Turbulent Combustion: Theory and Modelling

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Lecture 60
Combustion in 2 phase flows (Contd...)

Welcome back. So, let us continue the discussion on the spray and spray modelling challenges. So, what we have so far discuss on the single droplet combustion, evaporation rate their lifetime and all these now, from single droplet combustion, we are now trying to look at what happens in this frame.

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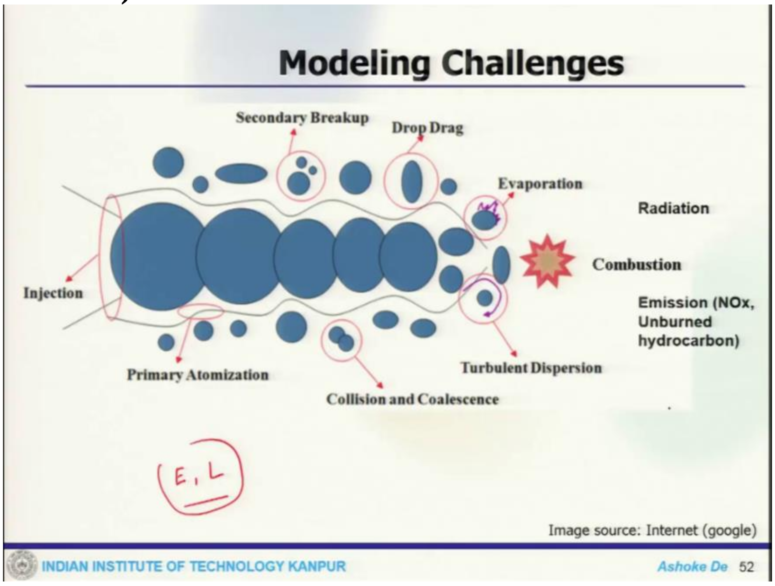

Modeling Challenges

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Image source: Internet (google)

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So, this is where we have actually stopped in the last class, like the spray goes to these primary atomization and secondary atomization and all these.

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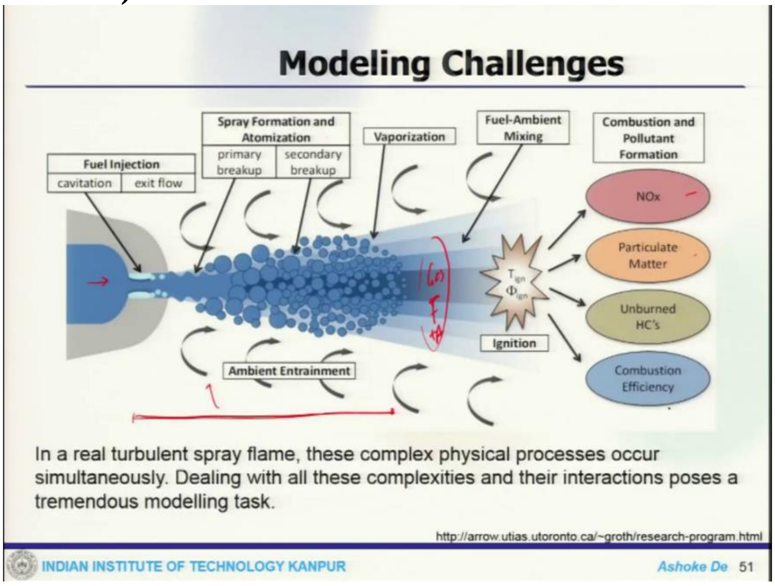

Modeling Challenges

Fuel Injection
cavitation | exit flow

Spray Formation and Atomization
primary breakup | secondary breakup

Vaporization

Fuel-Ambient Mixing

Combustion and Pollutant Formation

NOx

Particulate Matter

Unburned HC's

Combustion Efficiency

Ignition

T_{ign} Φ_{ign}

Ambient Entrainment

In a real turbulent spray flame, these complex physical processes occur simultaneously. Dealing with all these complexities and their interactions poses a tremendous modelling task.

http://arrow.utias.utoronto.ca/~groth/research-program.html

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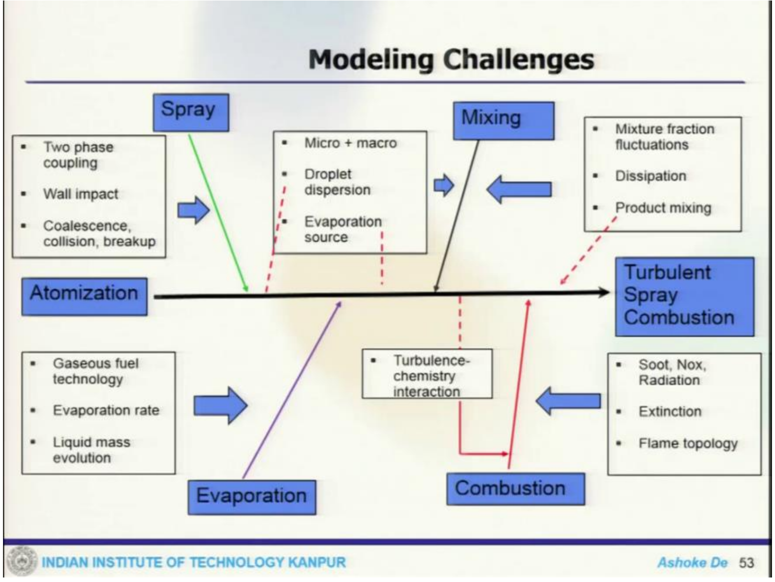

Modeling Challenges

Spray

- Two phase coupling
- Wall impact
- Coalescence, collision, breakup

- Micro + macro
- Droplet dispersion
- Evaporation source

Mixing

- Mixture fraction fluctuations
- Dissipation
- Product mixing

Atomization

Turbulent Spray Combustion

- Gaseous fuel technology
- Evaporation rate
- Liquid mass evolution

- Turbulence-chemistry interaction

- Soot, Nox, Radiation
- Extinction
- Flame topology

Evaporation

Combustion

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Now, this will give you a complete picture, how the turbulent spray combustion are actually handled. So, this is your atomization. Now, the spray comes in here, where there will be 2-phase coupling, there would be wall impact, breakup, then there will be droplet dispersion and then evaporation takes place.

So, where gaseous fuel technology, evaporation rate and then there could be a evaporation source and the mixing takes place then the combustion and where to do turbulence chemistry interaction and then finally, it goes to turbulent spray combustion where you get this soot and all these So, that gives you a complete picture. So, here the atomization to turbulent spray combustion in between there will be spray after that it evaporates, mixing then the combustion and finally, you have a complete picture of turbulent spray combustion.

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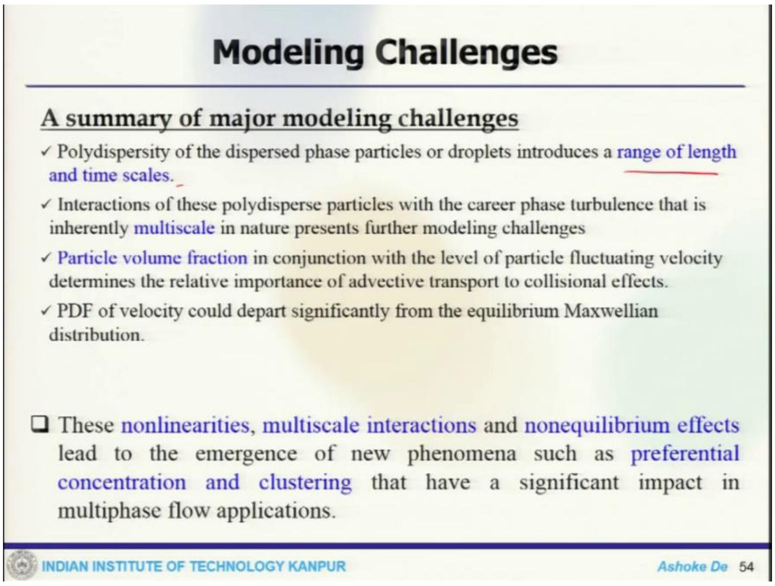

Modeling Challenges

A summary of major modeling challenges

- ✓ Polydispersity of the dispersed phase particles or droplets introduces a range of length and time scales.
- ✓ Interactions of these polydisperse particles with the career phase turbulence that is inherently multiscale in nature presents further modeling challenges
- ✓ Particle volume fraction in conjunction with the level of particle fluctuating velocity determines the relative importance of advective transport to collisional effects.
- ✓ PDF of velocity could depart significantly from the equilibrium Maxwellian distribution.

❑ These nonlinearities, multiscale interactions and nonequilibrium effects lead to the emergence of new phenomena such as preferential concentration and clustering that have a significant impact in multiphase flow applications.

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Now, if you put in summary of these things, now the polydispersity of dispersed phase particles and droplets introduces a range of length and time scales, which is very important. Then, the introduction of these polydispersed particles with the career phase turbulence that is inherently multiscale in nature, which complicates further the modelling part.

Then the particle volume fraction in conjunction with the level of particle fluctuating velocity determines the relative importance and their collisional effects and then the PDF of velocity could depart significantly from the equilibrium Maxwellian distribution. Now, these nonlinearities, multiscale interactions on non-equilibrium effects, which lead to actually new phenomena such as preferential concentration and clustering, that have a significant impact in the multiphase flow application.

So, essentially these are quite challenging. Now, it is not very uncommon to encounter a wide variation in the dispersed phase volume fraction in the same multi-phase flow. For example, particle volume fraction can range from near close pack to the base of the bed to less than 5% in the riser.

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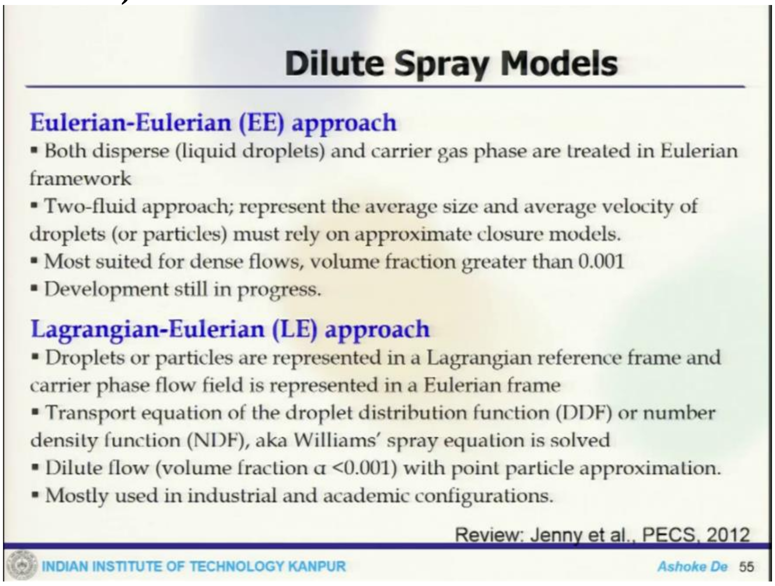

Dilute Spray Models

Eulerian-Eulerian (EE) approach

- Both disperse (liquid droplets) and carrier gas phase are treated in Eulerian framework
- Two-fluid approach; represent the average size and average velocity of droplets (or particles) must rely on approximate closure models.
- Most suited for dense flows, volume fraction greater than 0.001
- Development still in progress.

Lagrangian-Eulerian (LE) approach

- Droplets or particles are represented in a Lagrangian reference frame and carrier phase flow field is represented in a Eulerian frame
- Transport equation of the droplet distribution function (DDF) or number density function (NDF), aka Williams' spray equation is solved
- Dilute flow (volume fraction α <0.001) with point particle approximation.
- Mostly used in industrial and academic configurations.

Review: Jenny et al., PECS, 2012

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So, these are the things one has to know the approach when you go down to the dilute spray models, how to handle that. So, there is an Eulerian-Eulerian approach and there is a Lagrangian-Eulerian approach. So, as the Eulerian-Eulerian approach suggests that the both disperse and the carrier gas phase are treated in Eulerian framework. So, it is a 2 fluid approach and replacing the average size and average velocity of the droplets.

This is more suited for dense flows, volume fraction and greater than 0.001. Developments are still in progress. Now for Lagrangian-Eulerian approach, the droplets or particles are represented in Lagrangian reference frame and the carrier gas phase is handled or represented in Eulerian frame. Now, the transport equation of the droplet distribution DDF or a number density function NDF spray equation is solved dilute volume fraction with approximation of these.

Now, another advantage of the Lagrangian-Eulerian approach is what they 2 fluid theories its inability to accurately represent the collision represented flow. So, it is quite well on that interaction with them will flow can significantly alter the collision characteristics in particle laden or droplet laden flow and the effective restitution coefficient is a function of particle droplets stokes number.

So, these effects are incorporated in Lagrangian approach also from a numerical standpoint as it minimizes the numerical diffusion in disperse phase.

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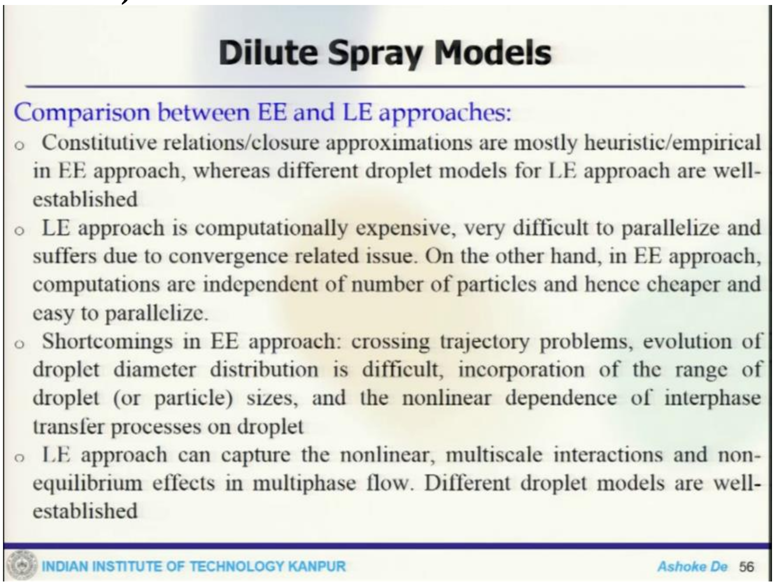

Dilute Spray Models

Comparison between EE and LE approaches:

- Constitutive relations/closure approximations are mostly heuristic/empirical in EE approach, whereas different droplet models for LE approach are well-established
- LE approach is computationally expensive, very difficult to parallelize and suffers due to convergence related issue. On the other hand, in EE approach, computations are independent of number of particles and hence cheaper and easy to parallelize.
- Shortcomings in EE approach: crossing trajectory problems, evolution of droplet diameter distribution is difficult, incorporation of the range of droplet (or particle) sizes, and the nonlinear dependence of interphase transfer processes on droplet
- LE approach can capture the nonlinear, multiscale interactions and non-equilibrium effects in multiphase flow. Different droplet models are well-established

Now, if we compare that both these phases Eulerian-Lagrangian approaches you have a constitutive relations closer approximations or mostly heuristic or empirical in Eulerian-Eulerian approach LE approach is computationally expensive, very difficult. So, one can think to capture the nonlinear multiscale interaction and knowledge benefits in multiphase flow accurately represent collisions.

In the face of the flow could be easily incorporated in the Lagrangian approach also minimises Lagrangian-Eulerian approach minimises a numerical diffusion in disperse phase, but it requires computationally higher cost. Now, one shortcoming in Eulerian-Eulerian approach is the crossing trajectory problem evolution of the droplet diameter distribution is also difficult incorporation of the range of droplet sizes, nonlinear dependence.

But Lagrangian-Eulerian approach can capture the nonlinear multiscale interaction and also there are different droplets model. Now, dilute flow point particle approximation these are the some other things.

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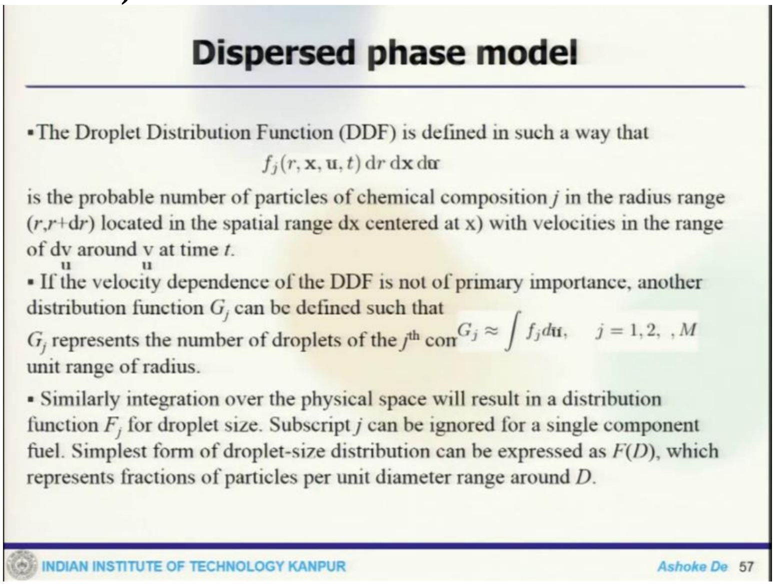

Dispersed phase model

- The Droplet Distribution Function (DDF) is defined in such a way that

$$f_j(r, \mathbf{x}, \mathbf{u}, t)\, dr\, d\mathbf{x}\, d\mathbf{u}$$

is the probable number of particles of chemical composition *j* in the radius range (*r*,*r*+d*r*) located in the spatial range dx centered at x) with velocities in the range of d$\underset{u}{v}$ around $\underset{u}{v}$ at time *t*.

- If the velocity dependence of the DDF is not of primary importance, another distribution function G_j can be defined such that

G_j represents the number of droplets of the j^{th} con $G_j \approx \int f_j d\mathbf{u}, \quad j = 1, 2, \ , M$

unit range of radius.

- Similarly integration over the physical space will result in a distribution function F_j for droplet size. Subscript *j* can be ignored for a single component fuel. Simplest form of droplet-size distribution can be expressed as *F*(*D*), which represents fractions of particles per unit diameter range around *D*.

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Now the droplet distribution function the DDF is defined in such a way that this is how you define now, the velocity dependence of the DDF is not primarily important, because this. So, this would be du this is also u. So, similarly integration of this will distribute the function the f(D) and the simplest form of droplet size distribution can be f(D) which represents the fraction of particles.

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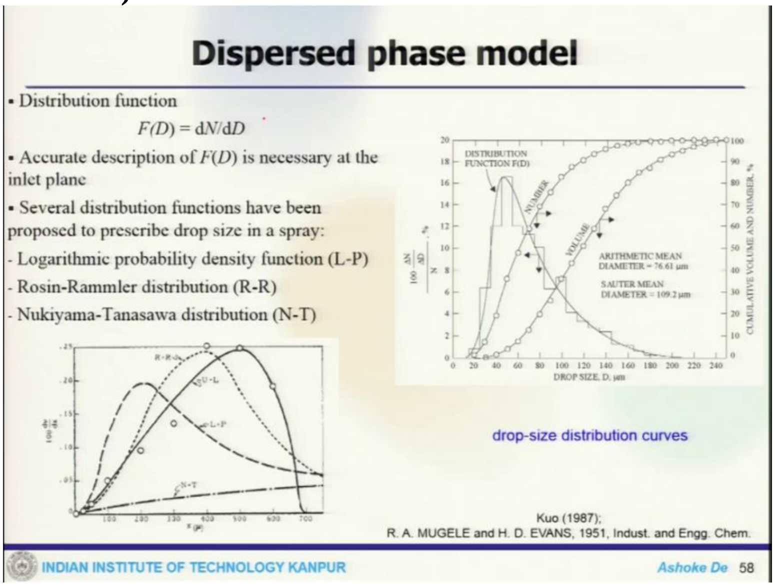

Dispersed phase model

- Distribution function

$$F(D) = dN/dD$$

- Accurate description of *F*(*D*) is necessary at the inlet plane
- Several distribution functions have been proposed to prescribe drop size in a spray:
- Logarithmic probability density function (L-P)
- Rosin-Rammler distribution (R-R)
- Nukiyama-Tanasawa distribution (N-T)

drop-size distribution curves

Kuo (1987);
R. A. MUGELE and H. D. EVANS, 1951, Indust. and Engg. Chem.

