Fundamentals of Combustion

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Lecture - 40

Laminar Premixed Flames - Part 8

Stability Maps and Worked Examples

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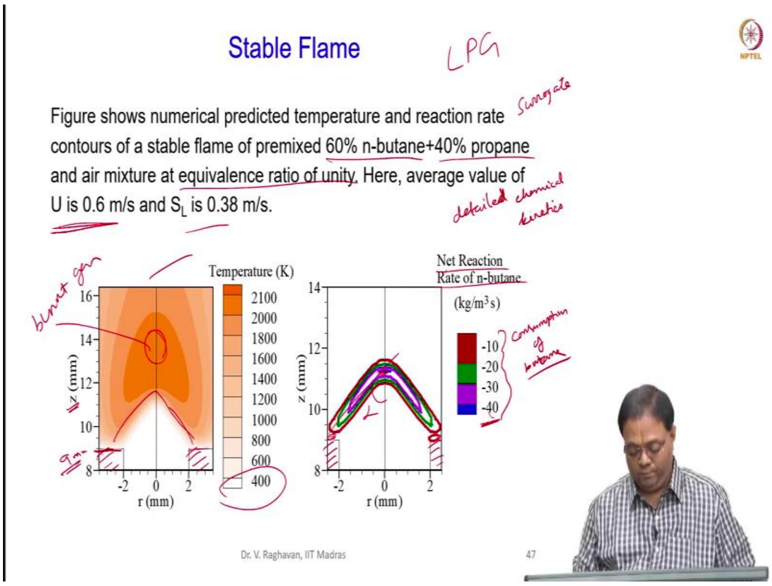

Stable Flame

LPG

Figure shows numerical predicted temperature and reaction rate contours of a stable flame of premixed 60% n-butane+40% propane and air mixture at equivalence ratio of unity. Here, average value of U is 0.6 m/s and S_L is 0.38 m/s.

Surrogate

detailed chemical kinetics

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So, now we have also predicted numerically. So, we have taken a surrogate of Liquefied petroleum gas (LPG), which is say 60% n-butane and 40% propane; this is called surrogate, surrogate of LPG. So, this is again a detailed mechanism is used, detailed chemical kinetics is used to simulate this. This is a axisymmetric burner, then premixed reactants comes in and burns.

Now the U, average value of the unburnt reactant velocity is 0.6 m/s and the value of S_L based upon these you can say, the half cone angle etcetera, α and you know U. So, you calculate the α and try to calculate S_L, that comes to about say 0.4 m/s and equivalence ratio is unity, so stoichiometric reactant is supplied.

And again, one atmosphere pressure and 298 K or maybe 300 K is the temperature of the reactant mixture. Now, these are the temperature contours; contour means it gives the map of the temperature. So, we can see that, the white is 400 K. So, very low temperature prevails and temperature increases here and this is the burnt gas temperature.

And this is the reaction zone. How is this reaction zone? Because plotting the net reaction of butane it coincides with the net reaction rate of propane also you can see this is the negative value you can see for consumption of butane.

So, butane is consumed here. So, according to the consumption of butane, you get negative values and you can see that the butane is consumed here and see the maximum value of consumption is -40, which occurs here and goes there.

So, this actually will give you the flame regime and now the temperature contour is given here. So, this is the stable flame; when you have a velocity of say 0.6 m/s, I get a stable flame which is anchoring slightly away from burner rim. So, this is the burner rim here. So, slightly away from the burner rim, you can see the flame is anchored properly.

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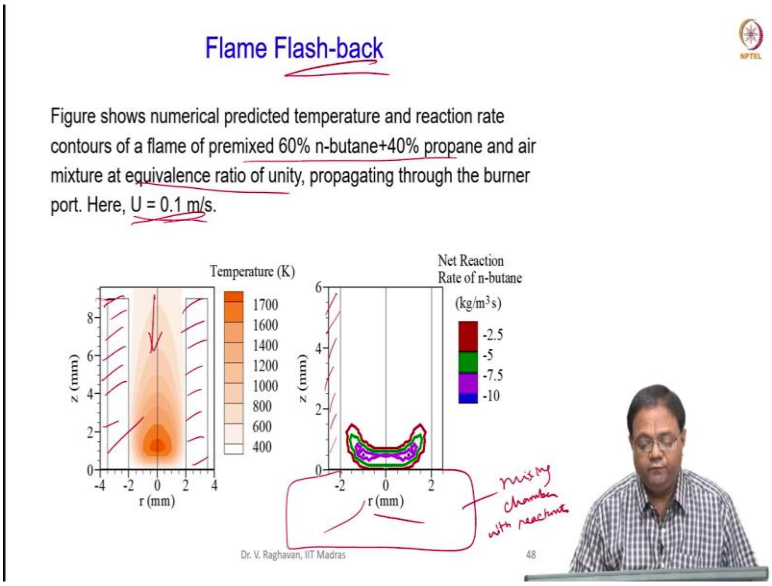

Flame Flash-back

Figure shows numerical predicted temperature and reaction rate contours of a flame of premixed 60% n-butane+40% propane and air mixture at equivalence ratio of unity, propagating through the burner port. Here, U = 0.1 m/s.

