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Lecture-59 Combustion in 2 Phase Flows (Contd...)

Welcome back. So, let us continue the discussion on 2 phase flow or combustion in 2 phase media. So, we started looking at the 2 phase media and how a single droplet combustion can be estimated, where we can actually estimate the evaporation rate and time.





So, we will continue the discussion. So, this is where we actually stopped.

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	$Y_{F,s} - Y_{F,\infty}$
Mass transfer based analysis:	$m = 4\pi r_s \rho D \ln(1 + B_Y)$, where, $B_Y = \frac{1}{1 - Y_{F,s}}$
Heat transfer based analysis:	$\dot{m} = \frac{4\pi \lambda_g r_s}{c_{pg}} \ln(B_q + 1), \text{ where, } B_q = \frac{c_{pg}(T_\infty - T_{\text{boil}})}{h_{fg}}$
For unity Lewis number $\lambda = \rho c_p L$ $\frac{c_p (T_{\infty} - h_{fg})}{h_{fg}}$	D, we have, $B_T = B_q$. $\frac{T_s}{Y_{F,s} - Y_{F,s}} = \frac{Y_{F,s} - Y_{F,s}}{Y_{F,s} - 1}$
$Y_{F,s}$ is function of the vapor pres	ssure of fuel and total pressure
$Y_{F,s} \equiv \frac{\rho_{F,s}}{\rho} = \frac{n_F}{n} \frac{M_H}{M}$	$\Sigma = \frac{P_F}{P} \frac{M_F}{M}$ where $P_{F,s} = Aexp(-B/T_s)$
1. A value of T_s is assumed -	
2. The vapor pressure of fuel is	determined using table
3. $Y_{F,s}$ is evaluated from Eq.	
4. Check whether the value of	T_s and Y_{Fs} satisfy $B_T = B_q$. Otherwise reiterate.
5. Calculate B_T or B_q using in lifetime.	itial conditions $T_{\infty}Y_{F,\infty}$. Estimate evaporation rate, drople

So, this is what we got from the mass transfer based analysis and the second one is the heat transfer based analysis. So, for now, the assumption here is that, if the Lewis number is infinity, then we can write this balance and then finally we can find out the fuel at the surface. So, that is 's' stands for this at surface. Now, how we estimate that, we can see this T_s is assumed.

The vapour pressure of the fuel is also determined using some table then $Y_{F,s}$ is evaluated from the equation and we can check whether T_s and $Y_{F,s}$ satisfy this. Otherwise, we will go for iterative. And then finally, we calculate B_Y and B_q using the initial condition of T_{∞} and $Y_{F,\infty}$. And then we can estimate the evaporation rate, droplet lifetime. So, these are the 2 important parameter that we wanted to calculate.

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Now, when you go to the single droplet combustion, there are also certain assumptions. So, one is that the first assumption is that it is spherical, burning droplet surrounded by spherical flame. Which means essentially we are assuming itself or simplifying to a 1-D problem, where \dot{m} is a constant and function of radius. Now, second one is that no interaction between droplets. That means, it does not take into account droplet collision and also sudden change in droplet size and number partially premixed combustion.

Therefore, diameter only function of \dot{m} and time, It is an Quasi steady stationary in the gas phase which clearly means that steady in the gaseous phase and we can use those assumption. Then one-component fuel, phase equilibrium at the surface. So, which means no mixing inside perfusion diffusion to the droplet surface if one know the temperature. Like Y_g.

Pressure is uniform and constant which simplifies the analysis. Fuel, oxidizer and products only. So that also is simplification. Then fast chemistry, reaction at stoichiometric surface which allows to use the concept killers approach like mixture fraction concept and then radiation is negligible. So, which also simplify the energy equation. Thermo-chemical properties are constant at Lewis number 0. No convection around the droplets. So, that mean all velocity is 0 and the size D_0 , temperature of the surroundings T_{∞} .