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And you can see the F(D)=dN/dD. This is an accurate description of the F(D) is necessary at the inlet plane several distribution functions have been proposed like logarithmic and probability density function, Rosin-Rammler distribution, Nukiyama-Tanasawa distribution N-T distribution. So, these are the distributions which are actually available. This is a droplet size distribution how that varies and this is a one case you can see how things actually for different these things they changes.

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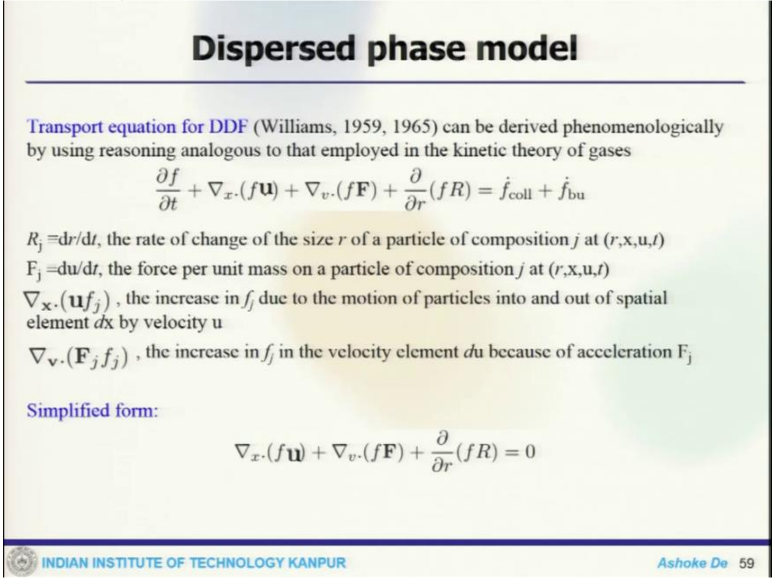

Dispersed phase model

Transport equation for DDF (Williams, 1959, 1965) can be derived phenomenologically by using reasoning analogous to that employed in the kinetic theory of gases

$$\frac{\partial f}{\partial t} + \nabla_x.(f\mathbf{u}) + \nabla_v.(f\mathbf{F}) + \frac{\partial}{\partial r}(fR) = \dot{f}_{\text{coll}} + \dot{f}_{\text{bu}}$$

$R_j = dr/dt$, the rate of change of the size r of a particle of composition j at (r,x,u,t)

$F_j = du/dt$, the force per unit mass on a particle of composition j at (r,x,u,t)

$\nabla_{\mathbf{x}}.(\mathbf{u}f_j)$, the increase in f_j due to the motion of particles into and out of spatial element dx by velocity u

$\nabla_{\mathbf{v}}.(\mathbf{F}_j f_j)$, the increase in f_j in the velocity element du because of acceleration F_j

Simplified form:

$$\nabla_x.(f\mathbf{u}) + \nabla_v.(f\mathbf{F}) + \frac{\partial}{\partial r}(fR) = 0$$

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Now, if you look at the transport of the DDF. This is derived for like this where there is a collision term is term R_j is that change of size r for a particle composition, F_j is the particle composition at j. This is the increase of F_j due to spatial element. So, the simplified form one can write in this.

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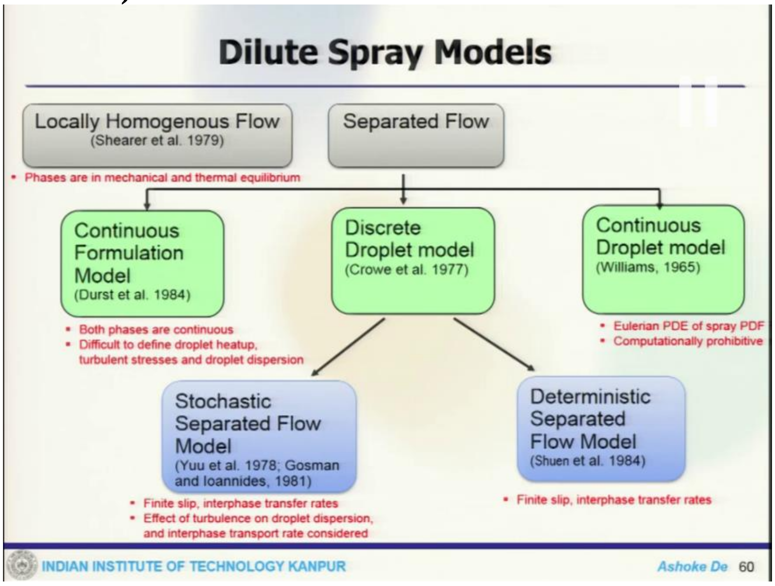

Dilute Spray Models

Locally Homogenous Flow (Shearer et al. 1979)

- Phases are in mechanical and thermal equilibrium

Separated Flow

Continuous Formulation Model (Durst et al. 1984)

- Both phases are continuous
- Difficult to define droplet heatup, turbulent stresses and droplet dispersion

Discrete Droplet model (Crowe et al. 1977)

Continuous Droplet model (Williams, 1965)

- Eulerian PDE of spray PDF
- Computationally prohibitive

Stochastic Separated Flow Model (Yuu et al. 1978; Gosman and Ioannides, 1981)

- Finite slip, interphase transfer rates
- Effect of turbulence on droplet dispersion, and interphase transport rate considered

Deterministic Separated Flow Model (Shuen et al. 1984)

- Finite slip, interphase transfer rates

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Now, if you look at this complete picture. So, either there could be locally homogeneous flow. So, the phases are in mechanical and thermal equilibrium or it is a separated flow then there could be continuous formulation model there would be discrete droplet model or continuous droplet model. Now, continuous formulation model both phases are continuous difficult to define droplet heat up turbulence stresses and dispersion.

Alternatively in continuous droplet model it is Eulerian PDF of spray PDF computationally prohibitive. Now, the approach which proposed by Crowe in 1977 that is discrete droplet where the stochastic separated flow model or deterministic separate flow model. So, this is finite slip, interphase transfer rate is also as a finite slip interface transfer rate effect of turbulence on dispersion these are considered.

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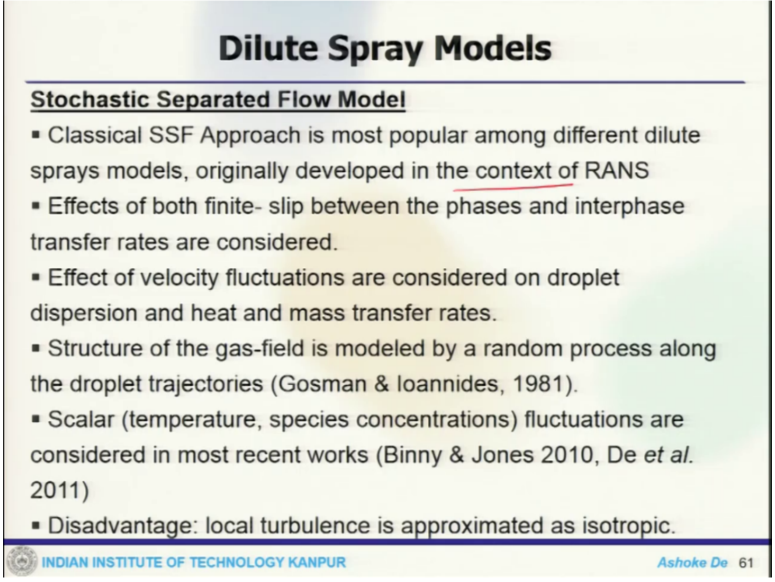

Dilute Spray Models

Stochastic Separated Flow Model

- Classical SSF Approach is most popular among different dilute sprays models, originally developed in the context of RANS
- Effects of both finite- slip between the phases and interphase transfer rates are considered.
- Effect of velocity fluctuations are considered on droplet dispersion and heat and mass transfer rates.
- Structure of the gas-field is modeled by a random process along the droplet trajectories (Gosman & Ioannides, 1981).
- Scalar (temperature, species concentrations) fluctuations are considered in most recent works (Binny & Jones 2010, De *et al.* 2011)
- Disadvantage: local turbulence is approximated as isotropic.

So, that gives you an idea what goes on. Now, classical SSF approach is most popular among different dilute spray models originally developed in context of RANS. Now, effect of both finite slip between the phases and interfaces transfer rates are considered effect of velocity fractures and are also all considered on droplet dispersion heat and mass transfer rate structure of the gas. So, these are some of the issues associated with the stochastic separated flow model which one can note it down.

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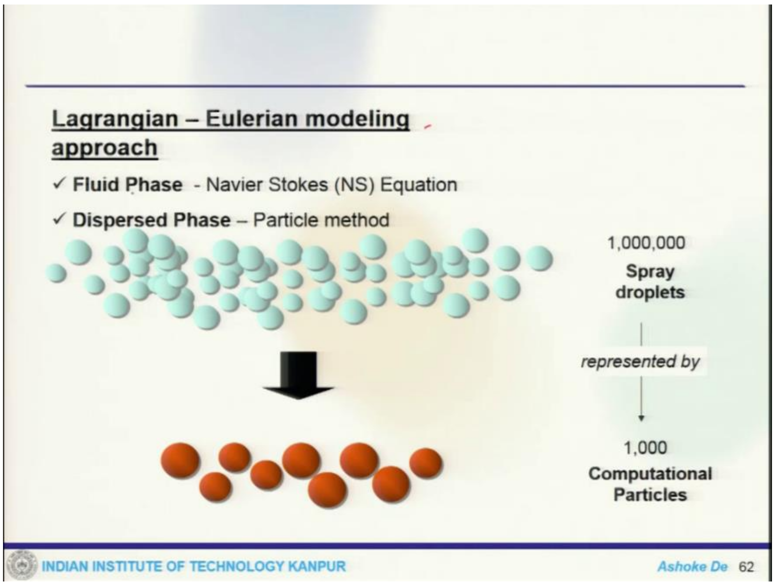

Lagrangian – Eulerian modeling approach

- ✓ **Fluid Phase** - Navier Stokes (NS) Equation
- ✓ **Dispersed Phase** – Particle method

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Now, you can have this Lagrangian-Eulerian modelling where your fluid phase or the gas phase is solved in all Eulerian framework and the liquid part is solved in the Lagrangian framework where we track the particles. And so, obviously, it becomes important that it is just like you are transported PDF calculation where you have so many particles to be tracked within the computational scale.

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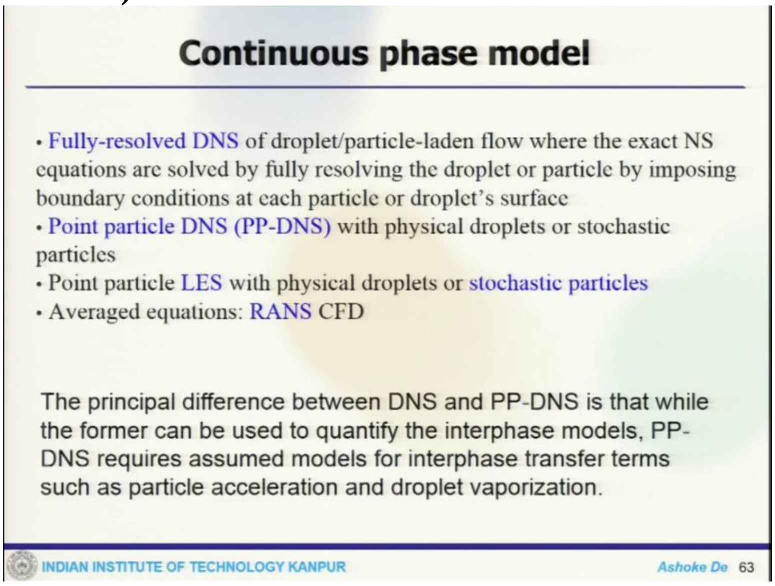

Continuous phase model

- Fully-resolved DNS of droplet/particle-laden flow where the exact NS equations are solved by fully resolving the droplet or particle by imposing boundary conditions at each particle or droplet's surface
- Point particle DNS (PP-DNS) with physical droplets or stochastic particles
- Point particle LES with physical droplets or stochastic particles
- Averaged equations: RANS CFD

The principal difference between DNS and PP-DNS is that while the former can be used to quantify the interphase models, PP-DNS requires assumed models for interphase transfer terms such as particle acceleration and droplet vaporization.

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Now, in a continuous phase model, there could be one can do fully resolved DNS, which is basically the droplet particle laden flow where the exact NS equations are solved or point particle DNS with physically droplets are stochastic particle or point particle LES. Now the LE approach discussed so far couple the Lagrangian and traffic of the commercial particle to a carrier gas flow based on the RANS or equation.

Now, these are the approaches one can actually adopt and take into consideration.

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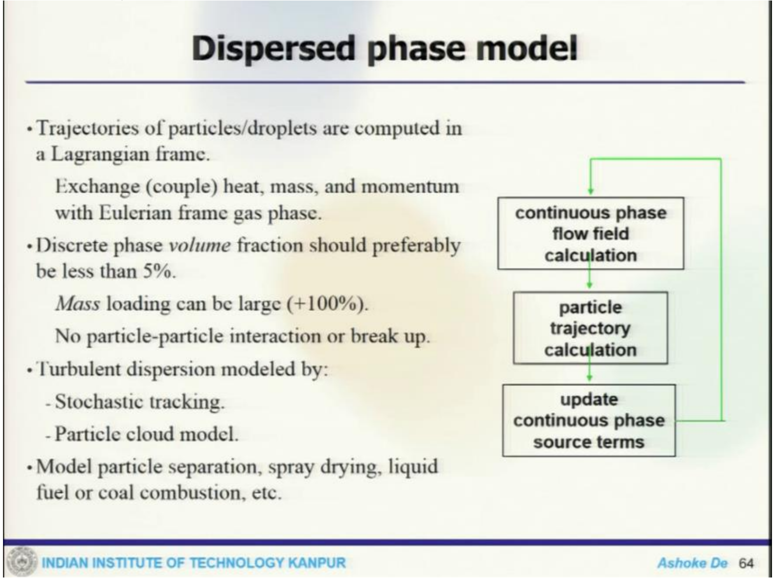

Dispersed phase model

- Trajectories of particles/droplets are computed in a Lagrangian frame.
  Exchange (couple) heat, mass, and momentum with Eulerian frame gas phase.
- Discrete phase *volume* fraction should preferably be less than 5%.
  Mass loading can be large (+100%).
  No particle-particle interaction or break up.
- Turbulent dispersion modeled by:
  - Stochastic tracking.
  - Particle cloud model.
- Model particle separation, spray drying, liquid fuel or coal combustion, etc.

continuous phase flow field calculation

particle trajectory calculation

update continuous phase source terms

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Now, we can start looking at the background on the descriptors model or DPM model the trajectory of particles or droplets are computed in Lagrangian frame. So, this is the trajectory and then we have calculators of coupling these particle to gas phase and now we can update the continuous space host term and move to the continuous phase calculation that there are certain specific requirements one has to keep in mind, if you are using the descriptors model.

It is I mean recommended that you keep your volume fraction less than 10%. So, the reason for that is because the displacement model does not take into account any particle-particle interaction. So, particle do not know about the another and if you are at a volume fraction much higher than 10% then the influence of particle interaction may become significant, which can alter them.

So, this is what you can calculate the trajectories in the heat and mass transfer receive volume fraction should be preferably less than 5%. So mass loading can be large, no particle-particle interaction or breakup. So, turbulent dispersion can be handled by stochastic tracking and multiple cloud model. So, the model particle separations, spray drying and all these things.

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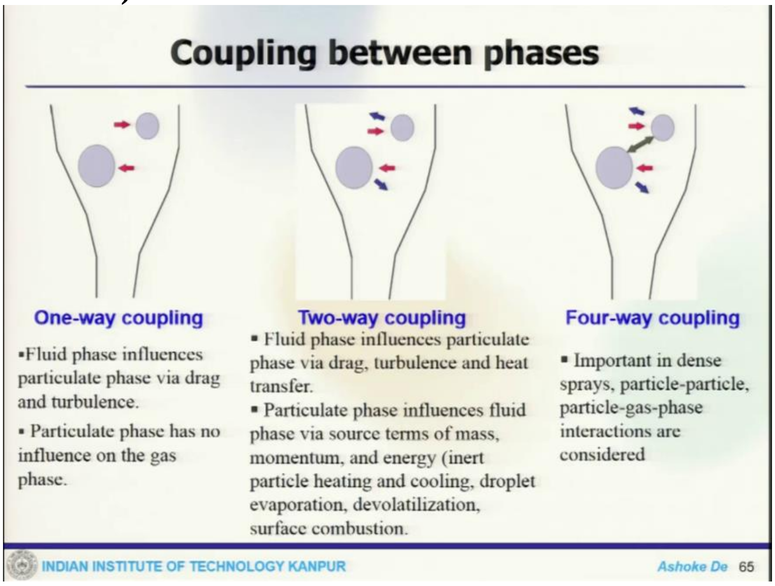

Coupling between phases

One-way coupling

- Fluid phase influences particulate phase via drag and turbulence.
- Particulate phase has no influence on the gas phase.

Two-way coupling

- Fluid phase influences particulate phase via drag, turbulence and heat transfer.
- Particulate phase influences fluid phase via source terms of mass, momentum, and energy (inert particle heating and cooling, droplet evaporation, devolatilization, surface combustion.

Four-way coupling

- Important in dense sprays, particle-particle, particle-gas-phase interactions are considered

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Now, the coupling process there could be one way coupling where fluid flow fluid phase influences a particular phase by a drag and turbulence. Particular phase has no influence or 2-way coupling where both fluid phase is influencing the liquid phase and the liquid phase also influencing the fluid phase. And 4 way coupling, so, this is dense sprays, particle-particle, particle-gas-phase and all these introductions are important.