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48

On the other hand, when I decrease U to 0.1, same scenario, same equivalence ratio, same mixture, decrease U; you can see that now this is the rim flame has come down, flame is propagating down, flame has come down and you can see that this is the rim, flame has already come in. So, you can see the dimension here.

So, the rim ends here, this is the end of the rim. So, about 9 mm, the rim ends. So, the burner exit is at 9 mm in z scale; whatever you put in the z direction, it is at 9 mm. So, now, we can see that, at the velocity of 0.6, the flame is above the burner rim burning slightly about 0.5 mm away from the burner rim, 1 mm away from the burner rim.

On the other hand, you can see that this is the burner rim and the flame has propagated down here towards the origin and reaction zone is formed right at the entry of the gas. Because velocity is so low, the unburnt gas velocity is 0.1 m/s, flame speed is about 0.4 m/s.

So, flame will not wait till the reactants reach. It has propagated down to consume the reactants; this is called flashback. So, numerically there is no harm in doing this flashback studies but experimentally we have to be careful.

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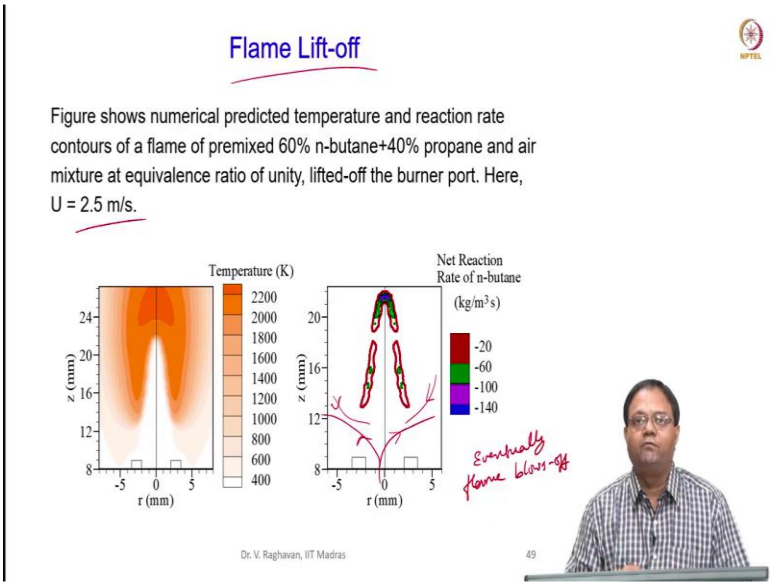

Flame Lift-off

Figure shows numerical predicted temperature and reaction rate contours of a flame of premixed 60% n-butane+40% propane and air mixture at equivalence ratio of unity, lifted-off the burner port. Here, U = 2.5 m/s.

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Now, lift off. So, I now abruptly increase from U 0.6 to 2.5; you can see that the reactants are going to enter at a very high velocity, moving the flame off and the flame is lifted off now, eventually it will blow off, eventually this flame will blow off. So, we can see that the flame, the flame zone tries to move away; it cannot sustain the incoming high velocity.

So, that is the flame lift off. So, it is dangerous, you can see that the reactants which is coming in can leak out and the atmosphere air can come in; this is the atmospheric air which has come in and reactant can leave, incomplete combustion can occur. There is no way you can sustain this flame easily. So, lift off is that type of instability, where there is no control provided for the flame.

And on the other hand, you can see that flashback is very dangerous; because the flame tries to propagate down. Now, if there is a mixing chamber here, mixing chamber with reactants it is very dangerous, because you can ignite this. So, these are the two instabilities which we have to avoid.