So, the whole idea is to calculate the evaporation rate, evaporation time and flame position. The approach here actually extends the development done for this spherically symmetric droplet evaporating in quiescent environment, as we have discussed earlier. So, I have written the assumption of stagnant environment and spherical symmetry in the initial development, but subsequently we can show how the spherically symmetric results can be adjusted to take into account the environment of burning caused by convection either all these things.





So that is essentially gives you this is how the inner region, this is the outer region from where oxidizer comes, this is fuel, temperature and the product and this is the surface from where it goes. So, this is the liquid zone, which is between the inner zone and the outer zone.

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So, we can write the mass conservation equation and then the mass flow rate would be this. So, one can write fuel mass transfer equation in terms of fuel mass fraction Y_F , oxidizer mass fraction equation which is Y_{Ox} , energy equation and then we can use the stoichiometric. So,

$$\dot{\omega}_F = \frac{\omega_{OX}}{v}$$

Single Droplet Combustion $\dot{m}_A'' = \dot{m}'' Y_A - \rho D \frac{\mathrm{d}Y_A}{\mathrm{d}r}$ Fick's law: Balance equation at the droplet surface $\dot{m}_{F}'' = \dot{m}_{F}''Y_{F,s} - \rho D \left. \frac{dY_{F}}{dr} \right|$ As $\dot{m}'' =$ Fuel: As $\dot{m}'' = \dot{m}''_F$ Using $\dot{m}_s'' = \rho_s u_s$, We obtain $\rho_s u_s(Y_{\mathrm{F},s} - 1) = \rho D \frac{\mathrm{d}Y_1}{\mathrm{d}r}$ Finally, $\rho_s \psi_{s,\text{Ox},s}^V = \rho D \frac{\mathrm{d}Y_{\text{Ox}}}{\mathrm{d}r}$ $0 = \dot{m}'' Y_{\text{Ox},s} - \rho D \left. \frac{\mathrm{d}Y_{\text{Ox}}}{\mathrm{d}r} \right|_{s}$ Oxidizer: $\rho_s u_{s,fg} = \lambda \left| \frac{\mathrm{d}T}{\mathrm{d}r} \right| = \rho D \left| \frac{\mathrm{d}(c_p T)}{\mathrm{d}r} \right|$ Energy: assuming droplet temperature is uniform at T_s Kuo (2005 INDIAN INSTITUTE OF TECHNOLOGY KANPUR ke De 22

Now, you also use the Fick's law of diffusion. So, which is like this and then we put it back in the equation system. So, what we get:

$$\dot{m}_A^{\prime\prime} = \dot{m}^{\prime\prime} Y_A - \rho D \, \frac{dY_A}{dr}$$

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where this is like this and using this what we get that $\rho_s u_s$ and this and here also finally, $\rho_s u_s$ this is also $u_s \rho D$ and energy equation becomes this is h_{fg} and if you look at the surface this is the droplet surface through which the heat transfer comes in. So, the droplet temperature here is uniform.



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So, we write the fuel equation, oxidizer equation and energy equation then multiply this 1 by Δh_c and adding to this, we get this from we calculate b_{F,T}. Similarly, we will do some algebra. We can also get b_{Ox,T}. So, this one can get. Again going back to this. So, for the b_{Ox,T} we can get.

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So, these are the calculations one can do and so, it just like fuel vapour multiply these oxygen doing these and then you do the algebra. So, you get these where $b_{F,T}$ you obtain like that.

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So, this is a simple algebra one can carry out and get it and now if the boundary condition if we put r tends to infinity, b would be b_{∞} . So, this will give me this at the interface. Now, we integrate this, first integration constant. Assuming ρD is this. Then we can get. Then substitute C in this equation and we get this 1 and separation of variable give us this and then finally, after integration.

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Then the second boundary condition r tends to infinity, b is b_{∞} . So, we will get C₂ we put it back this is what we get. And then finally, this is what it is. So, these is an evaporation rate:

$$\dot{m} = 4\pi r^2 \rho u_r$$

This is how it is estimated.