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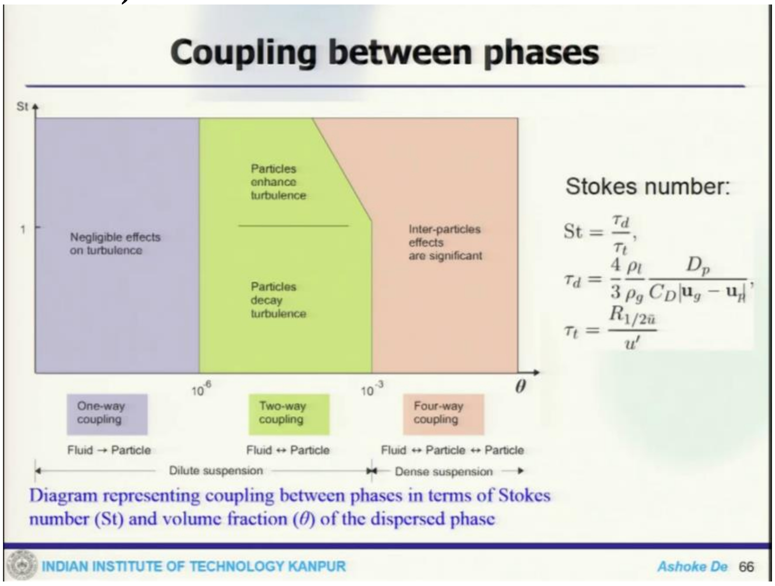

Coupling between phases

Stokes number:

$$\mathrm{St} = \frac{\tau_d}{\tau_t},$$

$$\tau_d = \frac{4}{3}\frac{\rho_l}{\rho_g}\frac{D_p}{C_D|\mathbf{u}_g - \mathbf{u}_p|},$$

$$\tau_t = \frac{R_{1/2\bar{u}}}{u'}$$

Diagram representing coupling between phases in terms of Stokes number (St) and volume fraction (θ) of the dispersed phase

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So, there are multiple ways one can couple this and this picture will give you an idea where you have a negligible effect of turbulence which is one way coupling and this is where particle enhanced turbulence, particle decay turbulence, so, this is 2-way coupling in particular interaction. So, these zone goes to dilute spray or dilute suspension and this is where the 4 way coupling is important in the dense region. So, there are Stokes number and the timescale of all this can be correlated.

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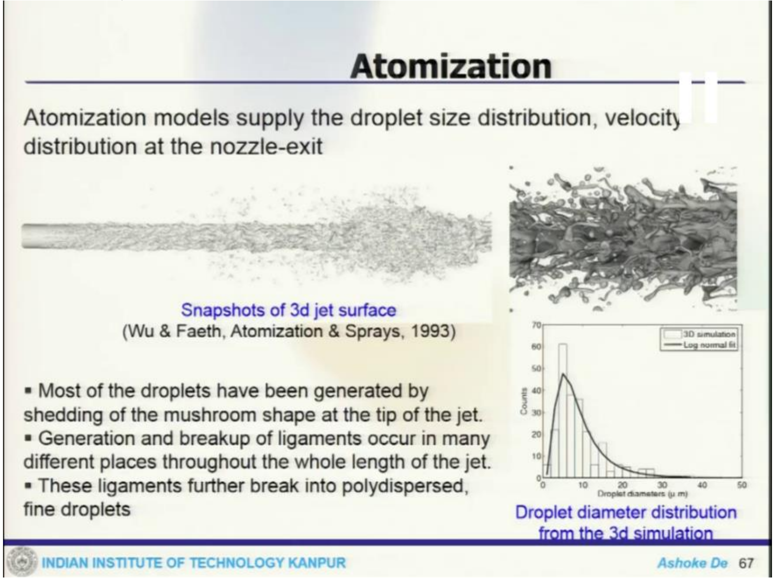

Atomization

Atomization models supply the droplet size distribution, velocity distribution at the nozzle-exit

Snapshots of 3d jet surface
(Wu & Faeth, Atomization & Sprays, 1993)

- Most of the droplets have been generated by shedding of the mushroom shape at the tip of the jet.
- Generation and breakup of ligaments occur in many different places throughout the whole length of the jet.
- These ligaments further break into polydispersed, fine droplets

Droplet diameter distribution from the 3d simulation

Now, atomization being show important one can look at this snapshot when it comes out of a nozzle-exit how it goes through. So, there is the initial sheet and then slowly becomes and then and this is how the droplet diameter distribution in that frame. So, this most of the droplets have been generated by shedding of mushroom shape a generation of the breakup of ligaments occur in many different places throughout the whole length of the jet.

These ligaments further break into poly dispersed, fine droplets. So, basically liquid comes in, there is a ligament and all these.

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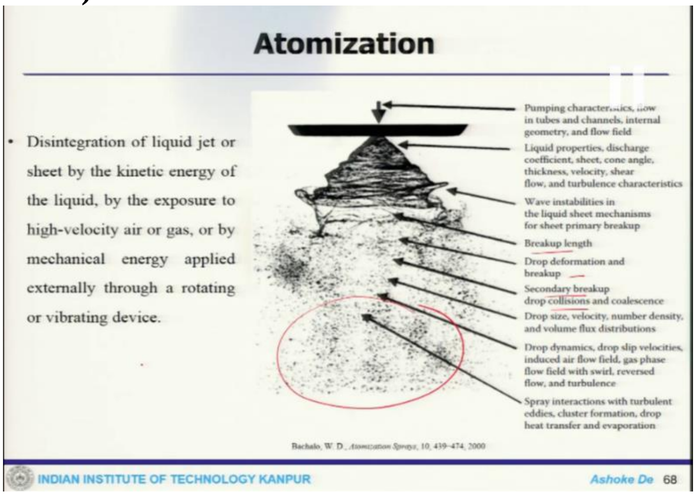

Atomization

- Disintegration of liquid jet or sheet by the kinetic energy of the liquid, by the exposure to high-velocity air or gas, or by mechanical energy applied externally through a rotating or vibrating device.

Pumping characteristics, flow in tubes and channels, internal geometry, and flow field

Liquid properties, discharge coefficient, sheet, cone angle, thickness, velocity, shear flow, and turbulence characteristics

Wave instabilities in the liquid sheet mechanisms for sheet primary breakup

Breakup length

Drop deformation and breakup

Secondary breakup drop collisions and coalescence

Drop size, velocity, number density, and volume flux distributions

Drop dynamics, drop slip velocities, induced air flow field, gas phase flow field with swirl, reversed flow, and turbulence

Spray interactions with turbulent eddies, cluster formation, drop heat transfer and evaporation

Bachalo, W. D., *Atomization Sprays*, 10, 439-474, 2000

So, this picture shows you more details, this is how it comes in then goes through like these and finally, you get this fine setup space. So, there is a primary breakup, there is a breakup length formation, secondary breakup and drop Collision. So everything is included. So, this integration of liquid jet or the seed by can emit kinetic energy of the liquid. So, do which is exposure to the high velocity air or gas or by mechanical energy.

So, this gives you an idea when the liquid is actually injected, what kind of process it goes through and what is them.

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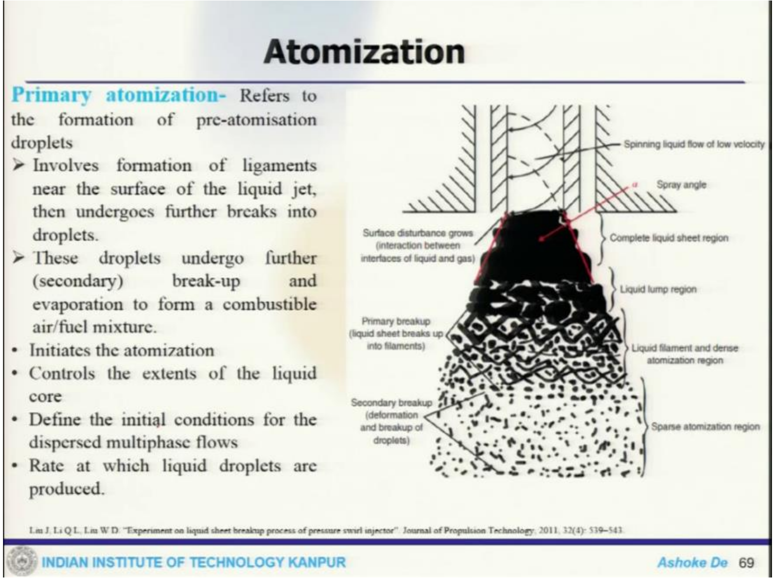

Atomization

Primary atomization- Refers to the formation of pre-atomisation droplets

- ➢ Involves formation of ligaments near the surface of the liquid jet, then undergoes further breaks into droplets.
- ➢ These droplets undergo further (secondary) break-up and evaporation to form a combustible air/fuel mixture.
- Initiates the atomization
- Controls the extents of the liquid core
- Define the initial conditions for the dispersed multiphase flows
- Rate at which liquid droplets are produced.

Liu J, Li Q L, Liu W D. "Experiment on liquid sheet breakup process of pressure swirl injector". Journal of Propulsion Technology, 2011, 32(4): 539–543.

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Now the primary atomization, which actually involves the formation of the ligament near the surface of the liquid jet and undergoes further breakup, these droplet undergo secondary breakup and then fuel mixture initiate the atomization controls the exit of the liquid core. So, now, this is how the sheet region the lump regions in the filament region and then the atomization which takes place.

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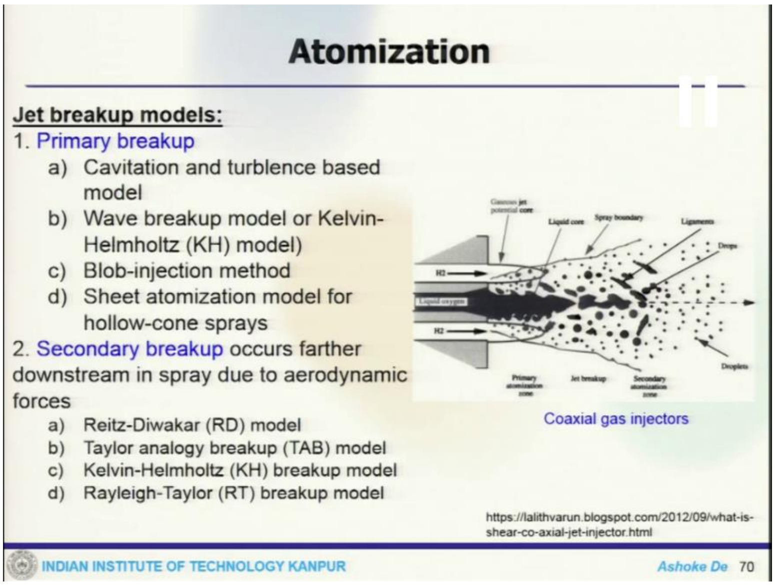

Atomization

Jet breakup models:

1. Primary breakup
    a) Cavitation and turblence based model
    b) Wave breakup model or Kelvin-Helmholtz (KH) model)
    c) Blob-injection method
    d) Sheet atomization model for hollow-cone sprays
2. Secondary breakup occurs farther downstream in spray due to aerodynamic forces
    a) Reitz-Diwakar (RD) model
    b) Taylor analogy breakup (TAB) model
    c) Kelvin-Helmholtz (KH) breakup model
    d) Rayleigh-Taylor (RT) breakup model

Coaxial gas injectors

https://lalithvarun.blogspot.com/2012/09/what-is-shear-co-axial-jet-injector.html

Now, there are jet breakup models in the primary breakup there could be cavitation and turbulence model, wave breakup models or Kelvin Helmholtz model, Blob-injection or sheet atomization model and there is another one which is quite popular this is a lesser. Secondary occurs downstream in the spray. So, this is the spray boundary this is somewhat the secondary breakup this is the primary breakup zone. So, Reitz-Diwakar model, TAB Model, Kelvin-Helmholtz Rayleigh-Taylor breakup model.

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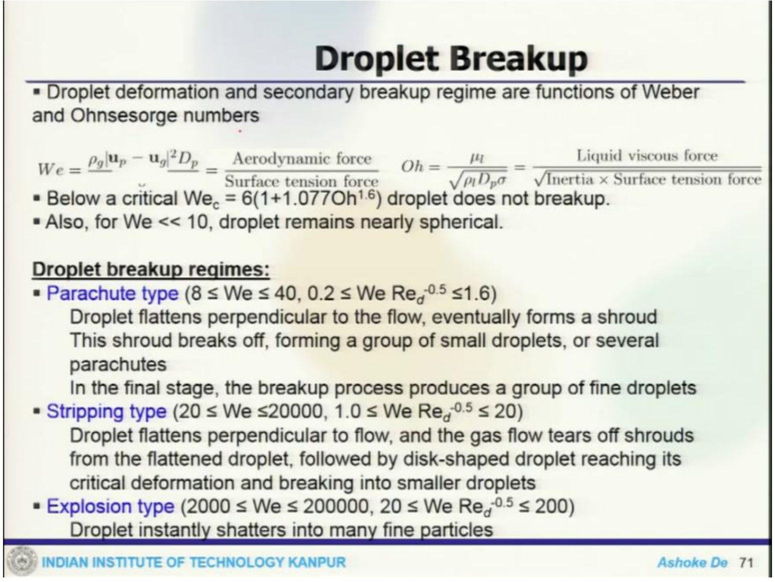

Droplet Breakup

- Droplet deformation and secondary breakup regime are functions of Weber and Ohnsesorge numbers

$$We = \frac{\rho_g |\mathbf{u}_p - \mathbf{u}_g|^2 D_p}{\sigma} = \frac{\text{Aerodynamic force}}{\text{Surface tension force}} \qquad Oh = \frac{\mu_l}{\sqrt{\rho_l D_p \sigma}} = \frac{\text{Liquid viscous force}}{\sqrt{\text{Inertia} \times \text{Surface tension force}}}$$

- Below a critical $We_c = 6(1+1.077Oh^{1.6})$ droplet does not breakup.
- Also, for We << 10, droplet remains nearly spherical.

Droplet breakup regimes:

- Parachute type ($8 \le We \le 40$, $0.2 \le We\, Re_d^{-0.5} \le 1.6$)
  Droplet flattens perpendicular to the flow, eventually forms a shroud
  This shroud breaks off, forming a group of small droplets, or several parachutes
  In the final stage, the breakup process produces a group of fine droplets
- Stripping type ($20 \le We \le 20000$, $1.0 \le We\, Re_d^{-0.5} \le 20$)
  Droplet flattens perpendicular to flow, and the gas flow tears off shrouds from the flattened droplet, followed by disk-shaped droplet reaching its critical deformation and breaking into smaller droplets
- Explosion type ($2000 \le We \le 200000$, $20 \le We\, Re_d^{-0.5} \le 200$)
  Droplet instantly shatters into many fine particles

So, these is the droplet formation and secondary breakup regime or function of the Weber and Ohnsesorge numbers. So, this is the weber number which is a proportionate to aerodynamics force to the surface tension force and which is liquid viscous force to surface tension force. So, the droplet breakup regimes there could be a parachute type with a droplet flattens. So, it depends on the Weber number range of the flow eventually forms a shroud there could be stripping type or the droplet flattens perpendicular to flow and the gas flow tears the shroud and explosion type.

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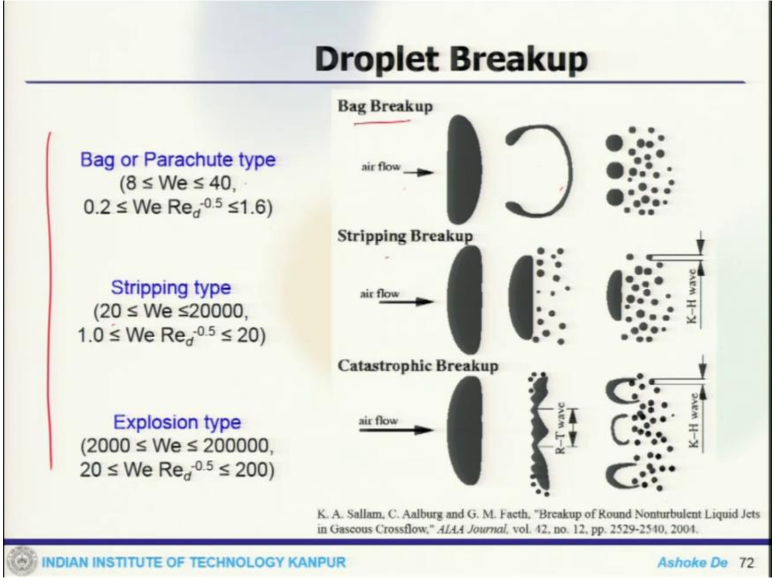

Droplet Breakup

Bag or Parachute type
($8 \le We \le 40$,
$0.2 \le We\, Re_d^{-0.5} \le 1.6$)

Stripping type
($20 \le We \le 20000$,
$1.0 \le We\, Re_d^{-0.5} \le 20$)

Explosion type
($2000 \le We \le 200000$,
$20 \le We\, Re_d^{-0.5} \le 200$)

K. A. Sallam, C. Aalburg and G. M. Faeth, "Breakup of Round Nonturbulent Liquid Jets in Gaseous Crossflow," *AIAA Journal*, vol. 42, no. 12, pp. 2529-2540, 2004.

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So, this picture will give you an idea. This is a bag breakup or the parachute type whether Weber number is like this, the air comes in and this kind of breakup takes place. Now, the stripping breakup this is a Weber number of 20 to 20,000 for these kind of breakups are the catastrophic breakup or which is they occur or explosion type. So, depending on the weber number, so, this is a very important non-dimensional number, which plays an important role in the atomization model.

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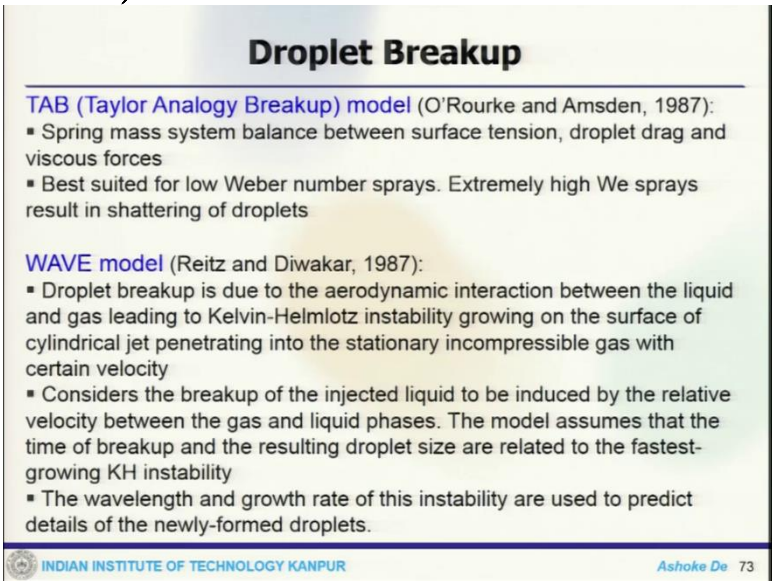

Droplet Breakup

TAB (Taylor Analogy Breakup) model (O'Rourke and Amsden, 1987):
- Spring mass system balance between surface tension, droplet drag and viscous forces
- Best suited for low Weber number sprays. Extremely high We sprays result in shattering of droplets

WAVE model (Reitz and Diwakar, 1987):
- Droplet breakup is due to the aerodynamic interaction between the liquid and gas leading to Kelvin-Helmlotz instability growing on the surface of cylindrical jet penetrating into the stationary incompressible gas with certain velocity
- Considers the breakup of the injected liquid to be induced by the relative velocity between the gas and liquid phases. The model assumes that the time of breakup and the resulting droplet size are related to the fastest-growing KH instability
- The wavelength and growth rate of this instability are used to predict details of the newly-formed droplets.

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Now, the TAB model this is proposed by O’Rourke on 1987. This is spring mass system balance between surface tension, droplet drag and the viscous forces. So, it is best suited for low Weber number sprays. Extremely high weber number sprays result in shattering of droplets. Now, the wave model here the droplet backup is due to aerodynamic interaction between the liquid and the gas leading to Kelvin-Helmholtz instability which is growing to the surface of the cylindrical jet here that it considers the breakup of the injected liquid to be induced by the relative velocity between the gas and the liquid phases and the model assumes that the time of breakup and the resulting droplet size that related to the KH instability growth.