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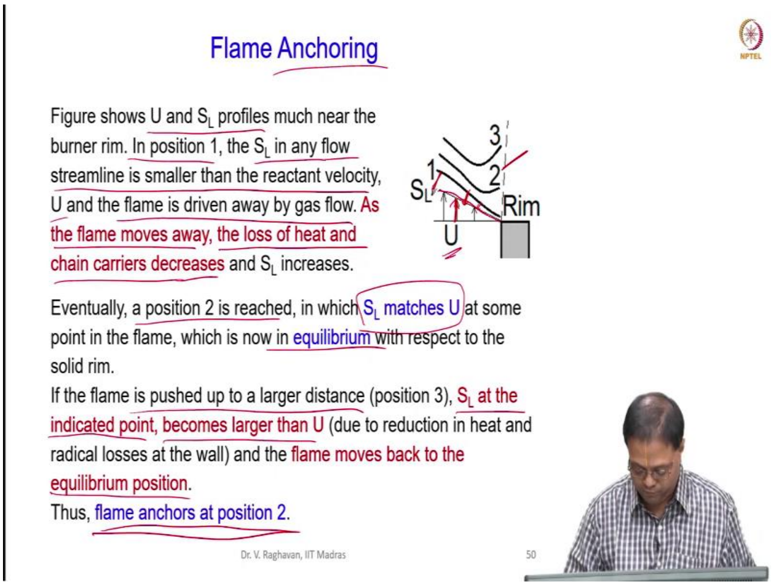

Flame Anchoring

Figure shows U and S_L profiles much near the burner rim. In position 1, the S_L in any flow streamline is smaller than the reactant velocity, U and the flame is driven away by gas flow. As the flame moves away, the loss of heat and chain carriers decreases and S_L increases.

Eventually, a position 2 is reached, in which S_L matches U at some point in the flame, which is now in equilibrium with respect to the solid rim.

If the flame is pushed up to a larger distance (position 3), S_L at the indicated point, becomes larger than U (due to reduction in heat and radical losses at the wall) and the flame moves back to the equilibrium position.

Thus, flame anchors at position 2.

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Now, next is what is called anchoring, how the anchoring occurs? Within the narrow range which we talked about the reactant flow rate; the flame can be stable. How the stability is achieved? Small velocity fluctuations may be there. So, small fluctuations in U can occur, if it occurs, that will not bother the flame; the flame can be perturbed, but again it will come and reach the equilibrium position.

Once this range is violated and the velocity is increased beyond this range or decreased beyond this range then there will be an instability. So, now again we are concentrating closer to the rim; you see this linear line that straight line here is the U profile and this S_L profile I am giving. Now, I am weighing S_L profiles; in the previous case we did the other way.

So, the equilibrium point, where the flame is stable, we are going to see. Now, figure shows the variation of U and S_L along the radius, radial profiles. Now, in position 1; what happens is the S_L is smaller. So, any flow, flow streamline is smaller than the reactant velocity U, and the flame is driven away by the blow gas; you can see this. S_L in any flow streamline is smaller than this.

Actually, here the S_L is smaller, here S_L is again smaller. So, if you take the local velocity here, their corresponding S_L is smaller than that, when you resolve it. So, either you resolve U to that direction or resolve S_L to this direction you will find that in the first position the flame, that means from a stable flame you are slightly increasing the velocity U, so that the flame is not able to match that speed of the reactants.

So, the flame is driven away from the gas. As the flame moves away, but since its only a small perturbation. So, this just moves away now due to the slight increase in the velocity. Now, it goes to some position 2, where when it moves away; the heat loss to the rim decreases, similarly the radical losses to the rim also decreases.

As the flame moves away, the loss of heat and chain carriers (chain carriers are radicals) loss decreases. So, S_L will increase. Now, at this position 2, it will have sufficient amount of S_L to match U values. So, position 2 is reached. That is the equilibrium position where locally S_L matches the U value and equilibrium is reached; that is flame will now sustain at that point.

Now, what you do? You decrease the velocity U then the flame will try to go to position 1, So, this is not discussed here, but we can discuss this. So, from the position 2, if you decrease the velocity slightly; then what happens is, you go to a position 1. Now, when the flame reaches the rim, it will lose more heat and radicals; then what happens, its velocity S_L will decrease.

Now, at this point, U will be more than S_L; again, U will push the flame out to position 2. So, again we reach the equilibrium position. Now, let us take the other condition; when the U is again increased more.

So, if the flame is pushed up to a larger distance, say position 3, by perturbation of the U to a higher value, then S_L at the indicated point 3 becomes larger than U. Why? Because S_L will increase; it will lose lesser heat and radicals to the wall, because it is away.

Now, what happens, the S_L will increase; so, it will try to come down again to the equilibrium position. So, this is the equilibrium position, 2 is equilibrium position, from that if we decrease the velocity, it may go to position 1, where the S_L will decrease due to the increase in the heat loss and radicals.