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Now, the mass conservation or mass evaporation rate also estimated like this and in order to determine the evaporation rate we calculate the spalding number $b_{\infty} - b_s$ using this information and this. So, these are standard calculations if you look at any textbook you can find this.

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So, more we can go into this what we observe here. The temperature of the flame did not appear in the burning rate directly. So, that is one of the observation that one can have. Secondly, the variation of B is not great among the different fuels that is second thing. Then the burning rate being proportional to the $ln(1 + \beta)$ will not change much as long as the oxidizing medium is kept the same.

So 10 times variation in B yields only 2 times variation in the burning rate, and, the diffusivity and gas density dominate the burning rate.



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So, these are the observation which allows and now these are the table which shows that the different transfer number for different fuels. So, this is the B or the Spalding number. So

temperature did not appear in the burning rate variation of B is not great, burning rate being proportional to $\ln(1 + \beta)$ will not change much as the medium is the same. And the diffusivity and the gas density dominate the burning rate and there is a 10 times variance in the diffusivity. So, that is what one get.

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Now from the combustion system $B_{Ox,T}$ is the most convenient form of B. So, one can write that there is a change in the resulting term. This particular term is less than the standard. So, basically the first term in the numerator is not that high compared to the second term. So, one can actually approximate this one like this. This is a fairly simple assumption and good enough assumption.

Now burning rate and the evaporation coefficient are readily evaluated. So it is not necessary. Now here one can note the form of $B_{Ox,T}$ or $B_{F,T}$ obtained in the analysis, assume that the fuel droplet has infinite thermal conductivity, that is temperature inside the droplet is throughout that is maintained as T_s . So, that is one of the assumption. Now at the interface if you do the heat balance, this is what coming out of the liquid. This goes as a vapour goes in. So, if we write down the heat balance this is what we get.

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Now, interface one can write:

$$\dot{Q}_{g-i} = \dot{m}_F h_{fg} + \dot{Q}_{i-l}$$

So the negligible thermal inertia simplest assume that the droplet rapidly heats up to temperature T_s . And there is an onion skin model which says that:

$$\dot{Q}_{i-l} = \dot{m}_F c_{pl} (T_s - T_0)$$

Here assumption is that the droplet as consisting of 2 zones an inner region existing uniformly at its initial temperature T_0 and a thin surface layer T_s . Then one can have transient heat up where it can be.

So, droplet behaves as a lumped parameter. Requires solving for energy and mass conservation equation for the droplet as a whole in order to obtain $\frac{dT_s}{dt}$. Now, alternative approach is that, one can estimate the B and that would give you a conservative results of the burning rate obtained by using this equation.

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Now, the estimation of the flame temperature and the flame radius T_f and r_f . So, we have $r_s^2 u_s$ by this already we have obtained. Now, using $r^2 \rho v_r$ here which is constant equals to $r_s^2 \rho_s v_s$. That is the essential at the surface and the so ρD is also constant. So, using this information in this equation, we get this. And then we recall the b_f value and that once we put. Now at the flame location, fuel and oxygen would be 0. Using this, the temperature of the flame and the r_f can be obtained.

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So, this boils down to this and we use this equation. So, the ratio of r_f by r_s is ln(1 + B) by this. So, that allow you to calculate the flame position r_f . Now, for the case of benzene just an example v is this using these Spalding number 6, we can calculate that this ratio to be 27. Now, for most of the fuel droplets burning in air, the flame standoff distance would be about 30 times the droplet radius.

This value is much larger than which is observed experimentally due to assumption made with respect to the thermo physical properties and the Lewis number that means the equal diffusivity unit Lewis number. So, these are the assumption made these things to happen like that.