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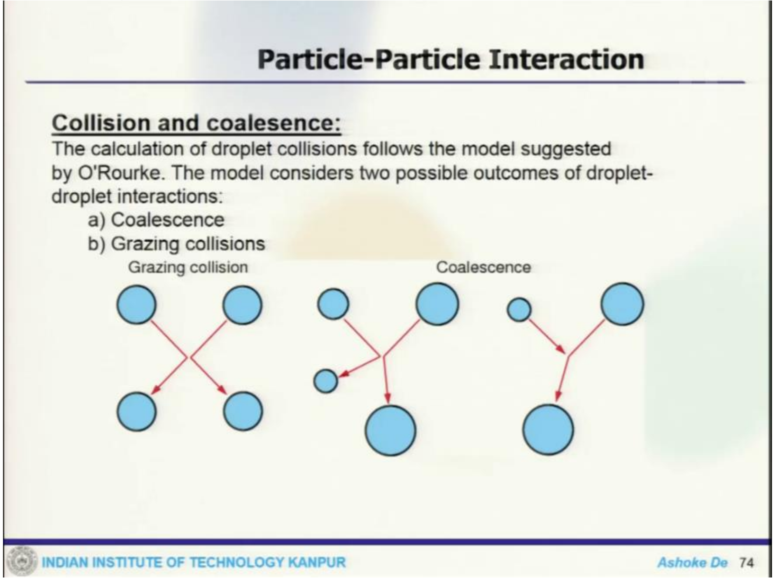

Particle-Particle Interaction

Collision and coalescence:

The calculation of droplet collisions follows the model suggested by O'Rourke. The model considers two possible outcomes of droplet-droplet interactions:

a) Coalescence
b) Grazing collisions

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So, here the collision and the coalescence. This is based on either there could be collisions or there could be grazing collisions. So the collision occurs if the impact parameter is lower than the critical value. So, the number of collisions for each collector is then found and used. Now, the diameter velocity temperature of the collected drop after coalescence is calculated from mass, momentum and energy conservation.

If the original number of the droplet in the droplet parcel is lower or equal to the droplet parcel is removed from the calculus, now, when you come to the regime calculation, collision, if the impact parameter is bigger than the critical value, so, the grazing collision usually occur between droplets of approximately equal sizes, when grazing collision occurs only momentum is exchanged between the droplets and the droplet diameters and temperature disagreements and change. So, this is what the actually the situation.

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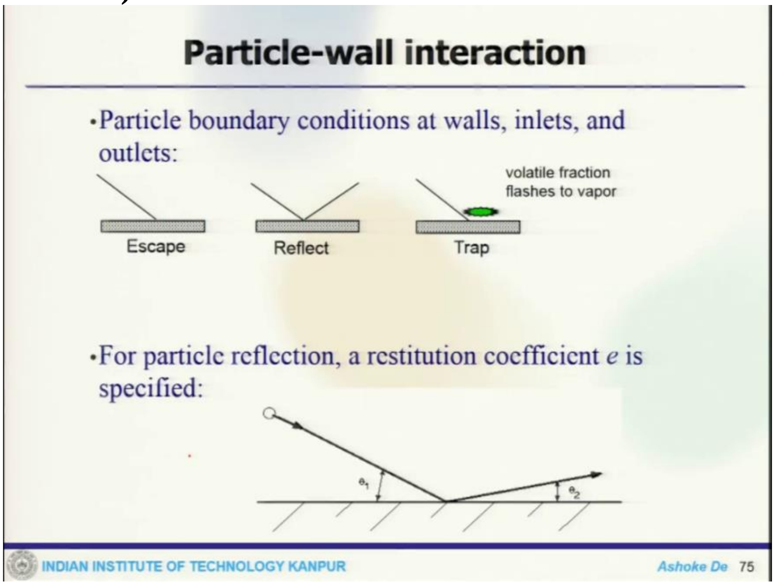

Particle-wall interaction

- Particle boundary conditions at walls, inlets, and outlets:

- For particle reflection, a restitution coefficient e is specified:

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Now, there could be particle conditions at walls so, it could escape or when it hits the wall it could reflect on this could be trapped. So, the particle the restitution coefficient can be specified and it can be estimated.

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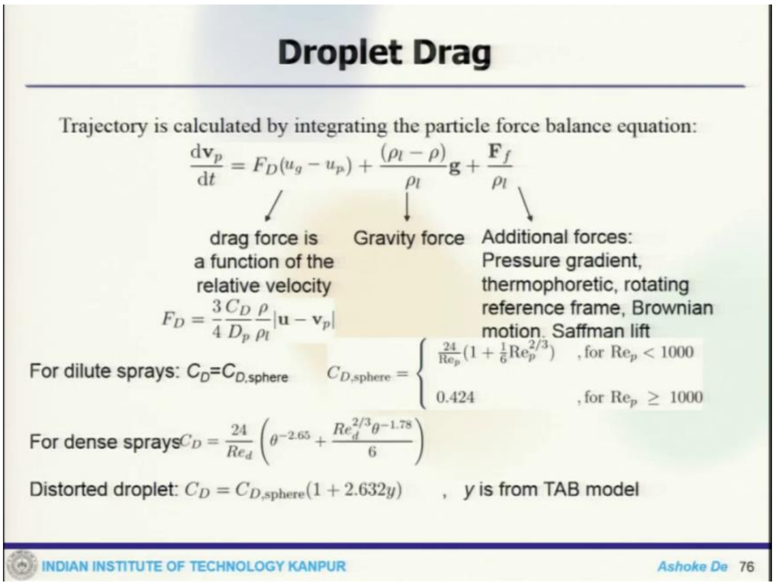

Droplet Drag

Trajectory is calculated by integrating the particle force balance equation:

$$\frac{d\mathbf{v}_p}{dt} = F_D(u_g - u_p) + \frac{(\rho_l - \rho)}{\rho_l}\mathbf{g} + \frac{\mathbf{F}_f}{\rho_l}$$

drag force is a function of the relative velocity

Gravity force

Additional forces: Pressure gradient, thermophoretic, rotating reference frame, Brownian motion. Saffman lift

$$F_D = \frac{3}{4}\frac{C_D}{D_p}\frac{\rho}{\rho_l}|\mathbf{u} - \mathbf{v}_p|$$

For dilute sprays: $C_D = C_{D,\text{sphere}}$ $\quad C_{D,\text{sphere}} = \begin{cases} \frac{24}{\text{Re}_p}\left(1 + \frac{1}{6}\text{Re}_p^{2/3}\right) & \text{, for Re}_p < 1000 \\ 0.424 & \text{, for Re}_p \geq 1000 \end{cases}$

For dense sprays $C_D = \frac{24}{Re_d}\left(\theta^{-2.65} + \frac{Re_d^{2/3}\theta^{-1.78}}{6}\right)$

Distorted droplet: $C_D = C_{D,\text{sphere}}(1 + 2.632y)$, y is from TAB model

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Now, that trajectory is calculated by integrating the particle force balance. So, this is the drag force, gravity force additional force due to pressure gradient, thermophoretic, rotating frame and then the dilute spray the C_D would be like this. Dense spray the C_D. So, these are the correlation, which are available in literature which is very common.

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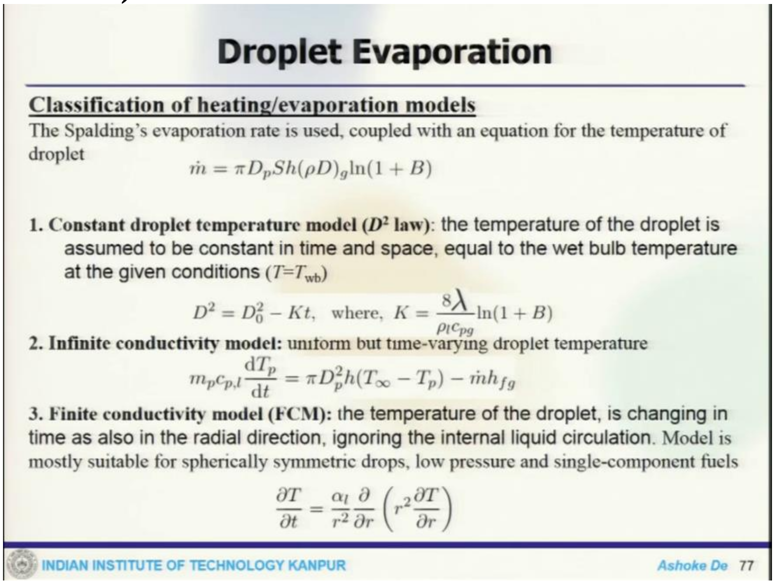

Droplet Evaporation

Classification of heating/evaporation models

The Spalding's evaporation rate is used, coupled with an equation for the temperature of droplet

$$\dot{m} = \pi D_p Sh(\rho D)_g \ln(1+B)$$

1. **Constant droplet temperature model (D^2 law)**: the temperature of the droplet is assumed to be constant in time and space, equal to the wet bulb temperature at the given conditions (T=T_{wb})

$$D^2 = D_0^2 - Kt, \quad \text{where,} \quad K = \frac{8\lambda}{\rho_l c_{pg}} \ln(1+B)$$

2. **Infinite conductivity model:** uniform but time-varying droplet temperature

$$m_p c_{p,l} \frac{\mathrm{d}T_p}{\mathrm{d}t} = \pi D_p^2 h(T_\infty - T_p) - \dot{m} h_{fg}$$

3. **Finite conductivity model (FCM):** the temperature of the droplet, is changing in time as also in the radial direction, ignoring the internal liquid circulation. Model is mostly suitable for spherically symmetric drops, low pressure and single-component fuels

$$\frac{\partial T}{\partial t} = \frac{\alpha_l}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right)$$

Now, the collision of heating and evaporation models so, you can have Spalding say of evaporation models like this the constant droplet temperature model D2 law, the infinite conductivity model or finite conductivity model.

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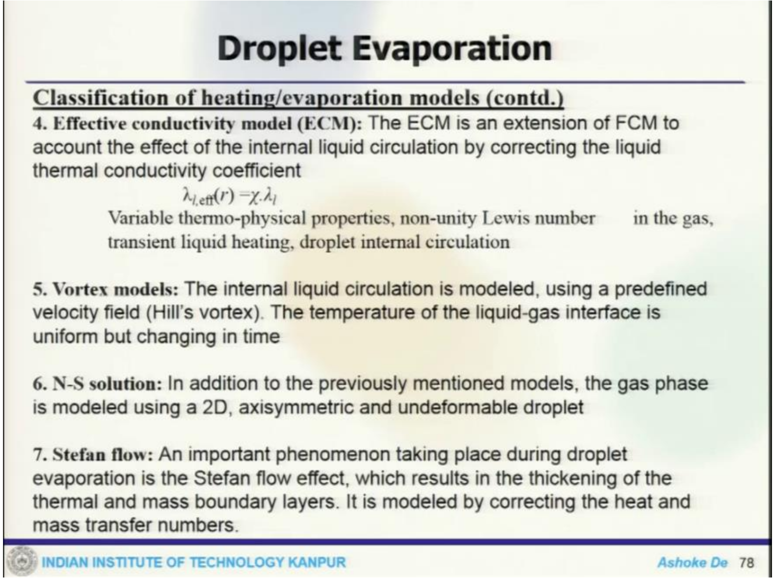

Droplet Evaporation

Classification of heating/evaporation models (contd.)

4. **Effective conductivity model (ECM):** The ECM is an extension of FCM to account the effect of the internal liquid circulation by correcting the liquid thermal conductivity coefficient

$$\lambda_{l,\text{eff}}(r) = \chi . \lambda_l$$

Variable thermo-physical properties, non-unity Lewis number in the gas, transient liquid heating, droplet internal circulation

5. **Vortex models:** The internal liquid circulation is modeled, using a predefined velocity field (Hill's vortex). The temperature of the liquid-gas interface is uniform but changing in time

6. **N-S solution:** In addition to the previously mentioned models, the gas phase is modeled using a 2D, axisymmetric and undeformable droplet

7. **Stefan flow:** An important phenomenon taking place during droplet evaporation is the Stefan flow effect, which results in the thickening of the thermal and mass boundary layers. It is modeled by correcting the heat and mass transfer numbers.

These are also well established or effective conducting model where the ECM is an extension of FCM amount of the internal liquid circulation there could be vortex models the internal liquid circulation is modelled using a predefined defined velocity field hills vortex or NS solution or Stefan flow. So, these are some of the ways one can classify the heating or evaporation models.

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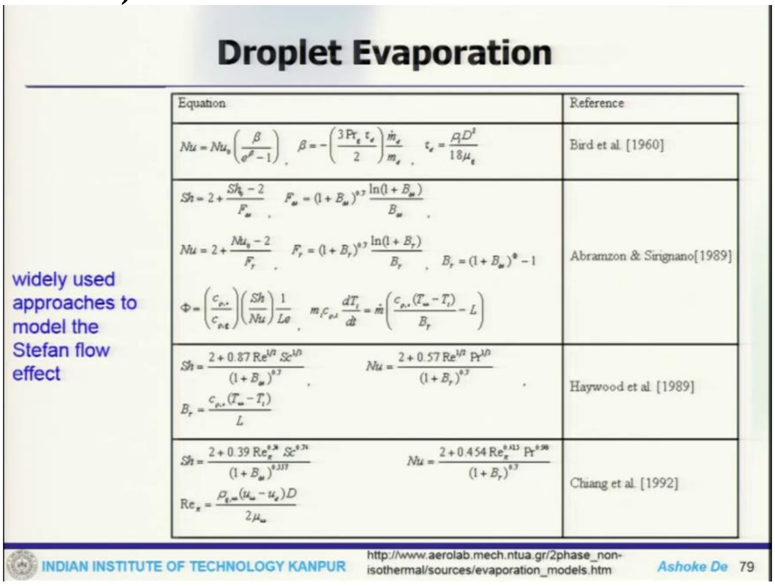

Droplet Evaporation

widely used approaches to model the Stefan flow effect

Equation	Reference
$Nu = Nu_0\left(\frac{\beta}{e^{\beta}-1}\right)$, $\beta = -\left(\frac{3\,\mathrm{Pr}_g\,\tau_d}{2}\right)\frac{\dot{m}_d}{m_d}$, $\tau_d = \frac{\rho_l D^2}{18\mu_g}$	Bird et al. [1960]
$Sh = 2 + \frac{Sh_0 - 2}{F_M}$, $F_M = (1+B_M)^{0.7}\frac{\ln(1+B_M)}{B_M}$, $Nu = 2 + \frac{Nu_0 - 2}{F_T}$, $F_T = (1+B_T)^{0.7}\frac{\ln(1+B_T)}{B_T}$, $B_T = (1+B_M)^{\Phi} - 1$ $\Phi = \left(\frac{c_{p,v}}{c_{p,g}}\right)\left(\frac{Sh}{Nu}\right)\frac{1}{Le}$, $m_l c_{p,l}\frac{dT_l}{dt} = \dot{m}\left(\frac{c_{p,v}(T_\infty - T_l)}{B_T} - L\right)$	Abramzon & Sirignano[1989]
$Sh = \frac{2 + 0.87\,\mathrm{Re}^{1/2}\,Sc^{1/3}}{(1+B_M)^{0.7}}$, $Nu = \frac{2 + 0.57\,\mathrm{Re}^{1/2}\,\mathrm{Pr}^{1/3}}{(1+B_T)^{0.7}}$. $B_T = \frac{c_{p,v}(T_\infty - T_l)}{L}$	Haywood et al. [1989]
$Sh = \frac{2 + 0.39\,\mathrm{Re}_g^{0.54}\,Sc^{0.76}}{(1+B_M)^{0.357}}$ $Nu = \frac{2 + 0.454\,\mathrm{Re}_g^{0.425}\,\mathrm{Pr}^{0.98}}{(1+B_T)^{0.7}}$ $\mathrm{Re}_g = \frac{\rho_{g,\infty}(u_\infty - u_d)D}{2\mu_\infty}$	Chiang et al. [1992]

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And these are now the widely used approaches to model the Stefan flow effect. So, these are the equations and this is the source of the information where you can see who has proposed based on what kind of these things.

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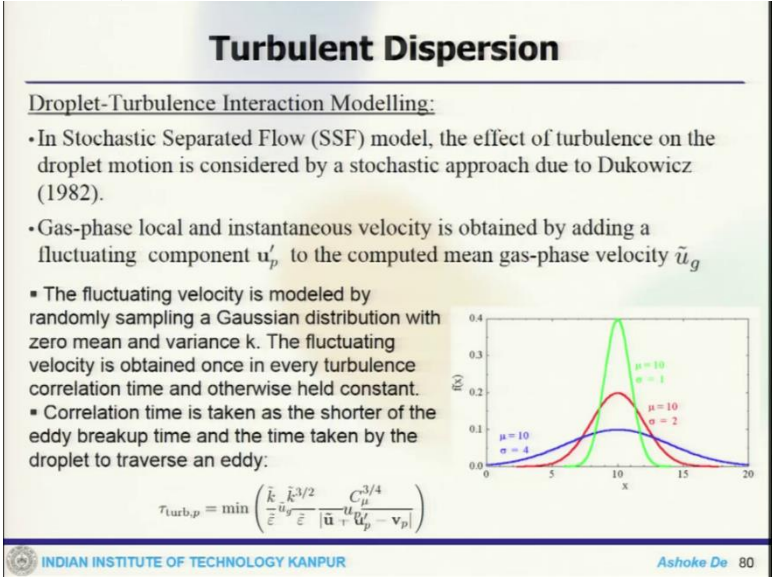

Turbulent Dispersion

Droplet-Turbulence Interaction Modelling:

- In Stochastic Separated Flow (SSF) model, the effect of turbulence on the droplet motion is considered by a stochastic approach due to Dukowicz (1982).
- Gas-phase local and instantaneous velocity is obtained by adding a fluctuating component $\mathbf{u}'_p$ to the computed mean gas-phase velocity $\tilde{u}_g$
  - The fluctuating velocity is modeled by randomly sampling a Gaussian distribution with zero mean and variance k. The fluctuating velocity is obtained once in every turbulence correlation time and otherwise held constant.
  - Correlation time is taken as the shorter of the eddy breakup time and the time taken by the droplet to traverse an eddy:

$$\tau_{\mathrm{turb},p} = \min\left(\frac{\tilde{k}}{\tilde{\varepsilon}}\tilde{u}_g \frac{\tilde{k}^{3/2}}{\tilde{\varepsilon}} \frac{C_\mu^{3/4}}{|\tilde{\mathbf{u}} + \mathbf{u}'_p - \mathbf{v}_p|} u_p\right)$$

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Now, the important thing is the interaction between droplet and turbulence. Now, the stochastic separated flow model or a SSF model, the effect of turbulence only droplet motion is considered by a stochastic approach due to Dukowicz and then the gas-phase is local and instantaneous velocity is often by adding the fluctuation component. So, then you can see how these turbulent timescale is actually. So, it is assumed by randomly sampling Gaussian distribution and then calculated.