Then, due to mismatch between U and S_L, it will again go to the position 2, which is equilibrium position. When it is lifted off to position 3, again due to the reduction in the radical and heat losses; S_L will actually increase and now try to come down to the position 2.

So, when we operate the burner in a small range of velocities, then we always have the flame within this position 2 which is the equilibrium position. The flame anchors at position 2 stably. But if you increase or decrease velocity more than this range; then we are not going to get a stable flame, either it will flash back with the velocity is reduced too much or it will lift off if the velocity is increased too much.

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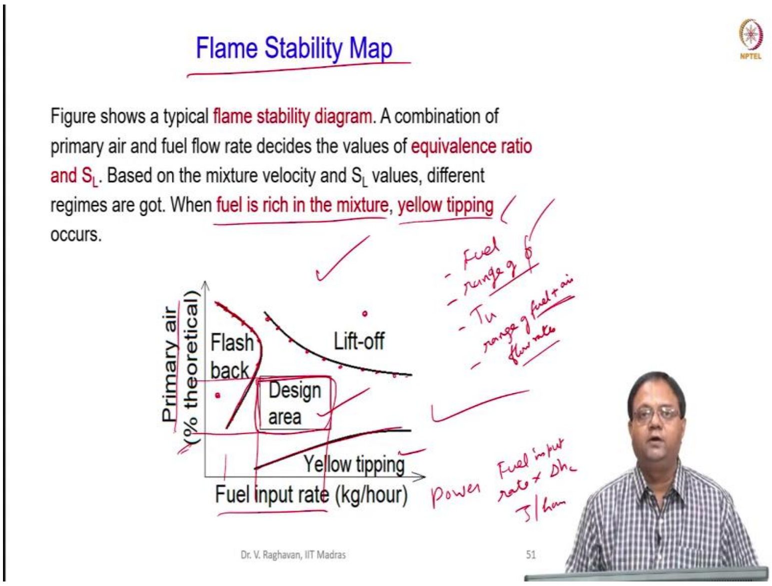

Flame Stability Map

Figure shows a typical flame stability diagram. A combination of primary air and fuel flow rate decides the values of equivalence ratio and S_L. Based on the mixture velocity and S_L values, different regimes are got. When fuel is rich in the mixture, yellow tipping occurs.

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51

So, the flame stability map, this is very important to do for all the burners, when you have a burner with premixed reactants. So, we have to select first fuel, then range of equivalence ratio; then T_u, unburnt temperature range, then see fuel. We will also know the range of flow rates. So, this you have to first fix.

So, there will be a range; why this range of fuel flow rates is required, fuel and air flow rate, range of phi? Because you have to have a range of power produced by the burner. So, when you fix this, we have to draw a map like this, which is called flame stability map.

What we try to do here is, the fuel input rate is given; we can also put fuel input rate or power rating here, power rating is nothing but fuel input rate into Δh_c or calorific value then you get say J/hr.

So, that is what we can plot here. So, this is a range of operation we should decide on first. Similarly, for the fuel flow rate, we have to supply air; why I call primary air? Because normally in big combustion chambers, there will be stages of combustion. So, we will have primary air and we will also have some secondary air to cool the hot products and so on. So, secondary air, tertiary air; zonal air will be supplied.

So, primary air basically is the air which you supply along with the fuel. So, that is called primary air. So, this is actually calculated percentage theoretical; stochiometric is 100% So, whether it is 80% stochiometric or 120% stochiometric etcetera, it will vary like this.

So, now if you see, if you have a mixture which is ignitable mixture and there is a fuel flow rate and air flow rate, but the velocities are low. If we have in this, the velocity of the mixture is very low, so, for the given equivalence ratio etcetera, the flame velocity will be higher. So, flashback occurs. So, you note these points where flashback occur and put a boundary like this.

So, to the left of this boundary, flashback will occur. So, I should not go to this. Similarly, I note the points where the lift off initiates and draw this line; this boundary we will avoid, see crossing this boundary for a given fuel flow rate and air flow rate, if I am here, it will surely lift off. For a given fuel flow rate and air flow rate, I am in this point, it will flashback. So, I should not go to this.

So, similarly when I do not provide enough air, then yellow tipping will occur; yellow tipping will occur in a fuel rich mixture. When you increase the Φ value, equivalence ratio value to say, 2, 2.2, 2.5 etcetera yellow tipping; that means that yellow tipping indicates that there is a probability for incomplete combustion, because some CO can be released or soot can be formed in some fuels and so on.

So, in some fuels, in all fuels it will not occur; in some fuels like LPG etcetera, higher order hydrocarbons, unsaturated hydrocarbons yellow tipping can occur if you starve the mixture with too much of air, starve the mixture with air or supply too much of fuel.