We have,	$\frac{r_s^2 \rho_s u_s}{\rho_s D_s r_f} = \ln(1 + \frac{Y_{\text{Ox},\infty}}{\nu})$	Eq. 2.13
tarting again fr	om $\frac{r_s^2 u_\delta}{r D_s} = \ln \frac{b_\infty - b_s + 1}{b - b_s - 1}$ (using $b = b_{\text{Ox}, 2}$	$T = \frac{Y_{\text{Ox}} \Delta h_c / \nu + c_p T}{\Delta h_c Y_{\text{Ox},s} / \nu + h_{fg}})$
nd making use	of Eq.(2.13),	
Tame temperati	$\operatorname{rre:} c_p(T_f - T_s) = \frac{\Delta h_c Y_{\mathrm{Ox},\infty} / \nu + c_p(T_s)}{1 + Y_{\mathrm{Ox},\infty}}$	$\int_{\infty}^{\infty} -T_s) + h_{fg} - h_{fg}$
T_f obtained can	be higher than the adiabatic flame temper	ature, since the nitrogen
iffused into the	inner region is preheated, which can in the	irn heat the fuel vapor

Now, we have these. Now, again we are starting from there. So, using these we can find out the flame temperature. So, T_f obtained can be higher than the adiabatic flame temperature, since the nitrogen diffused in this.

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And then the droplet lifetime, we have already seen the droplet lifetime in the radius can be obtained from the mass balance. So,

$$\frac{Dm_d}{Dt} = -\dot{m}_F$$

Which is $4\pi\lambda_D$ divided by this and once we integrate we get this. So, this is the well-known D² law and you can see four different fuels if you plot that how it varies actually. So, the droplet lifetime can be easily obtained that t. So, that is the lifetime of the droplet.

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Now, we look at the heat and mass transfer balance, so, the heat conduction which takes place. So this is our droplet radius, this is the flame sheet. So, in between this is the inner zone. Now, there is a heat transfer which comes in then the mass diffusion analogue process to heat conduction and using Fick's law, we can write this.

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There is the mass diffusion and then this is the convection. This is applicable since at surface no fluid motion and energy transfer occurs only through conduction. Here the f stands for fluid. So, the energy transfer not only by diffusion also by macroscopic motion of the fluid. The difference in droplet and gas space velocity exists. Convection is mode of heat transfer. So, this would be heat flux would be $h_T(T_s - T_\infty)$ which is like that.

Next is the convection heat transfer coefficient. And this is the thermal boundary layer and the temperature profile how and the T_s is the surface temperature.



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Similarly, the convection of mass which is there. There will be boundary layer thickness and the diffusion coefficient one can find out.

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Now, in boundary layer flows constant heat transfer h_T that can be expressed in terms of dimensionless variable like this. So, these come from the boundary layer equations where the non-dimensional is done and one can get those things. So, the non-dimensional number Nusselt number which is at the boundaries surface $\frac{\partial T}{\partial y}$ is 0 or hysteresis function of this for given geometry hence this derivative would be also function of like this.

And the Nusselt number and function of x^* , Reynolds number and Prandtl number. So, the average Nusselt number can be obtained by integration over the surface of the body.



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Now analogy. So, if boundary layer flow if you assume that you can find out the h_m and then you can find out the Sherwood number and this. So, essentially it means that the convective heat transfer is only function of Nusselt number and Sherwood number for a given geometry. So, it should be a similar for a variety of fluids. Length scale is not only dependent on this Reynolds number, Prandtl number and Schmidt number parameters.

So, Nusselt number you can see it is a function of also I mean by analogy we can see the Nusselt number would be also function of x, Re_L , Sherwood number is also function of x*, Re_L , Sc So, like that.



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Now, we can see the effect of combustion against the boundary layer of type width so, this is the surface outer region. This is flame surface or flame length. This is how oxidizer varying, fuel varying, this is temperature and all these things. So, this you can see when there is a boundary layer, the profile actually changes and that change takes place because of this boundary layer both and all these things.

