\text{ft}^3}$$

$$WB = \frac{1050}{\sqrt{\frac{333}{425}}} = \frac{1050}{0.885} \cong 1186 \frac{\text{Btu}}{\text{ft}^3}$$



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Now, we have another correlation for finding out the Wobbe index which a definition that the definition is goes like that the ratio of the high heating value to this specific gravity, and here we have the rho g as 333 kg per meter cube, which can be obtained from our earlier tutorial on the thermo physical property measurement.

And here we have the density of the air and this value has been given in the problem. With these values we find out the Wobbe index to be 11886 Btu per cubic feet.

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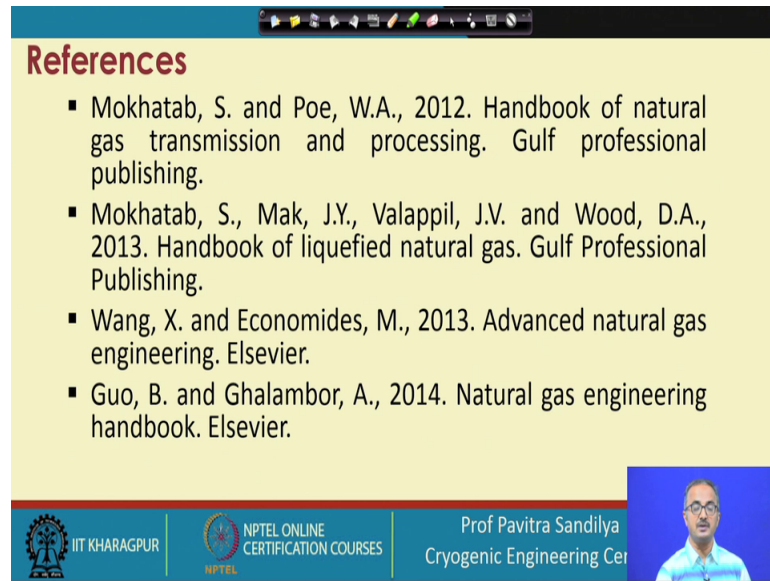
Estimation of CARI from A/F ratio

$$\text{CARI} = \frac{\text{A/F Ratio}}{\sqrt{\text{specific gas gravity}}}$$
$$\text{CARI} = \frac{12.56}{\sqrt{0.69}} = 15$$

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After finding Wobbe index we go to estimate the value of the combustion air ratio index from the air to fuel ratio. Here is the formula that we use and we put plug in the values of the given natural gas and we find that CARI is coming to be 15.

(Refer Slide Time: 10:43)



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Now, these are the references which we which we refer to and this has been also given in our earlier lecture on the estimation of these properties from which we have taken the correlations and the various tables for the various types of parameters.

Thank you.