So, this also you should avoid. Now, this is the range you have to operate; but normally we take a stable range, this is the range which you take and I call this design area. So, now, I will only supply fuel in this and the air only in this range. So that I get proper stable combustion. So, this stability map has to be done for different fuel type, for a given burner you have to check this.

In a given burner itself if you want to change the fuel from methane, natural gas to LPG; you have to conduct this experiment and get the map and get this design range for operation. So, this is very important. So, this is the end of the topic.

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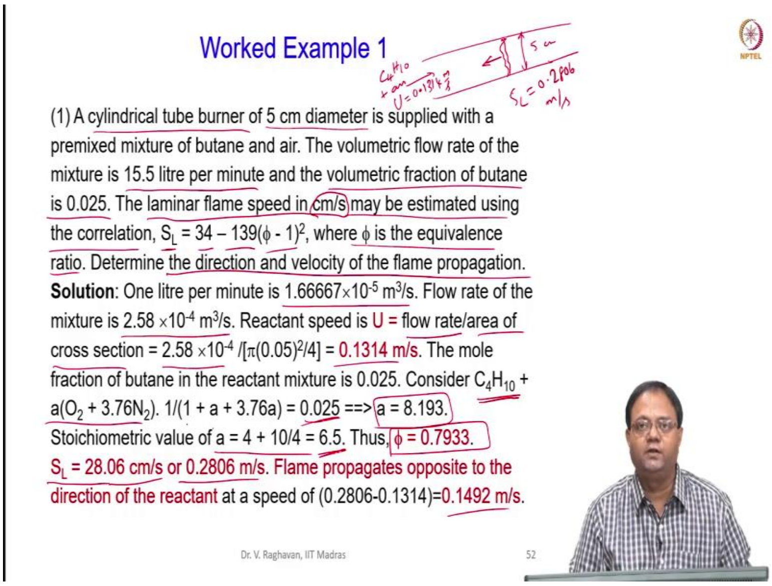

Worked Example 1

(1) A cylindrical tube burner of 5 cm diameter is supplied with a premixed mixture of butane and air. The volumetric flow rate of the mixture is 15.5 litre per minute and the volumetric fraction of butane is 0.025. The laminar flame speed in cm/s may be estimated using the correlation, $S_L = 34 – 139(\phi - 1)^2$, where ϕ is the equivalence ratio. Determine the direction and velocity of the flame propagation.

Solution: One litre per minute is 1.66667×10^{-5} m^3/s. Flow rate of the mixture is 2.58×10^{-4} m^3/s. Reactant speed is U = flow rate/area of cross section = $2.58 \times 10^{-4} /[\pi(0.05)^2/4]$ = 0.1314 m/s. The mole fraction of butane in the reactant mixture is 0.025. Consider C_4H_{10} + $a(O_2 + 3.76N_2)$. 1/(1 + a + 3.76a) = 0.025 ==> a = 8.193. Stoichiometric value of a = 4 + 10/4 = 6.5. Thus, ϕ = 0.7933. S_L = 28.06 cm/s or 0.2806 m/s. Flame propagates opposite to the direction of the reactant at a speed of (0.2806-0.1314)=0.1492 m/s.

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52

Let us see a worked example. A cylindrical tube burner, diameter of the burner is 5 cm tube, it is supplied with a premixed mixture of butane and air; the volumetric flow rate is 15.5 lpm and the volumetric fraction of butane is 0.025.

Now, the laminar flame speed in cm/s may be estimated using the correlation which is $S_L = 34 – 139(\Phi-1)^2$, where Φ is the equivalence ratio. Now, it is ignited somewhere and the flame is formed. Determine the direction and velocity of the flame propagation that is what we need to find.

Now, to determine the direction and the velocity of the flame propagation. So, 1 lpm = 1.66667×10^5 m^3/s, SI units convert that.

So, flow rate is 2.54×10^{-4} corresponding to 15.5 lpm, it is 2.58×10^{-4} m^3/s. So, reactant velocity is nothing but the flow rate, volumetric flow rate divided by the area of cross section which is $2.58 \times 10^{-4}/(\pi d^2/4)$.