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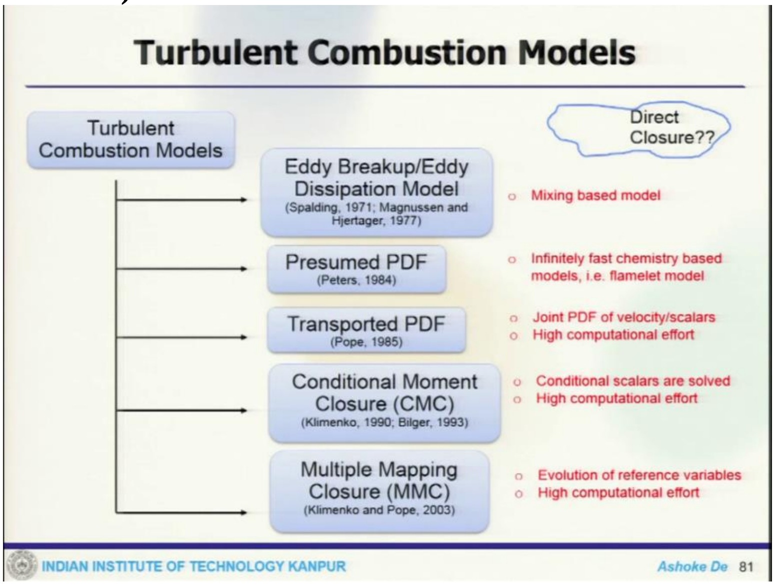

Turbulent Combustion Models

Turbulent Combustion Models

Direct Closure??

- Eddy Breakup/Eddy Dissipation Model (Spalding, 1971; Magnussen and Hjertager, 1977)
  - Mixing based model
- Presumed PDF (Peters, 1984)
  - Infinitely fast chemistry based models, i.e. flamelet model
- Transported PDF (Pope, 1985)
  - Joint PDF of velocity/scalars
  - High computational effort
- Conditional Moment Closure (CMC) (Klimenko, 1990; Bilger, 1993)
  - Conditional scalars are solved
  - High computational effort
- Multiple Mapping Closure (MMC) (Klimenko and Pope, 2003)
  - Evolution of reference variables
  - High computational effort

These are the different turbulent combustion model where we already have Eddy breakup, presumed PDF, transported PDF model. So, these are the 2 advanced models which are conditional moment closure for the conditional scalars are solved high computational effort evolution of reference variables and high computational effort.

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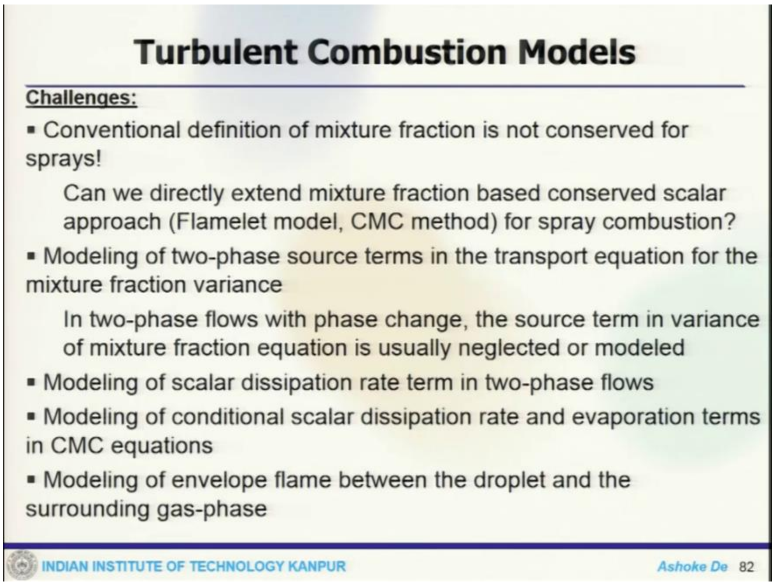

Turbulent Combustion Models

Challenges:

- Conventional definition of mixture fraction is not conserved for sprays!

  Can we directly extend mixture fraction based conserved scalar approach (Flamelet model, CMC method) for spray combustion?
- Modeling of two-phase source terms in the transport equation for the mixture fraction variance

  In two-phase flows with phase change, the source term in variance of mixture fraction equation is usually neglected or modeled
- Modeling of scalar dissipation rate term in two-phase flows
- Modeling of conditional scalar dissipation rate and evaporation terms in CMC equations
- Modeling of envelope flame between the droplet and the surrounding gas-phase

Now, the challenges your conventional definition of mixture fraction and is not conserved for sprays. So, we can directly extend mixture fraction based on the conserved scalar approach to CMC and all these. Now 2-phase source terms in the transport equation for mixture fraction variance. So, scalar dissipation rate is another thing and flame envelope and all these things.

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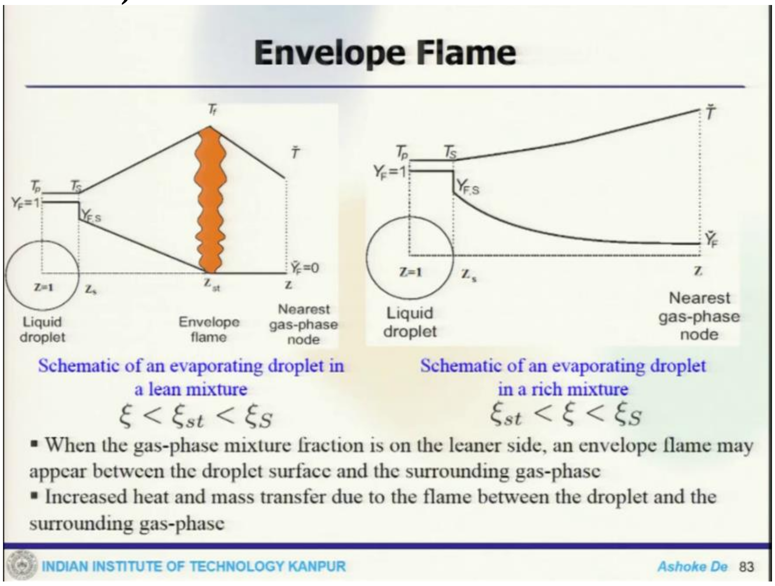

Envelope Flame

Schematic of an evaporating droplet in a lean mixture

$$\xi < \xi_{st} < \xi_S$$

Schematic of an evaporating droplet in a rich mixture

$$\xi_{st} < \xi < \xi_S$$

- When the gas-phase mixture fraction is on the leaner side, an envelope flame may appear between the droplet surface and the surrounding gas-phase
- Increased heat and mass transfer due to the flame between the droplet and the surrounding gas-phase

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So, flame envelope one can look at these things.

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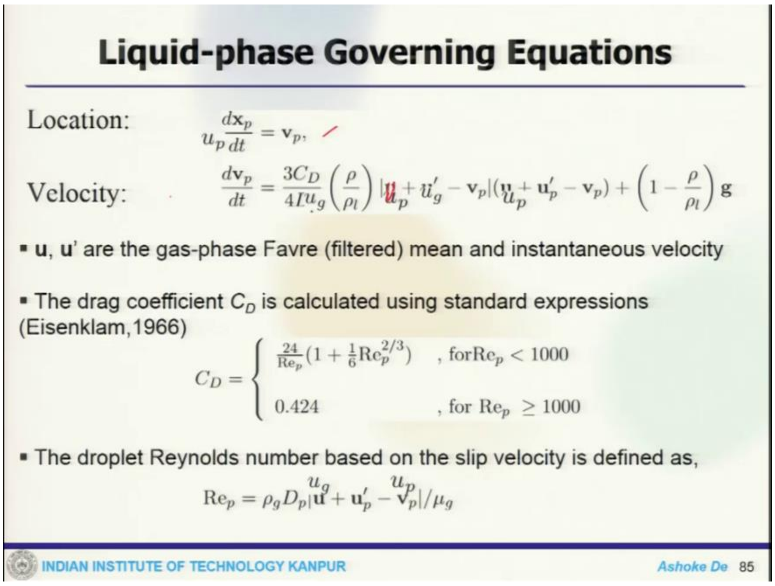

Liquid-phase Governing Equations

Location: $u_p\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p,$

Velocity: $\frac{d\mathbf{v}_p}{dt} = \frac{3C_D}{4Iu_g}\left(\frac{\rho}{\rho_l}\right)|\underset{u_p}{\mathbf{u}} + u'_g - \mathbf{v}_p|(\underset{u_p}{\mathbf{u}} + \mathbf{u}'_p - \mathbf{v}_p) + \left(1 - \frac{\rho}{\rho_l}\right)\mathbf{g}$

- **u**, **u'** are the gas-phase Favre (filtered) mean and instantaneous velocity
- The drag coefficient C_D is calculated using standard expressions (Eisenklam,1966)

$$C_D = \begin{cases} \frac{24}{Re_p}(1 + \frac{1}{6}Re_p^{2/3}) & , \text{for} Re_p < 1000 \\ 0.424 & , \text{for } Re_p \geq 1000 \end{cases}$$

- The droplet Reynolds number based on the slip velocity is defined as,

$$Re_p = \rho_g D_p|\overset{u_g}{\mathbf{u}} + \mathbf{u}'_p - \overset{u_p}{\mathbf{v}_p}|/\mu_g$$

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Now, we can quickly go through the RANS and LES of spray combustion what is available or what have been people doing it. This is the particle upload their locations and their velocity how it is estimated. So, this is up then you can get the drag coefficient like this and this is the droplet Reynolds number.

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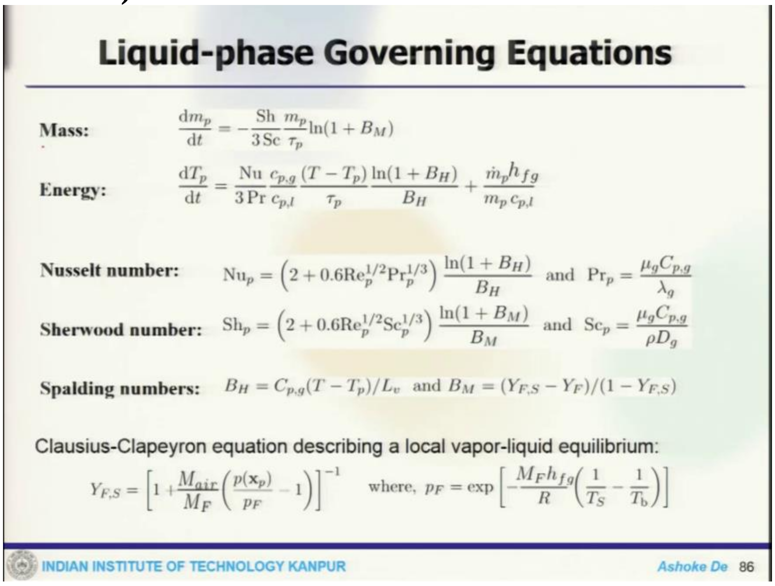

Liquid-phase Governing Equations

Mass: $$\frac{\mathrm{d}m_p}{\mathrm{d}t} = -\frac{\mathrm{Sh}}{3\,\mathrm{Sc}}\frac{m_p}{\tau_p}\ln(1+B_M)$$

Energy: $$\frac{\mathrm{d}T_p}{\mathrm{d}t} = \frac{\mathrm{Nu}}{3\,\mathrm{Pr}}\frac{c_{p,g}}{c_{p,l}}\frac{(T-T_p)}{\tau_p}\frac{\ln(1+B_H)}{B_H} + \frac{\dot{m}_p h_{fg}}{m_p c_{p,l}}$$

Nusselt number: $$\mathrm{Nu}_p = \left(2+0.6\mathrm{Re}_p^{1/2}\mathrm{Pr}_p^{1/3}\right)\frac{\ln(1+B_H)}{B_H} \quad \text{and} \quad \mathrm{Pr}_p = \frac{\mu_g C_{p,g}}{\lambda_g}$$

Sherwood number: $$\mathrm{Sh}_p = \left(2+0.6\mathrm{Re}_p^{1/2}\mathrm{Sc}_p^{1/3}\right)\frac{\ln(1+B_M)}{B_M} \quad \text{and} \quad \mathrm{Sc}_p = \frac{\mu_g C_{p,g}}{\rho D_g}$$

Spalding numbers: $$B_H = C_{p,g}(T-T_p)/L_v \quad \text{and} \quad B_M = (Y_{F,S}-Y_F)/(1-Y_{F,S})$$

Clausius-Clapeyron equation describing a local vapor-liquid equilibrium:

$$Y_{F,S} = \left[1+\frac{M_{air}}{M_F}\left(\frac{p(\mathbf{x}_p)}{p_F}-1\right)\right]^{-1} \quad \text{where, } p_F = \exp\left[-\frac{M_F h_{fg}}{R}\left(\frac{1}{T_S}-\frac{1}{T_b}\right)\right]$$

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Now, we have mass balance, energy balance, Nusselt number calculation, Sherwood number, Spalding number and Clausius-Clapeyron equation for vapour liquid equilibrium.

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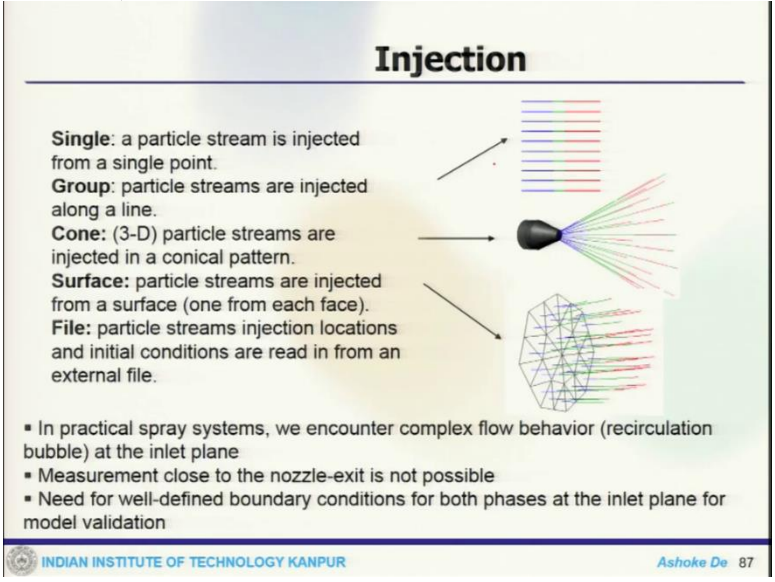

Injection

Single: a particle stream is injected from a single point.
Group: particle streams are injected along a line.
Cone: (3-D) particle streams are injected in a conical pattern.
Surface: particle streams are injected from a surface (one from each face).
File: particle streams injection locations and initial conditions are read in from an external file.

- In practical spray systems, we encounter complex flow behavior (recirculation bubble) at the inlet plane
- Measurement close to the nozzle-exit is not possible
- Need for well-defined boundary conditions for both phases at the inlet plane for model validation

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So, these are the important equations and then there could be single or group injection, how the particles are injected there could be cone injection and there could be surface injection. So, depending on that, and in practical spray systems we encounter complex flow behaviour. So, measurement close to the nozzle is not possible. So, we need well-defined boundary conditions for both phases or the inlet plane of the model validation. So, this is an important point because these measurements on these planes are not that easy.

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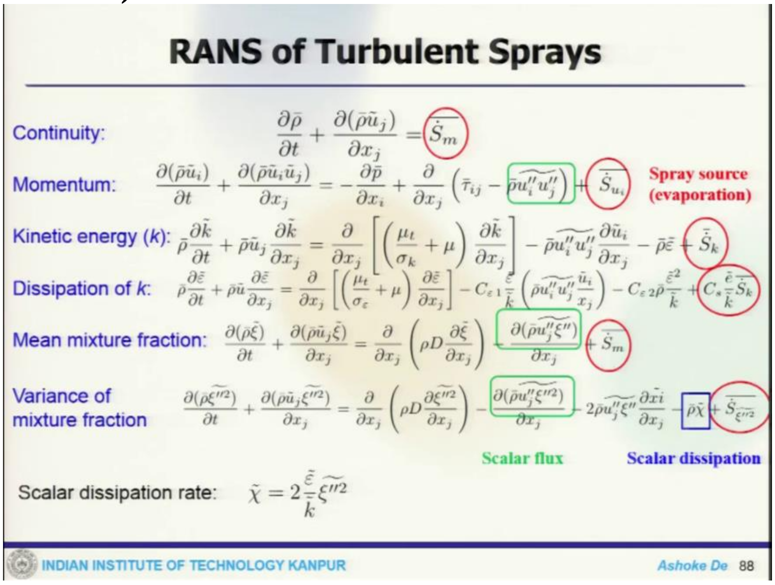

RANS of Turbulent Sprays

Continuity: $$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j)}{\partial x_j} = \boxed{\overline{\dot{S}_m}}$$

Momentum: $$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\bar{\tau}_{ij} - \boxed{\bar{\rho}\widetilde{u_i''u_j''}}\right) + \boxed{\overline{\dot{S}_{u_i}}}$$

Spray source (evaporation)

Kinetic energy (*k*): $$\bar{\rho}\frac{\partial \tilde{k}}{\partial t} + \bar{\rho}\tilde{u}_j\frac{\partial \tilde{k}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\frac{\mu_t}{\sigma_k} + \mu\right)\frac{\partial \tilde{k}}{\partial x_j}\right] - \bar{\rho}\widetilde{u_i''u_j''}\frac{\partial \tilde{u}_i}{\partial x_j} - \bar{\rho}\bar{\varepsilon} + \boxed{\overline{\dot{S}_k}}$$

Dissipation of *k*: $$\bar{\rho}\frac{\partial \bar{\varepsilon}}{\partial t} + \bar{\rho}\bar{u}\frac{\partial \bar{\varepsilon}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\frac{\mu_t}{\sigma_\varepsilon} + \mu\right)\frac{\partial \bar{\varepsilon}}{\partial x_j}\right] - C_{\varepsilon 1}\frac{\bar{\varepsilon}}{\tilde{k}}\left(\bar{\rho}\widetilde{u_i''u_j''}\frac{\tilde{u}_i}{x_j}\right) - C_{\varepsilon 2}\bar{\rho}\frac{\bar{\varepsilon}^2}{\tilde{k}} + \boxed{C_s\frac{\bar{\varepsilon}}{\tilde{k}}\overline{\dot{S}_k}}$$

Mean mixture fraction: $$\frac{\partial(\bar{\rho}\tilde{\xi})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{\xi})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D\frac{\partial \tilde{\xi}}{\partial x_j}\right) - \boxed{\frac{\partial(\bar{\rho}\widetilde{u_j''\xi''})}{\partial x_j}} + \boxed{\overline{\dot{S}_m}}$$

Variance of mixture fraction $$\frac{\partial(\bar{\rho}\widetilde{\xi''^2})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\widetilde{\xi''^2})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D\frac{\partial \widetilde{\xi''^2}}{\partial x_j}\right) - \boxed{\frac{\partial(\bar{\rho}\widetilde{u_j''\xi''^2})}{\partial x_j}} - 2\bar{\rho}\widetilde{u_j''\xi''}\frac{\partial \tilde{x}i}{\partial x_j} - \boxed{\bar{\rho}\tilde{\chi}} + \boxed{\overline{\dot{S}_{\xi''^2}}}$$

Scalar flux **Scalar dissipation**

Scalar dissipation rate: $$\tilde{\chi} = 2\frac{\bar{\varepsilon}}{\tilde{k}}\widetilde{\xi''^2}$$

These are the set of equations. So, you have continuity equation with the source term, momentum equations with spray source term, evaporation term, kinetic energy for they will be source term dissipation source term mixture fraction, there is a source term because of the second phase and variance equation also and this is your scalar. So, the equation system we have discussed in details, but what I am trying to mark here is that these are the changes that one will encounter due to the second phase.