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Effects of Convection	
The idea is to move the heat- and conditions from infinity inwards to the and δ_T for energy. The film radius st temperature gradients and hence, heat a increased. This means that convection rates.	mass transfer boundary film radius δ_M for species eepens concentration and and mass transfer rates are enhances droplet burning
The film radii are expressed as function and mass transfer respectively.	ons of Nu and Sh for heat
$\frac{\delta_T}{r_s} = \frac{Nu}{Nu - 2}$	Eq. 3.1
$\frac{\delta_M}{\delta_M} = \frac{Sh}{\delta_M}$	Fg 32

Idea have moved to heat and mass transfer boundary conditions from flame radius δ_M for species and for energy flame radius stiffens the concentration and temperature gradient and heat and mass transfer rate are increased. So, the $\frac{\delta_T}{r_s}$ is expressed as Nusselt number function and the δ_M is a function of Sherwood number.

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Now, if you have a convective environments for a quiescent medium the Nusselt number equals to 2 and in general δ_T / δ_M equals to Prandtl number to power one third. If Prandtl number is one then Sherwood number equals to Nusselt number. So, this would be estimated. So, there are different correlations which actually exist and one may look at that thing how.

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Now, again we can come back and look at the evaporation with convection. So, we have:

$$r^{2}\rho u_{r}\frac{db}{dr} = \frac{d}{dr}\left(r^{2}\rho D\frac{db}{dr}\right)$$

The boundary condition at the liquid gas interface that is r equals r_s now, we have $\rho_s u_s$ because to this for integrating this one will get C_1 assuming they are always D_s this at r_s we get this then get this C_1 putting back to get this separate the variable and finally, after integration and get the C_2 .

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Now, in the presence of convection the energy equation however, the boundary condition at the infinity are replaced by the boundary condition at δ_T and δ_M . So, we have already seen solving the energy equation we can find out now due to the convection now, instead of r tends

to infinity use at that thermal boundary layer. So, oxygen profile at the mass boundary layer thickness would be this.

So, this one will get me back these one side put it this. So, the burning rate then results in:

$$\dot{m}_F = \frac{2\pi\lambda r_s N u}{c_p} \ln(1 + B_{q,0})$$

One can note here this is not the only way to do these things. So, one can also do this by starting from the other equations or integrating the different equation and then apply the boundary condition, we can get this variable 2.

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Now, we can see the effects. So, one of this variable parameters the gas-phase thermophysical properties exhibit strong temperature and composition dependence. So, this is an important parameter and thermophysical properties, which actually control this droplet in combustion, then there will be unsteady effect of fuel-vapour accumulation. So, this is an unrealistic large flame stand-off distances predicted by D^2 law droplet heating.

Now, the evaporation rate depends on time bind temperature field within the droplet. So, we required more sophisticated model to capture that. Then it is a multicomponent fuel which is very important. So, if you look at these liquid fuels, they are not whether it is taking kerosene or petrol, diesel or something, they are really a multi component fuel there would be aromatic ring there would be other rings so the rate of evaporation of different component in a multi component fuel could be significantly different which actually alter the fuel consumption rate. So, this is very important property because in the practical system that we burn, we burn these

fuels which are having actually multi component ingredients and that changes the whole properties that we estimate from a single component fuel. Now, the interaction among multi component droplet is primary issue in spray combustion.

The variable ambient conditions to which the droplet is exposed during its lifetime. Then, another very specific case which may occur in our space application, or the semi cryo or cryogenic application, where there is supercritical droplet combustion. Here the pressure is higher than the critical pressure. So, the latent heat of the vaporization becomes 0 and the evaporation rate becomes infinity.

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So, that means, as soon as the liquid comes out it evaporates. Transient term in the energy equation is no longer negligible as the gaseous mass in the region influenced by the droplet increases with pressure then the abrupt change of liquid phase to the gas phase and the droplet outer radius is replaced by the gradual density change.

Then the radiation effect. So, radiation also increases overall heat transfer at the droplet surface because some fuels when they burn actually there is a lot of heat radiation effect that can change those things. And then the internal circulation in practically high pressure combustor shear stress at the liquid gas interface could be high enough to induce internal circulation within the liquid phase.