So, that is 0.1314 m/s. So, U is 0.1314 m/s. Now, what is Φ? When I want to calculate S_L, I need value of Φ as per the correlation. What is Φ? You know the reactant mixture is butane, 1 kmol of butane + a kmol of the air, that is a kmol of O_2 and 3.76×a N_2, kilo moles of nitrogen.

$$C_4H_{10} + 6.5(O_2 + 3.76N_2) \rightarrow 4CO_2 + 5H_2O + 6.5 \times 3.76\, N_2.$$

Now, what is given is the volumetric fraction of butane, which is the mole fraction of butane. So, number of moles of butane is 1, so, 1/(1+a+3.76a) will be the mole fraction of butane given as 0.025.

$$C_4H_{10} + a(O_2 + 3.76N_2).\ 1/(1 + a + 3.76a) = 0.025 \Longrightarrow a = 8.193.$$

So, from this, a value is estimated as 8.193. Now, stochiometric value of a is x + y/4. So, 4 + 10/4 is 6.5. Now, from this stochiometric a value you know; actual a value is 8.19 stoichiometric a value is 6.5.

So, what is the Φ? Φ is close to 0.8.

$$\phi = 0.7933$$

So, once you know the Φ, calculate S_L in cm/s convert into m/s, so, 0.2806. That means the reactants are flowing at this and the flame is formed here and the flame propagates with S_L of 0.2806.

Flame propagates opposite to the direction of the reactant at a speed of (0.2806 - 0.1314) = 0.1492 m/s.

So, the reactants are coming at a speed of 0.13, the flame can propagate at a speed of this 0.28 m/s so that the flame actually will propagate in the direction opposite to the mixture at a velocity of 0.15 m/s. So, this is the first example, where you use a correlation to find the S_L value.

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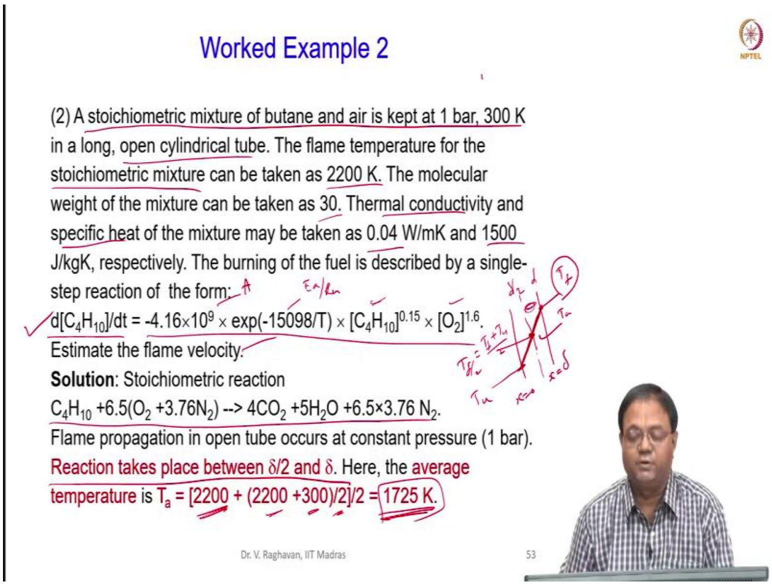

Worked Example 2

(2) A stoichiometric mixture of butane and air is kept at 1 bar, 300 K in a long, open cylindrical tube. The flame temperature for the stoichiometric mixture can be taken as 2200 K. The molecular weight of the mixture can be taken as 30. Thermal conductivity and specific heat of the mixture may be taken as 0.04 W/mK and 1500 J/kgK, respectively. The burning of the fuel is described by a single-step reaction of the form:

$d[C_4H_{10}]/dt = -4.16\times10^9 \times \exp(-15098/T) \times [C_4H_{10}]^{0.15} \times [O_2]^{1.6}$.

Estimate the flame velocity.

Solution: Stoichiometric reaction

$C_4H_{10} + 6.5(O_2 + 3.76N_2) \text{-->} 4CO_2 + 5H_2O + 6.5\times3.76\ N_2$.

Flame propagation in open tube occurs at constant pressure (1 bar).

Reaction takes place between δ/2 and δ. Here, the average temperature is $T_a = [2200 + (2200 + 300)/2]/2 = 1725\ K$.

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53

Second example, a stochiometric mixture of butane and air is kept at 1 bar and 300 K, in a long open cylindrical tube. Flame temperature is given as 2200 K, it is an approximate; you can find the adiabatic flame temperature. Molecular weight of the mixture is given as 30 kg/kmol, thermal conductivity and the specific heat is given as 0.04 W/m-K and 1500 J/kg-K.