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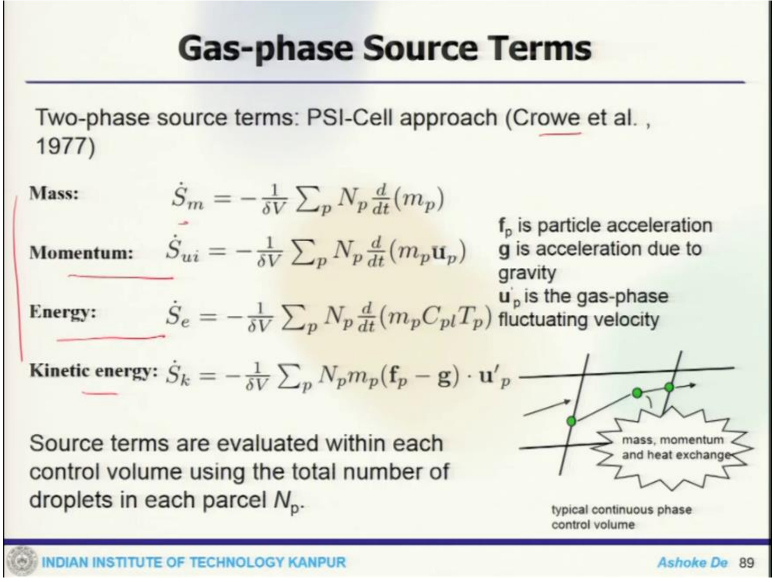

Gas-phase Source Terms

Two-phase source terms: PSI-Cell approach (Crowe et al. , 1977)

Mass: $$\dot{S}_m = -\frac{1}{\delta V}\sum_p N_p\frac{d}{dt}(m_p)$$

Momentum: $$\dot{S}_{ui} = -\frac{1}{\delta V}\sum_p N_p\frac{d}{dt}(m_p\mathbf{u}_p)$$

Energy: $$\dot{S}_e = -\frac{1}{\delta V}\sum_p N_p\frac{d}{dt}(m_pC_{pl}T_p)$$

Kinetic energy: $$\dot{S}_k = -\frac{1}{\delta V}\sum_p N_pm_p(\mathbf{f}_p - \mathbf{g}) \cdot \mathbf{u}'_p$$

$\mathbf{f}_p$ is particle acceleration
$\mathbf{g}$ is acceleration due to gravity
$\mathbf{u}'_p$ is the gas-phase fluctuating velocity

Source terms are evaluated within each control volume using the total number of droplets in each parcel N_p.

Now 2-phase, this is Crowe et al., proposed the mass is m would be number of particles and calculated momentum energy source. So, there is a fairly good amount of literature which is rather fairly established literature which is available to close those terms.

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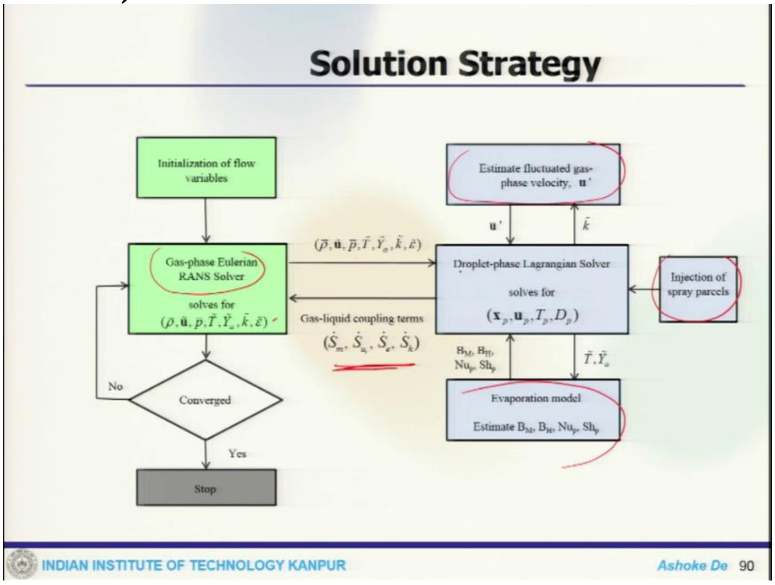

Solution Strategy

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How this things work. So, we have initialize the flow, we solve in the gas phase, then these information of the meaningful pass to the second phase, where we use the evaporation model using the midfield. If evaporation model that comes back, we use our injection of the spray then estimate the fluctuating velocity and finally, get back up and then finally, the gas liquid coupling comes the source from goes back here and again it solves.

It is gone did not stop others goes back. So, that means one and the main flow will send the information back here and then it goes back like this.

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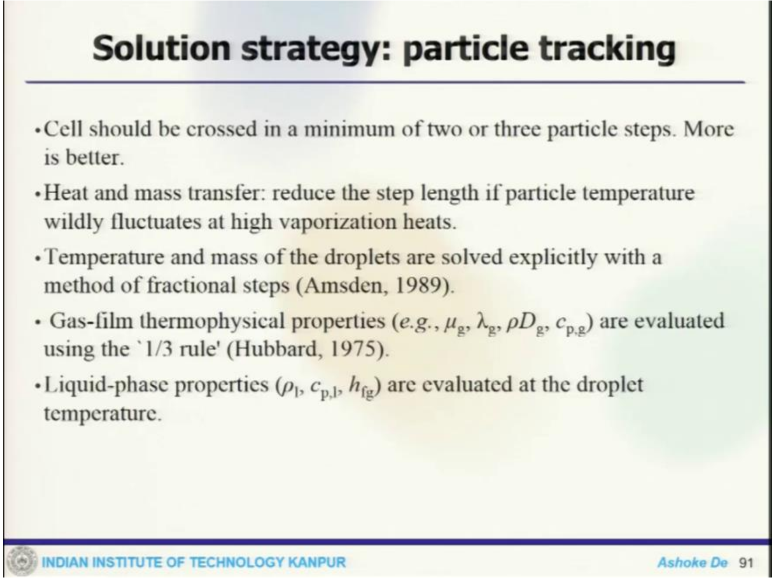

Solution strategy: particle tracking

- Cell should be crossed in a minimum of two or three particle steps. More is better.
- Heat and mass transfer: reduce the step length if particle temperature wildly fluctuates at high vaporization heats.
- Temperature and mass of the droplets are solved explicitly with a method of fractional steps (Amsden, 1989).
- Gas-film thermophysical properties (*e.g.*, μ_g, λ_g, ρD_g, $c_{p,g}$) are evaluated using the `1/3 rule' (Hubbard, 1975).
- Liquid-phase properties (ρ_l, $c_{p,l}$, h_{fg}) are evaluated at the droplet temperature.

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Ashoke De 91

So, particle touching cells should be crossed in a minimum 2 cell. So, this is typically the way we have handled in the transported phase actually this similar way one can handle this.

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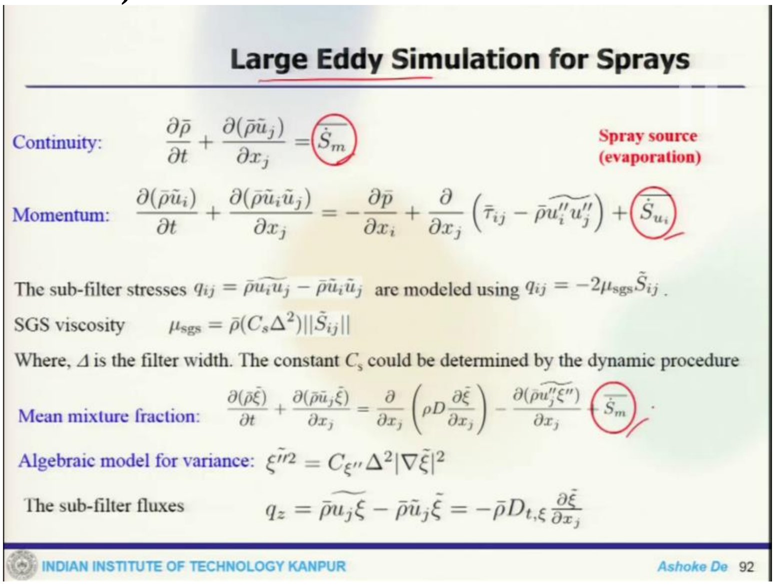

Large Eddy Simulation for Sprays

Continuity: $\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho}\tilde{u}_j)}{\partial x_j} = \overline{\dot{S}_m}$

Spray source (evaporation)

Momentum: $\frac{\partial (\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial (\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\bar{\tau}_{ij} - \bar{\rho}\widetilde{u_i'' u_j''}\right) + \overline{\dot{S}_{u_i}}$

The sub-filter stresses $q_{ij} = \bar{\rho}\widetilde{u_i u_j} - \bar{\rho}\tilde{u}_i\tilde{u}_j$ are modeled using $q_{ij} = -2\mu_{sgs}\tilde{S}_{ij}$.

SGS viscosity $\mu_{sgs} = \bar{\rho}(C_s\Delta^2)||\tilde{S}_{ij}||$

Where, Δ is the filter width. The constant C_s could be determined by the dynamic procedure

Mean mixture fraction: $\frac{\partial (\bar{\rho}\tilde{\xi})}{\partial t} + \frac{\partial (\bar{\rho}\tilde{u}_j\tilde{\xi})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial \tilde{\xi}}{\partial x_j}\right) - \frac{\partial (\bar{\rho}\widetilde{u_j''\xi''})}{\partial x_j} + \overline{\dot{S}_m}$.

Algebraic model for variance: $\widetilde{\xi''^2} = C_{\xi''}\Delta^2|\nabla\tilde{\xi}|^2$

The sub-filter fluxes $q_z = \bar{\rho}\widetilde{u_j\xi} - \bar{\rho}\tilde{u}_j\tilde{\xi} = -\bar{\rho}D_{t,\xi}\frac{\partial \tilde{\xi}}{\partial x_j}$

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Now, similarly, LES case your resource term here in the momentum one source term, there is a source term in the mixture of fraction and variance.

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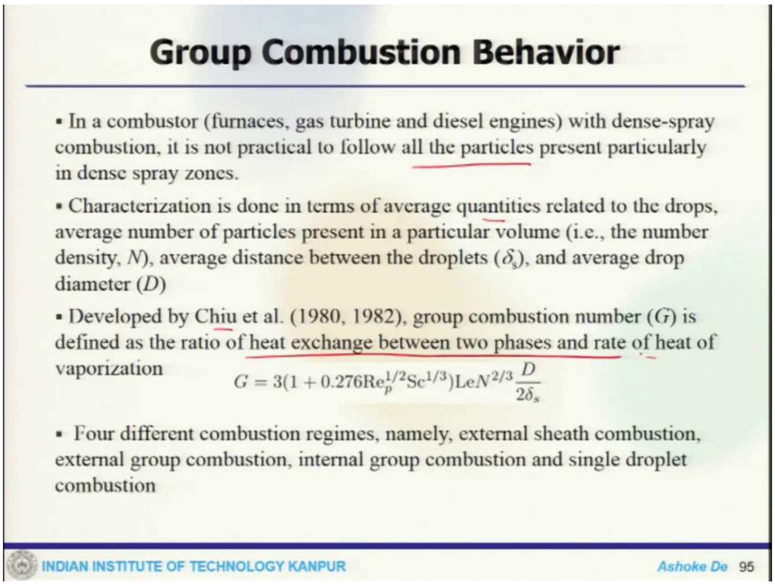

Group Combustion Behavior

- In a combustor (furnaces, gas turbine and diesel engines) with dense-spray combustion, it is not practical to follow all the particles present particularly in dense spray zones.
- Characterization is done in terms of average quantities related to the drops, average number of particles present in a particular volume (i.e., the number density, N), average distance between the droplets (δ_s), and average drop diameter (D)
- Developed by Chiu et al. (1980, 1982), group combustion number (G) is defined as the ratio of heat exchange between two phases and rate of heat of vaporization $G = 3(1 + 0.276\mathrm{Re}_p^{1/2}\mathrm{Sc}^{1/3})\mathrm{Le}N^{2/3}\frac{D}{2\delta_s}$
- Four different combustion regimes, namely, external sheath combustion, external group combustion, internal group combustion and single droplet combustion

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Then the variance equations, now another is the group conversion. So, in a particular conversion it is quite difficult to follow each particle which are present. So, there are the ways calculation is done in terms of average quantities related to the drops ever this numbers and all these. So, this is developed by that group. Combustion number was defined as the ratio of heat exchange between 2 phases and rate of heat of vaporization.

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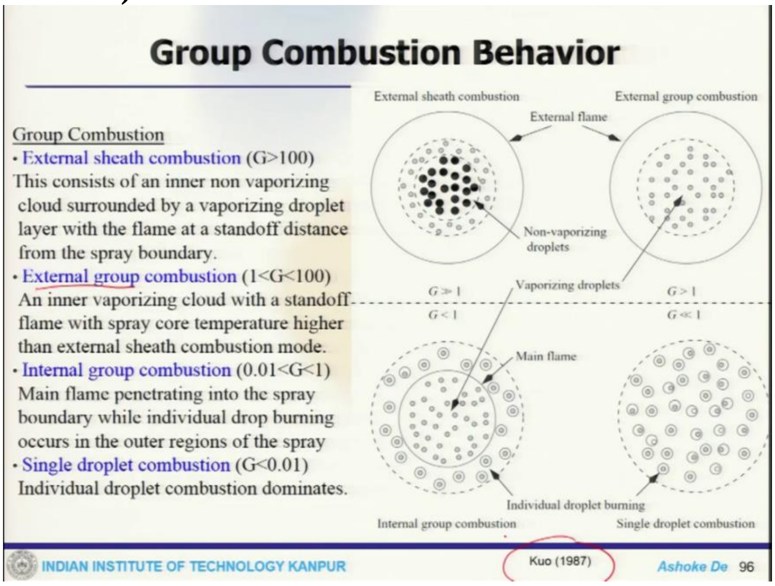

Group Combustion Behavior

Group Combustion

- External sheath combustion (G>100)
This consists of an inner non vaporizing cloud surrounded by a vaporizing droplet layer with the flame at a standoff distance from the spray boundary.
- External group combustion (1<G<100)
An inner vaporizing cloud with a standoff flame with spray core temperature higher than external sheath combustion mode.
- Internal group combustion (0.01<G<1)
Main flame penetrating into the spray boundary while individual drop burning occurs in the outer regions of the spray
- Single droplet combustion (G<0.01)
Individual droplet combustion dominates.

Kuo (1987)

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So, depending on this one can have external sheath combustion where this group combustion number G greater than 100. So, this consists of an inner non-vaporizing cloud surrounded by a vaporizing droplet. Now, there could be external group combustion where it it between 1 greater then G greater than 100 and in our vaporizing cloud with standoff flame with spray core temperature higher than this or internal group combustion or the single. So, you can find out in these details that what these are.

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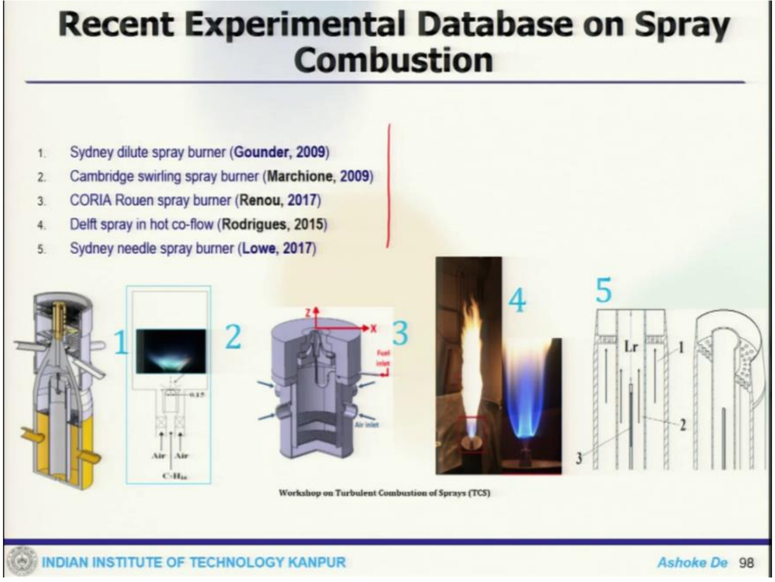

Recent Experimental Database on Spray Combustion

1. Sydney dilute spray burner (**Gounder, 2009**)
2. Cambridge swirling spray burner (**Marchione, 2009**)
3. CORIA Rouen spray burner (**Renou, 2017**)
4. Delft spray in hot co-flow (**Rodrigues, 2015**)
5. Sydney needle spray burner (**Lowe, 2017**)

Workshop on Turbulent Combustion of Sprays (TCS)

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Now, these are the some of the free downloads which are available in literature, I mean people have done calculations on these burners. So, some of the examples. This is an LES of gas phase.