So, these are the factors one can think about then in realistic situation, they can change the complete evaporation phenomena the bonding rate consumption and all these things, it is not that simple. So, as you can see, as long as you are looking at the gas-phase combustion and when you are coming here in the multiphase combustion, things are quite different, because in the liquid phase there are so many other things that needs to be considered.

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Now, when you look at this internal circulation this is a Hill's spherical vortex. This one is the Hill's spherical vortex and the different regions which are considered in Prakash and Sirignano's model so this is a boundary layer region. This is the Hill's spherical vortex, this is behind the wake region near the axis of symmetry and all this. So, Prakash and Sirignano they developed a theoretical model or this liquid phase, this is within the droplet.

So, the liquid phase is divided in a thin boundary layer, near the droplet surface in the liquid phase. So, this is what the thin boundary layer then the core region for the liquid motion was approximated by Hill's spherical vortex that means, there is a region where the spherical vortex would be there and the wake region near the axis of symmetry.

Now, when you look at the system, the gas phase analysis or the motion near the surface analysed by three different regions stagnation point boundary layer and the separation region and for boundary layer Karman-Pohlhausen integral approach can be used. So, this is quite important while determining the heat and mass transfer within the droplet. And that is why it also altered the evaporation rate. So, this is an important phenomena that takes place within the droplet. And there is another thing also within the droplet which actually happens is the flux boiling. So that we will talk a little bit when you go to actually the breakup and all these things, and we will see how that.



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Now the application point of view, we have already seen this is a gas turbine application industrial furnace, this is your liquid rocket, gasoline spray in the engine, spray dryer, diesel engine. So, these are all using different kind of fuels, which are actually multi component. So, simplified analysis is good enough to give you some idea, but the realistic situation is quite different as this multi component system play an important role.



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Now, coming to another important picture when this actual show. So for our discussion was on the single droplet combustion the evaporation looking at the surface now, whole point is that before we get the single component droplet or single droplet, it has to because the liquid is injected like this or the fuel is injected like this as a form of fuel injector that does not produce these single droplets, it goes through a process and the process is first the fuel is injected.

So, there could be exit flow there could be cavitation these are the things which may occur then primary there would be ignition and where there is a primary breakup takes place or the primary atomization. So, this is where the spray formation takes place. And then there would be entrainment from the ambient and then there would be secondary breakup that means from the primary, your sheet break into smaller.

I mean the large size droplet and then this will evaporate and mix I mean rather the secondary breakup and the smaller size droplets are formed and then it evaporates. So, that is why the vaporisation is there, once it evaporates, so, it is becoming the gas phase. So, this is the gas phase, where the fuel and air is mixed. And then once you ignite the ignition takes place and the combustion goes on.

So, from these to these there are so you can see we talk about the single droplet combustion going from the gas phase to heat transfer and all these which is actually in this position, but before that the liquid which is also injected that also goes through different stages. And that is why and once it burns you have a pollutant formation like NOx, particulate matter, unburned hydrocarbon and you can look at these.

So, the physical process occurs very simultaneously. So dealing with all these complexities, so that is why to but in order to advance with current modelling capabilities.

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So, it seems reasonable to aim for progress individuals are various like one can look up the breakup, somebody can look up the dispersion, mixing and combustion but, which in other way cannot be viewed in complete isolation. Moreover, one has to consider the advantages and disadvantages of the different modelling approaches like the DNS, LES and simulation based on RANS, property density function kind of approach and all these things.

So, and also important is that you have injection and primary atomization and secondary then drop collisions and all these things dispersion the important is that you have both Eulerian framework and Lagrangian framework, so the coupling between that 2 or completely handling in Lagrangian framework. So these are the challenges that one has to look at it. So we will see how these things are handled from the modelling perspective, and we will stop here today and continue the discussion in the next lecture.