Now, the reaction rate of consumption of butane; so negative is because of the consumption of butane here. This is the A value, this is E_a/R_u value and this is concentration of butane power m, concentration of oxygen power n, so single step reaction.

$$d[C_4H_{10}]/dt = -4.16\times10^9 \times \exp(-15098/T) \times [C_4H_{10}]^{0.15} \times [O_2]^{1.6}$$

So, what is the flame velocity or the laminar flame speed? So, this is actually stochiometric mixture. So, write the equation for the stoichiometric mixture like this; this is what is taking place. Now, you know that this is the reaction zone and in the simplified analysis, we used this. So, this is $x = 0$, this is $x = \delta$ and this is say T_u and this is T_f, so linear variation.

Now, please understand this, calculation of temperatures, average temperatures etcetera is very important here. So, this is the reaction rate which is given but the reaction rate or the concentrations at what temperature you will calculate? What we assume is, this is half of the reaction zone.

So, we say that the reaction takes place between $\delta/2$ and δ; obviously because in our simplified analysis, we assume that from $-\infty$ to $\delta/2$ no reaction takes place. So, predominantly reaction takes place between this point which is $\delta/2$ and δ. So, what is the temperature between this? You know this is a linear profile, linear variation of temperature.

So, at this point the temperature will be $(T_f + T_u)/2$. So, this temperature at $\delta/2 = (T_f + T_u)/2$ and here this is T_f. So, the average temperature here is T_a, which is nothing but $(T_f + T_u)/2$, both added up and divided by 2, that is 1725 K, that is the average temperature at which the concentrations are evaluated and the reaction rate is calculated.

You can also calculate the temperature, the reaction happening at T_f; but obviously the reaction has started well before that. So, you have to take an average temperature; we are requiring only the average reaction rate. Maximum reaction rate will be at T_f, what we calculate at T_f, but we are now interested in the average reaction rate which is calculated at this temperature. How to calculate concentrations?

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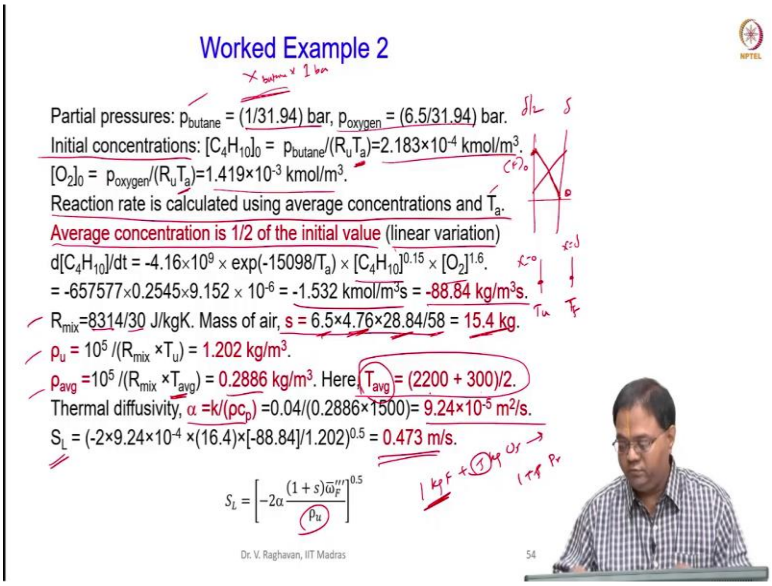

Worked Example 2

Partial pressures: p_{butane} = (1/31.94) bar, p_{oxygen} = (6.5/31.94) bar.

Initial concentrations: $[C_4H_{10}]_0$ = $p_{butane}/(R_uT_a)$=2.183×10^{-4} kmol/m^3.

$[O_2]_0$ = $p_{oxygen}/(R_uT_a)$=1.419×10^{-3} kmol/m^3.

Reaction rate is calculated using average concentrations and T_a.

Average concentration is 1/2 of the initial value (linear variation)

$d[C_4H_{10}]/dt = -4.16\times10^9 \times \exp(-15098/T_a) \times [C_4H_{10}]^{0.15} \times [O_2]^{1.6}$.

$= -657577\times0.2545\times9.152 \times 10^{-6} = -1.532$ kmol/m^{3}s = -88.84 kg/m^{3}s.

R_{mix}=8314/30 J/kgK. Mass of air, s = 6.5×4.76×28.84/58 = 15.4 kg.

$\rho_u = 10^5/(R_{mix} \times T_u)$ = 1.202 kg/m^3.

$\rho_{avg} = 10^5/(R_{mix} \times T_{avg})$ = 0.2886 kg/m^3. Here, T_{avg} = (2200 + 300)/2.

Thermal diffusivity, $\alpha = k/(\rho c_p)$ =0.04/(0.2886×1500)= 9.24×10^{-5} m^2/s.