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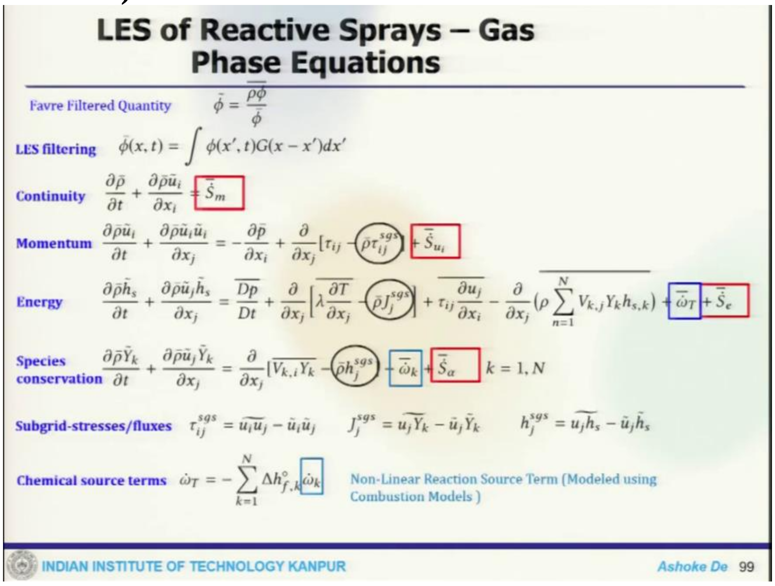

LES of Reactive Sprays – Gas Phase Equations

Favre Filtered Quantity $\tilde{\phi} = \frac{\overline{\rho\phi}}{\bar{\phi}}$

LES filtering $\bar{\phi}(x,t) = \int \phi(x',t)G(x-x')dx'$

Continuity $\frac{\partial\bar{\rho}}{\partial t} + \frac{\partial\bar{\rho}\tilde{u}_i}{\partial x_i} = \boxed{\bar{\dot{S}}_m}$

Momentum $\frac{\partial\bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial\bar{\rho}\tilde{u}_i\tilde{u}_i}{\partial x_j} = -\frac{\partial\bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}[\tau_{ij} - \bar{\rho}\tau_{ij}^{sgs}] \boxed{+\bar{\dot{S}}_{u_i}}$

Energy $\frac{\partial\bar{\rho}\tilde{h}_s}{\partial t} + \frac{\partial\bar{\rho}\tilde{u}_j\tilde{h}_s}{\partial x_j} = \overline{\frac{Dp}{Dt}} + \frac{\partial}{\partial x_j}\left[\overline{\lambda\frac{\partial T}{\partial x_j}} - \bar{\rho}J_j^{sgs}\right] + \overline{\tau_{ij}\frac{\partial u_j}{\partial x_i}} - \frac{\partial}{\partial x_j}\overline{(\rho\sum_{n=1}^{N} V_{k,j}Y_k h_{s,k})} + \boxed{\bar{\dot{\omega}}_T} \boxed{+\bar{\dot{S}}_e}$

Species conservation $\frac{\partial\bar{\rho}\tilde{Y}_k}{\partial t} + \frac{\partial\bar{\rho}\tilde{u}_j\tilde{Y}_k}{\partial x_j} = \frac{\partial}{\partial x_j}[\overline{V_{k,i}Y_k} - \bar{\rho}h_j^{sgs}] + \boxed{\bar{\dot{\omega}}_k} + \boxed{\bar{\dot{S}}_\alpha} \quad k = 1, N$

Subgrid-stresses/fluxes $\tau_{ij}^{sgs} = \widetilde{u_i u_j} - \tilde{u}_i\tilde{u}_j$ $\quad J_j^{sgs} = \widetilde{u_j Y_k} - \tilde{u}_j\tilde{Y}_k$ $\quad h_j^{sgs} = \widetilde{u_j h_s} - \tilde{u}_j\tilde{h}_s$

Chemical source terms $\dot{\omega}_T = -\sum_{k=1}^{N}\Delta h_{f,k}^{\circ}\boxed{\dot{\omega}_k}$ Non-Linear Reaction Source Term (Modeled using Combustion Models)

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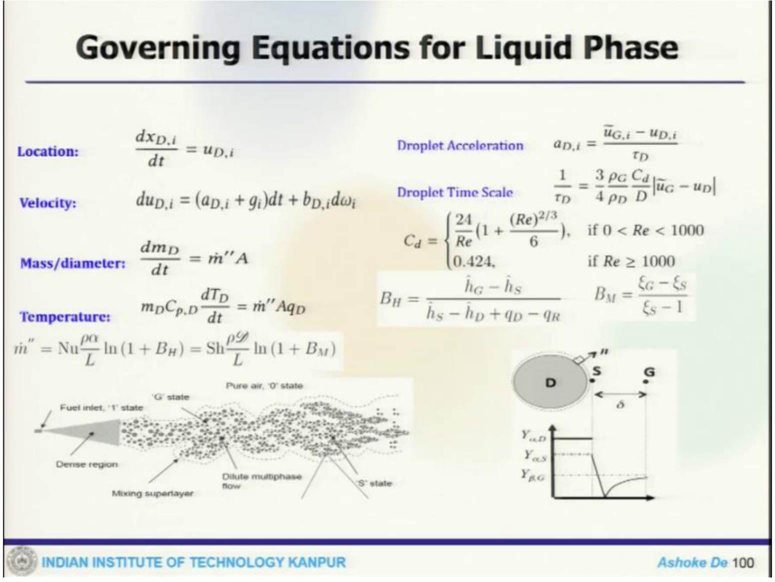

Governing Equations for Liquid Phase

Location: $\frac{dx_{D,i}}{dt} = u_{D,i}$

Velocity: $du_{D,i} = (a_{D,i} + g_i)dt + b_{D,i}d\omega_i$

Mass/diameter: $\frac{dm_D}{dt} = \dot{m}''A$

Temperature: $m_D C_{p,D}\frac{dT_D}{dt} = \dot{m}''Aq_D$

$\dot{m}'' = \mathrm{Nu}\frac{\rho\alpha}{L}\ln(1+B_H) = \mathrm{Sh}\frac{\rho\mathscr{D}}{L}\ln(1+B_M)$

Droplet Acceleration $a_{D,i} = \frac{\tilde{u}_{G,i} - u_{D,i}}{\tau_D}$

Droplet Time Scale $\frac{1}{\tau_D} = \frac{3}{4}\frac{\rho_G}{\rho_D}\frac{C_d}{D}|\tilde{u}_G - u_D|$

$$C_d = \begin{cases} \frac{24}{Re}(1 + \frac{(Re)^{2/3}}{6}), & \text{if } 0 < Re < 1000 \\ 0.424, & \text{if } Re \geq 1000 \end{cases}$$

$B_H = \frac{\hat{h}_G - \hat{h}_S}{\hat{h}_S - \hat{h}_D + q_D - q_R}$ $\quad B_M = \frac{\xi_G - \xi_S}{\xi_S - 1}$

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I will show you some, I mean how it is handled.

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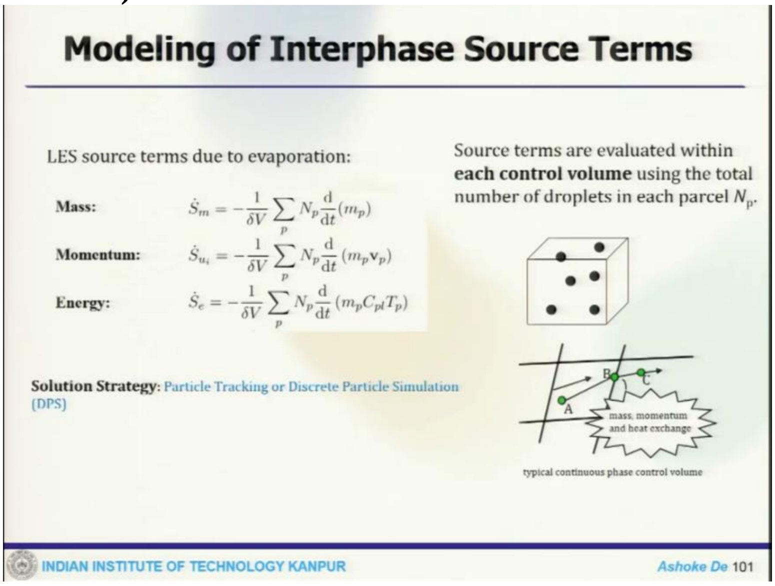

Modeling of Interphase Source Terms

LES source terms due to evaporation:

Mass: $\dot{S}_m = -\frac{1}{\delta V}\sum_p N_p \frac{\mathrm{d}}{\mathrm{d}t}(m_p)$

Momentum: $\dot{S}_{u_i} = -\frac{1}{\delta V}\sum_p N_p \frac{\mathrm{d}}{\mathrm{d}t}(m_p \mathbf{v}_p)$

Energy: $\dot{S}_e = -\frac{1}{\delta V}\sum_p N_p \frac{\mathrm{d}}{\mathrm{d}t}(m_p C_{pl} T_p)$

Source terms are evaluated within **each control volume** using the total number of droplets in each parcel N_p.

Solution Strategy: Particle Tracking or Discrete Particle Simulation (DPS)

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Ashoke De 101

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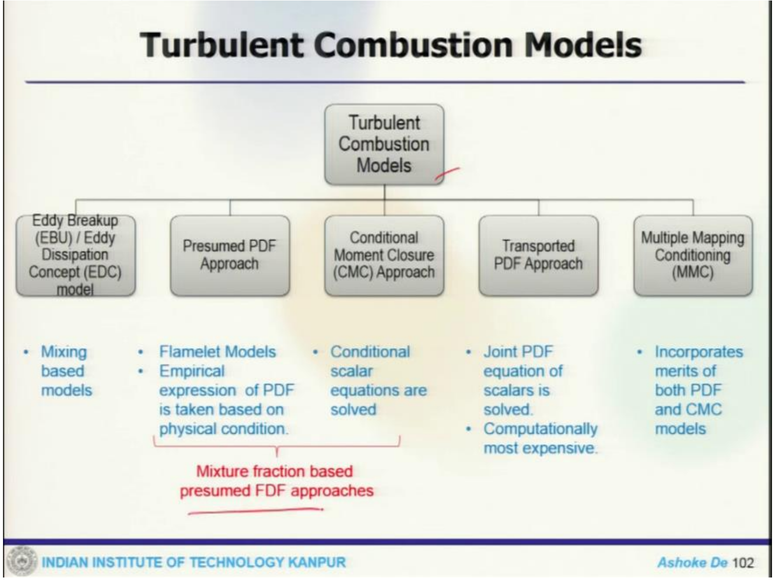

Turbulent Combustion Models

Turbulent Combustion Models

- Eddy Breakup (EBU) / Eddy Dissipation Concept (EDC) model
  - Mixing based models
- Presumed PDF Approach
  - Flamelet Models
  - Empirical expression of PDF is taken based on physical condition.
- Conditional Moment Closure (CMC) Approach
  - Conditional scalar equations are solved
- Transported PDF Approach
  - Joint PDF equation of scalars is solved.
  - Computationally most expensive.
- Multiple Mapping Conditioning (MMC)
  - Incorporates merits of both PDF and CMC models

Mixture fraction based presumed FDF approaches

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Ashoke De 102

So, this is not your models where you had. This is based on mixture fraction LES.

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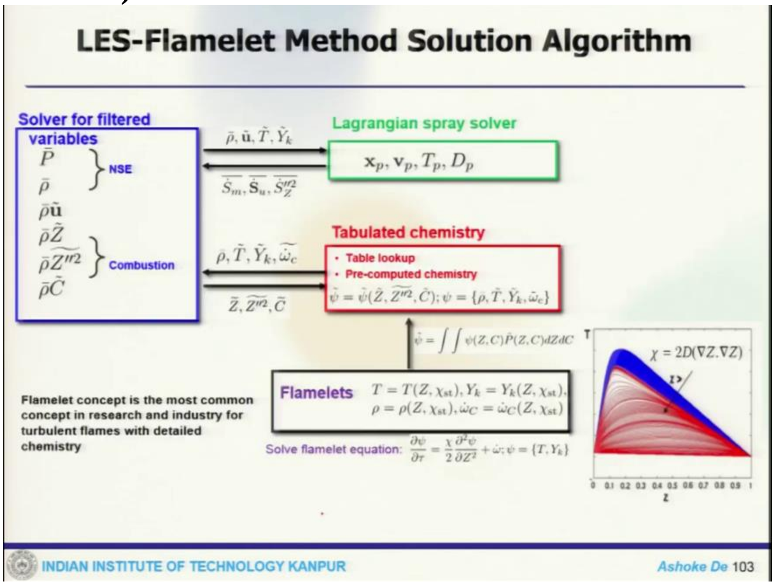

LES-Flamelet Method Solution Algorithm

Solver for filtered variables

$\bar{P}$, $\bar{\rho}$ } NSE

$\bar{\rho}\tilde{\mathbf{u}}$

$\bar{\rho}\tilde{Z}$, $\bar{\rho}\widetilde{Z''^2}$ } Combustion

$\bar{\rho}\tilde{C}$

$\bar{\rho}, \tilde{\mathbf{u}}, \tilde{T}, \tilde{Y}_k$

$\overline{\dot{S}_m}, \overline{\dot{\mathbf{S}}_u}, \overline{\dot{S}_Z''^2}$

Lagrangian spray solver

$\mathbf{x}_p, \mathbf{v}_p, T_p, D_p$

Tabulated chemistry

- Table lookup
- Pre-computed chemistry

$\tilde{\psi} = \tilde{\psi}(\tilde{Z}, \widetilde{Z''^2}, \tilde{C}); \psi = \{\bar{\rho}, \tilde{T}, \tilde{Y}_k, \tilde{\dot{\omega}}_c\}$

$\bar{\rho}, \tilde{T}, \tilde{Y}_k, \widetilde{\dot{\omega}_c}$

$\tilde{Z}, \widetilde{Z''^2}, \tilde{C}$

$\tilde{\psi} = \int\int \psi(Z,C)\tilde{P}(Z,C)dZdC$

Flamelets $T = T(Z, \chi_{st}), Y_k = Y_k(Z, \chi_{st}),$
$\rho = \rho(Z, \chi_{st}), \dot{\omega}_C = \dot{\omega}_C(Z, \chi_{st})$

Solve flamelet equation: $\frac{\partial \psi}{\partial \tau} = \frac{\chi}{2}\frac{\partial^2 \psi}{\partial Z^2} + \dot{\omega}; \psi = \{T, Y_k\}$

Flamelet concept is the most common concept in research and industry for turbulent flames with detailed chemistry

So, this is how LES you have filtered equation, you pass the equation in the Lagrangian spray solver when you have a local flamelet structure which is tabulated and sent back and they are coupled.

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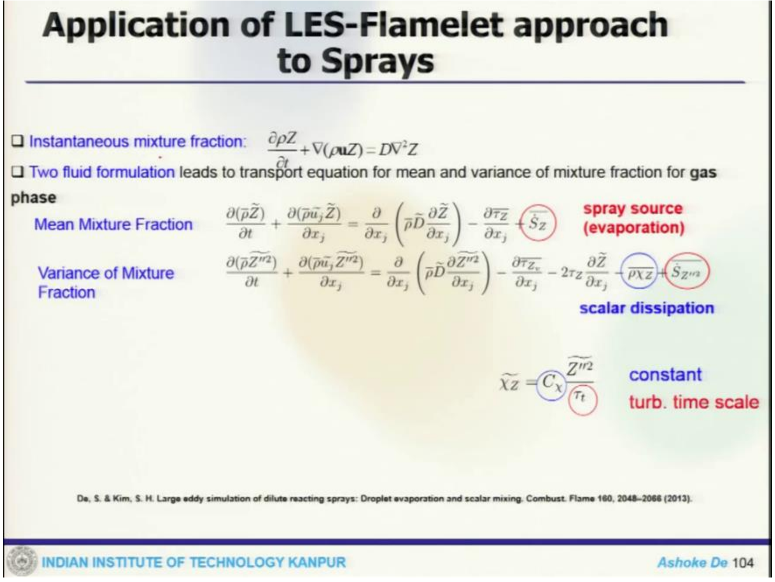

Application of LES-Flamelet approach to Sprays

- ☐ Instantaneous mixture fraction: $\frac{\partial \rho Z}{\partial t} + \nabla(\rho \mathbf{u} Z) = D\nabla^2 Z$
- ☐ Two fluid formulation leads to transport equation for mean and variance of mixture fraction for **gas phase**

Mean Mixture Fraction

$$\frac{\partial(\bar{\rho}\tilde{Z})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{D}\frac{\partial \tilde{Z}}{\partial x_j}\right) - \frac{\partial \tau_Z}{\partial x_j} + \overline{\dot{S}_Z}$$

spray source (evaporation)

Variance of Mixture Fraction

$$\frac{\partial(\bar{\rho}\widetilde{Z''^2})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\widetilde{Z''^2})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{D}\frac{\partial \widetilde{Z''^2}}{\partial x_j}\right) - \frac{\partial \tau_{Z_v}}{\partial x_j} - 2\tau_Z\frac{\partial \tilde{Z}}{\partial x_j} - \overline{\rho\chi_Z} + \overline{\dot{S}_{Z''^2}}$$

scalar dissipation

$$\tilde{\chi}_Z = C_\chi \frac{\widetilde{Z''^2}}{\tau_t}$$

constant

turb. time scale

De, S. & Kim, S. H. Large eddy simulation of dilute reacting sprays: Droplet evaporation and scalar mixing. Combust. Flame 160, 2048–2066 (2013).

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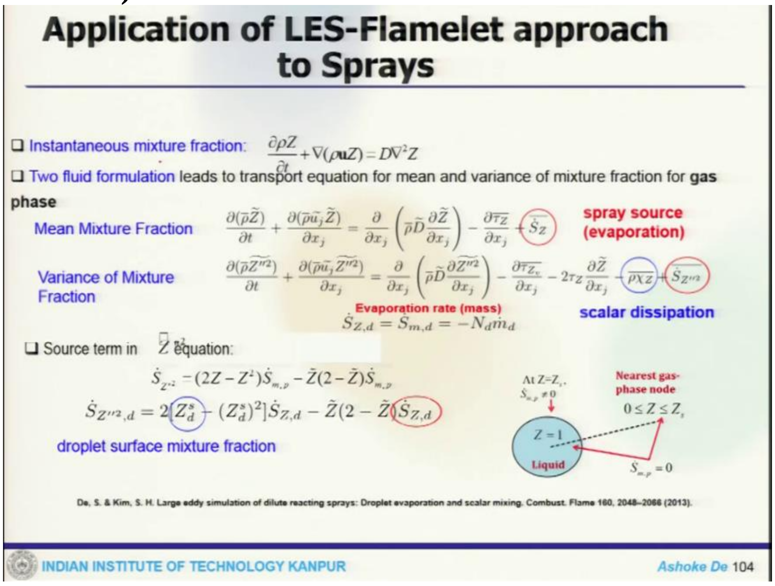

Application of LES-Flamelet approach to Sprays

❑ Instantaneous mixture fraction: $\frac{\partial \rho Z}{\partial t} + \nabla(\rho \mathbf{u} Z) = D\nabla^2 Z$

❑ Two fluid formulation leads to transport equation for mean and variance of mixture fraction for **gas phase**

Mean Mixture Fraction $\frac{\partial(\bar{\rho}\tilde{Z})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{D}\frac{\partial \tilde{Z}}{\partial x_j}\right) - \frac{\partial \tau_Z}{\partial x_j} + \overline{\dot{S}_Z}$ **spray source (evaporation)**

Variance of Mixture Fraction $\frac{\partial(\bar{\rho}\widetilde{Z''^2})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\widetilde{Z''^2})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{D}\frac{\partial \widetilde{Z''^2}}{\partial x_j}\right) - \frac{\partial \tau_{Z_v}}{\partial x_j} - 2\tau_Z\frac{\partial \tilde{Z}}{\partial x_j} - \overline{\rho\chi_Z} + \overline{\dot{S}_{Z''^2}}$

Evaporation rate (mass)

$\dot{S}_{Z,d} = \dot{S}_{m,d} = -N_d\dot{m}_d$

scalar dissipation

❑ Source term in $\widetilde{Z''^2}$ equation:

$$\dot{S}_{Z''^2} = (2Z - Z^2)\dot{S}_{m,p} - \tilde{Z}(2-\tilde{Z})\dot{S}_{m,p}$$

$$\dot{S}_{Z''^2,d} = 2[Z_d^s - (Z_d^s)^2]\dot{S}_{Z,d} - \tilde{Z}(2-\tilde{Z})\dot{S}_{Z,d}$$

droplet surface mixture fraction

De, S. & Kim, S. H. Large eddy simulation of dilute reacting sprays: Droplet evaporation and scalar mixing. Combust. Flame 160, 2048–2066 (2013).

And this is how you couple that in the continuity mixture fraction momentum the second phase or the spray source term.

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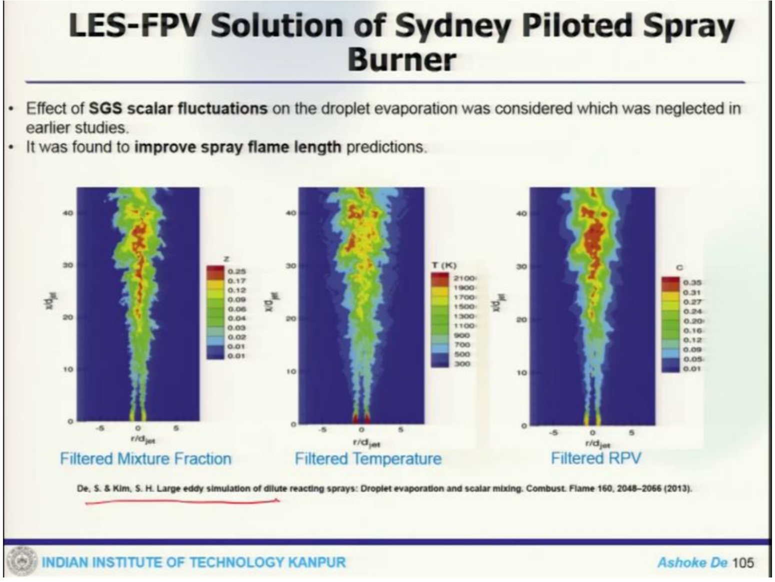

LES-FPV Solution of Sydney Piloted Spray Burner

- Effect of **SGS scalar fluctuations** on the droplet evaporation was considered which was neglected in earlier studies.
- It was found to **improve spray flame length** predictions.