S_L = (-2×9.24×10^{-4} ×(16.4)×[-88.84]/1.202)$^{0.5}$ = 0.473 m/s.

$$S_L = \left[-2\alpha\frac{(1+s)\bar{\omega}_F'''}{\rho_u}\right]^{0.5}$$

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54

Now, I calculate initial concentrations; initial concentrations are we know the partial pressure of butane that is the mole fraction into total pressure, total pressure is 1 bar. So, mole fraction of butane, this is x butane into 1 bar. So, that will be the partial pressure of butane.

$$p_{butane} = (1/31.94)\text{ bar}, p_{oxygen} = (6.5/31.94)\text{ bar}$$

Similarly, partial pressure of oxygen you calculate that. What is concentration? Concentration is P/R_uT. So, this is the again when you calculate the concentration as I told you; you have to take the average temperature which you calculated here.

The flame zone averaged temperature, this temperature you have to take, that is 1725 K. So, use that temperature here to calculate the concentrations of this. This is the initial concentration. So, we can also assume that concentration also varies from a high value to a low value linearly. So, reaction rate is calculated using average concentration and average temperature.

$$[C_4H_{10}]_0 = p_{butane}/(R_uT_a)=2.183\times10^{-4}\text{ kmol/m}^3.$$

$$[O_2]_0 = p_{oxygen}/(R_uT_a)=1.419\times10^{-3}\text{ kmol/m}^3.$$

So, initial concentration, see for example, this is δ/2 and this is δ the concentration, initial concentration is this; concentration falls to 0 here. So, this is 0, and this is initial concentration. So, from initial concentration, the reactant reactants concentration decreased to 0 value.

$$d[C_4H_{10}]/dt = -4.16\times10^9 \times \exp(-15098/T_a) \times [C_4H_{10}]^{0.15} \times [O_2]^{1.6}.$$

$$= -657577\times0.2545\times9.152 \times 10^{-6} = -1.532\text{ kmol/m}^3\text{s} = -88.84\text{ kg/m}^3\text{s}.$$

R_{mix}=8314/30 J/kgK. Mass of air, s = 6.5×4.76×28.84/58 = 15.4 kg. $\rho_u = 10^5/(R_{mix} \times T_u) = 1.202\ \text{kg/m}^3$.

$$\rho_{avg} = 10^5/(R_{mix} \times T_{avg}) = 0.2886\ \text{kg/m}^3$$

So, what is the average concentration? Average concentration can be taken as half of the initial value because this concentration plus 0 by 2, so half of the initial value, assuming linear variation. So, temperature also we have assumed like this, it increases linearly; concentration also decreases linearly from initial value to a 0 value, so average concentration is half of the initial value.

So, using this half of the concentration for this, the initial concentrations which is subscript 0 then you can calculate the reaction rate in kmol/m^3s or in kg/m^3s. So, now, you have to find the s, 1 kg of fuel 1 kg fuel + s kg oxidizer → 1 + s kg products.

So, what is s? This s is nothing, but the mass of air. So, that is 6.5a × molecular weight of air × 4.76 / molecular weight of the fuel. So, 1 kg of fuel, you require 15.4 kg of air that is value of s, the oxidizer which is air.

So, now that you calculate. Then similarly mixtures, specific gas constant, universal gas constant by the molecular weight of mixture which is given as 30 kg/kmol. Similarly, calculate the unburnt reactant density which is required for S_L and the average density for which you are going to calculate the value of α.

$$\alpha = k/(\rho c_p) = 0.04/(0.2886 \times 1500) = 9.24 \times 10^{-5}\ \text{m}^2/\text{s}$$

So, the average value now is entire reaction zone this is x = 0, this is x = δ. In the entire reaction zone, what is the average temperature here? This is T_u, this is T_f. So, what is the average temperature $(T_f + T_u)/2$? That will be the average temperature in the entire reaction zone.

$$S_L = \left[-2\alpha \frac{(1+s)\bar{\omega}_F'''}{\rho_u}\right]^{0.5}$$

$$S_L = (-2 \times 9.24 \times 10^{-4} \times (16.4) \times [-88.84]/1.202)^{0.5} = 0.473\ \text{m/s}$$

At that average temperature, calculate density, calculate the value of α; because the k and c_p values are given at an average temperature. Now, this is the thermal diffusivity. So, substituting all these you get S_L as 0.473; we are over predicting this. So, this is the way you calculate the S_L based upon the simplified analysis. The main important point to note here is, the values of the properties have to be evaluated at some average temperature. Similarly, the reaction rates, concentration of the reactants have to be calculated at some average temperature which is very close to the reaction zone. So, we will stop this now.