Filtered Mixture Fraction Filtered Temperature Filtered RPV

De, S. & Kim, S. H. Large eddy simulation of dilute reacting sprays: Droplet evaporation and scalar mixing. Combust. Flame 160, 2048–2066 (2013).

And these are the some of the results, which is from this literature for you can see LES earliest progress variable kind of approach to compute them.

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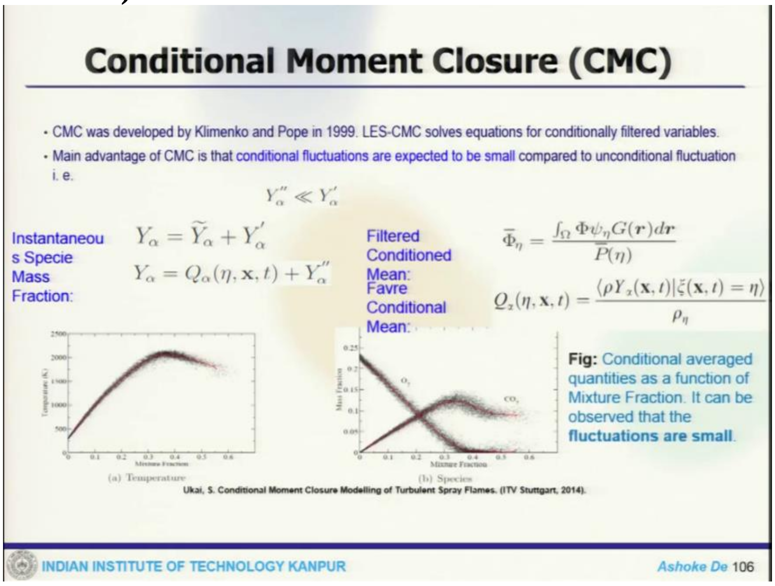

Conditional Moment Closure (CMC)

- CMC was developed by Klimenko and Pope in 1999. LES-CMC solves equations for conditionally filtered variables.
- Main advantage of CMC is that conditional fluctuations are expected to be small compared to unconditional fluctuation i. e.

$$Y_\alpha'' \ll Y_\alpha'$$

Instantaneous Specie Mass Fraction:

$$Y_\alpha = \widetilde{Y}_\alpha + Y_\alpha'$$

$$Y_\alpha = Q_\alpha(\eta, \mathbf{x}, t) + Y_\alpha''$$

Filtered Conditioned Mean:

$$\overline{\Phi}_\eta = \frac{\int_\Omega \Phi \psi_\eta G(\boldsymbol{r}) d\boldsymbol{r}}{\overline{P}(\eta)}$$

Favre Conditional Mean:

$$Q_\alpha(\eta, \mathbf{x}, t) = \frac{\langle \rho Y_\alpha(\mathbf{x}, t) | \xi(\mathbf{x}, t) = \eta \rangle}{\rho_\eta}$$

(a) Temperature (b) Species

Fig: Conditional averaged quantities as a function of Mixture Fraction. It can be observed that the **fluctuations are small**.

Ukai, S. Conditional Moment Closure Modelling of Turbulent Spray Flames. (ITV Stuttgart, 2014).

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Then there is another one in the conditional moment closure which is initially proposed by Klimenko and Pope.

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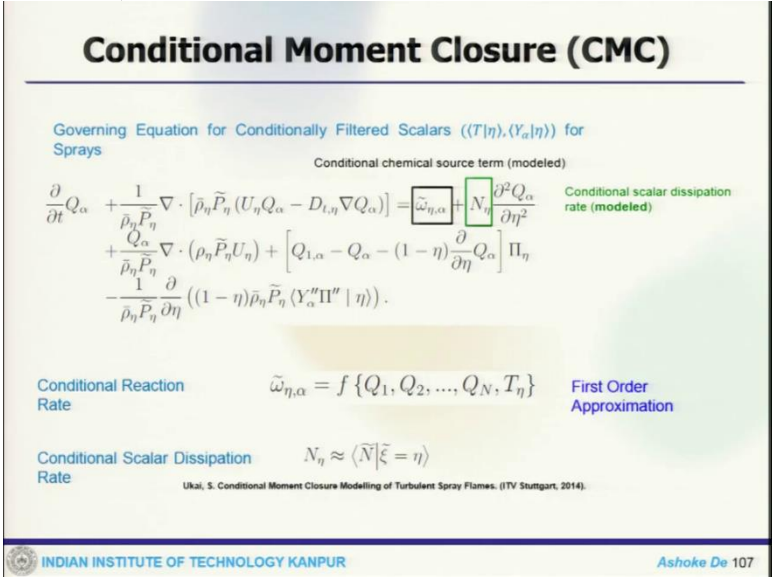

Conditional Moment Closure (CMC)

Governing Equation for Conditionally Filtered Scalars ($\langle T|\eta\rangle, \langle Y_\alpha|\eta\rangle$) for Sprays

Conditional chemical source term (modeled)

Conditional scalar dissipation rate (**modeled**)

$$\frac{\partial}{\partial t} Q_\alpha + \frac{1}{\bar{\rho}_\eta \widetilde{P}_\eta} \nabla \cdot \left[\bar{\rho}_\eta \widetilde{P}_\eta \left(U_\eta Q_\alpha - D_{t,\eta} \nabla Q_\alpha \right) \right] = \boxed{\widetilde{\omega}_{\eta,\alpha}} + \boxed{N_\eta} \frac{\partial^2 Q_\alpha}{\partial \eta^2}$$
$$+ \frac{Q_\alpha}{\bar{\rho}_\eta \widetilde{P}_\eta} \nabla \cdot \left(\rho_\eta \widetilde{P}_\eta U_\eta \right) + \left[Q_{1,\alpha} - Q_\alpha - (1-\eta) \frac{\partial}{\partial \eta} Q_\alpha \right] \Pi_\eta$$
$$- \frac{1}{\bar{\rho}_\eta \widetilde{P}_\eta} \frac{\partial}{\partial \eta} \left((1-\eta) \bar{\rho}_\eta \widetilde{P}_\eta \langle Y_\alpha'' \Pi'' \mid \eta \rangle \right).$$

Conditional Reaction Rate

$$\widetilde{\omega}_{\eta,\alpha} = f\{Q_1, Q_2, ..., Q_N, T_\eta\}$$

First Order Approximation

Conditional Scalar Dissipation Rate

$$N_\eta \approx \langle \widetilde{N} | \widetilde{\xi} = \eta \rangle$$

Ukai, S. Conditional Moment Closure Modelling of Turbulent Spray Flames. (ITV Stuttgart, 2014).

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But later on it was used by different groups and we are actually the gaseous phase we have seen that conditional moment closure of course this is now extended for multi-phase and there will be some terms and you can look at these references for details and you can see the predictions, how that comes through.

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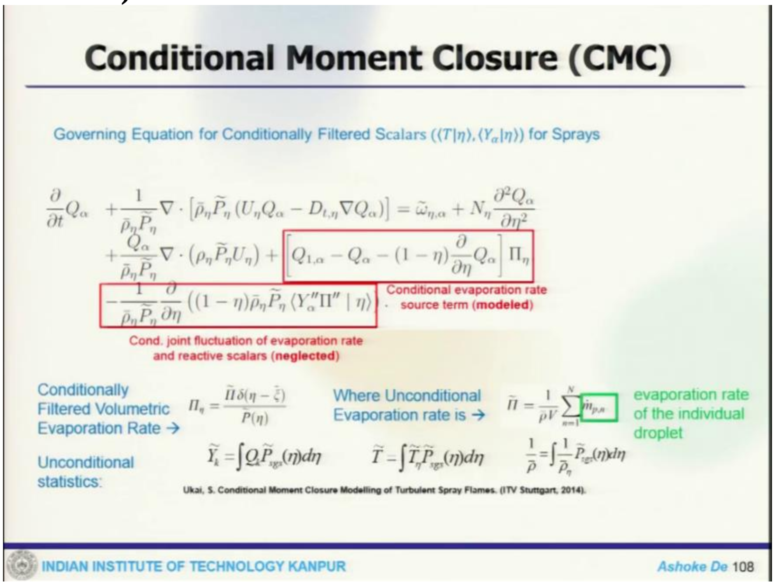

Conditional Moment Closure (CMC)

Governing Equation for Conditionally Filtered Scalars ($(\langle T|\eta\rangle, \langle Y_\alpha|\eta\rangle)$) for Sprays

$$\frac{\partial}{\partial t}Q_\alpha + \frac{1}{\bar{\rho}_\eta \widetilde{P}_\eta}\nabla\cdot\left[\bar{\rho}_\eta \widetilde{P}_\eta\left(U_\eta Q_\alpha - D_{t,\eta}\nabla Q_\alpha\right)\right] = \widetilde{\omega}_{\eta,\alpha} + N_\eta\frac{\partial^2 Q_\alpha}{\partial\eta^2}$$
$$+\frac{Q_\alpha}{\bar{\rho}_\eta \widetilde{P}_\eta}\nabla\cdot\left(\rho_\eta \widetilde{P}_\eta U_\eta\right) + \boxed{\left[Q_{1,\alpha} - Q_\alpha - (1-\eta)\frac{\partial}{\partial\eta}Q_\alpha\right]\Pi_\eta}$$
$$\boxed{-\frac{1}{\bar{\rho}_\eta \widetilde{P}_\eta}\frac{\partial}{\partial\eta}\left((1-\eta)\bar{\rho}_\eta \widetilde{P}_\eta\left\langle Y_\alpha''\Pi'' \mid \eta\right\rangle\right)}\ .$$

Conditional evaporation rate source term (**modeled**)

Cond. joint fluctuation of evaporation rate and reactive scalars (**neglected**)

Conditionally Filtered Volumetric Evaporation Rate → $\Pi_\eta = \frac{\widetilde{\Pi}\,\delta(\eta-\tilde{\xi})}{\widetilde{P}(\eta)}$

Where Unconditional Evaporation rate is → $\widetilde{\Pi} = \frac{1}{\bar{\rho}V}\sum_{n=1}^{N}\boxed{\dot{m}_{p,n}}$ evaporation rate of the individual droplet

Unconditional statistics: $\widetilde{Y}_k = \int Q_k \widetilde{P}_{sgs}(\eta)d\eta$ $\quad \widetilde{T} = \int \widetilde{T}_\eta \widetilde{P}_{sgs}(\eta)d\eta$ $\quad \frac{1}{\bar{\rho}} = \int \frac{1}{\bar{\rho}_\eta}\widetilde{P}_{sgs}(\eta)d\eta$

Ukai, S. Conditional Moment Closure Modelling of Turbulent Spray Flames. (ITV Stuttgart, 2014).

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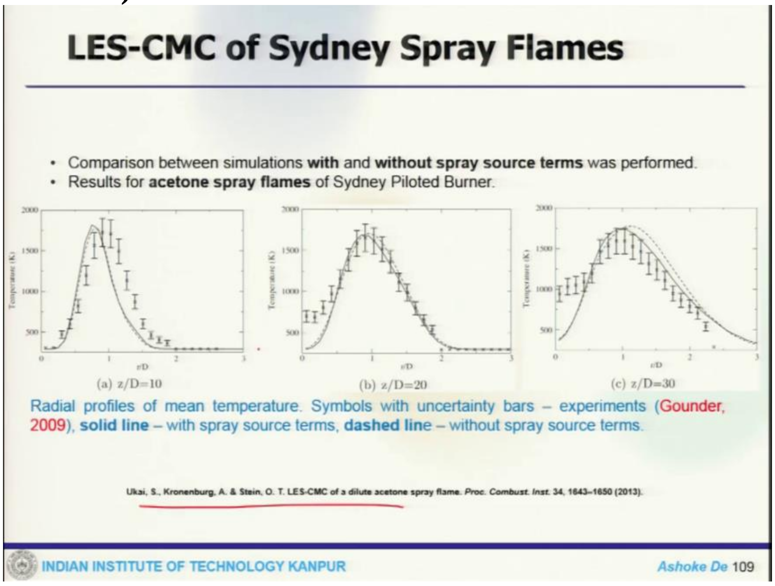

LES-CMC of Sydney Spray Flames

- Comparison between simulations **with** and **without spray source terms** was performed.
- Results for **acetone spray flames** of Sydney Piloted Burner.

(a) z/D=10 (b) z/D=20 (c) z/D=30

Radial profiles of mean temperature. Symbols with uncertainty bars – experiments (Gounder, 2009), **solid line** – with spray source terms, **dashed line** – without spray source terms.

Ukai, S., Kronenburg, A. & Stein, O. T. LES-CMC of a dilute acetone spray flame. *Proc. Combust. Inst.* 34, 1643–1650 (2013).

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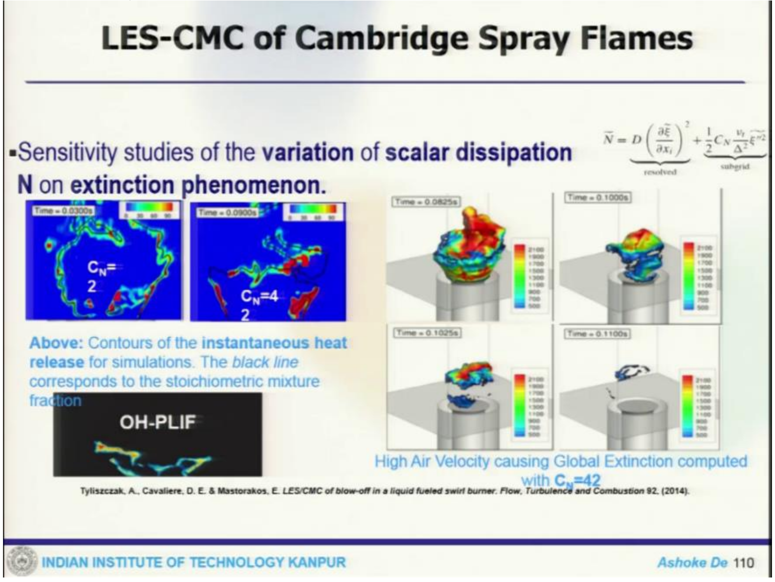

LES-CMC of Cambridge Spray Flames

- Sensitivity studies of the **variation of scalar dissipation N** on **extinction phenomenon.**

$$\widetilde{N} = \underbrace{D\left(\frac{\partial\tilde{\xi}}{\partial x_i}\right)^2}_{\text{resolved}} + \underbrace{\frac{1}{2}C_N\frac{\nu_t}{\Delta^2}\widetilde{\xi''^2}}_{\text{subgrid}}$$

Above: Contours of the **instantaneous heat release** for simulations. The *black line* corresponds to the stoichiometric mixture fraction

High Air Velocity causing Global Extinction computed with C_N=42

Tyliszczak, A., Cavaliere, D. E. & Mastorakos, E. *LES/CMC of blow-off in a liquid fueled swirl burner. Flow, Turbulence and Combustion* 92, (2014).

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These are the some of the images from that.

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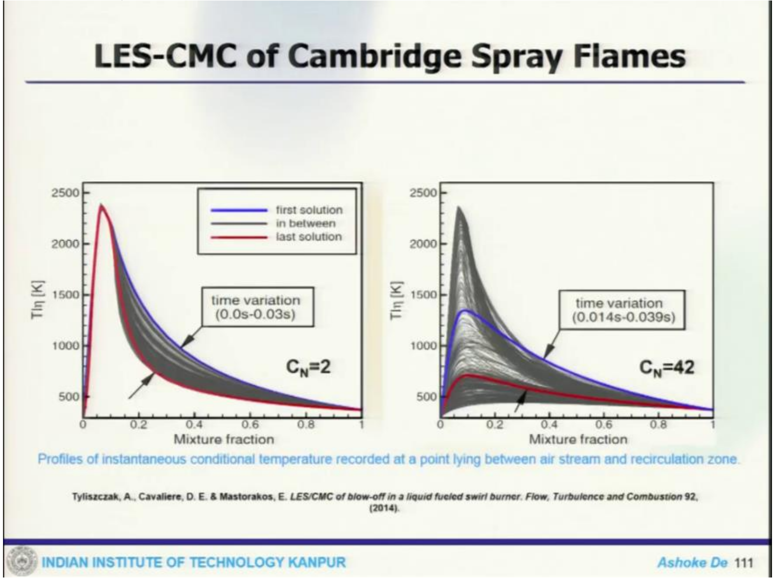

LES-CMC of Cambridge Spray Flames

Profiles of instantaneous conditional temperature recorded at a point lying between air stream and recirculation zone.

Tyliszczak, A., Cavaliere, D. E. & Mastorakos, E. *LES/CMC of blow-off in a liquid fueled swirl burner. Flow, Turbulence and Combustion* 92, (2014).

And after that there is a one more advancement which has been taken place there, or this one could do the transported PDF approach, you can go through the literature, but they have used the LES.

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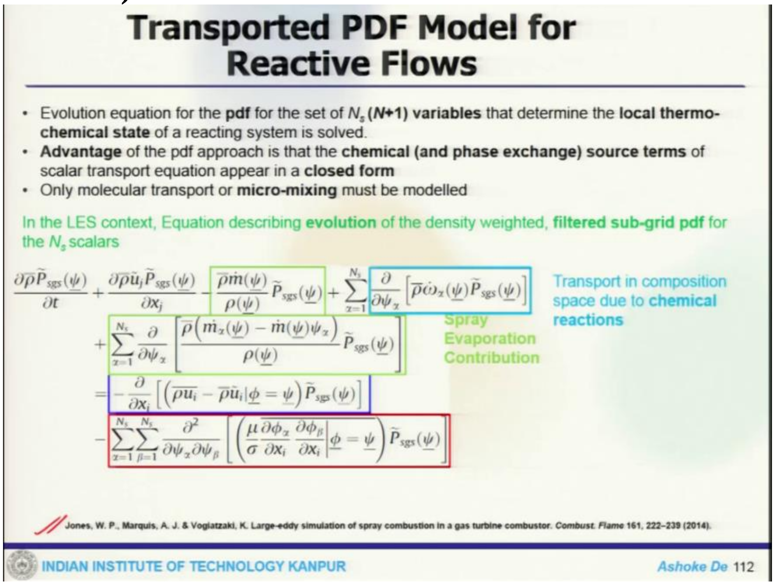

Transported PDF Model for Reactive Flows

- Evolution equation for the **pdf** for the set of N_s **(N+1) variables** that determine the **local thermo-chemical state** of a reacting system is solved.
- **Advantage** of the pdf approach is that the **chemical (and phase exchange) source terms** of scalar transport equation appear in a **closed form**
- Only molecular transport or **micro-mixing** must be modelled

In the LES context, Equation describing **evolution** of the density weighted, **filtered sub-grid pdf** for the N_s scalars

$$\frac{\partial \overline{\rho}\tilde{P}_{sgs}(\underline{\psi})}{\partial t}+\frac{\partial \overline{\rho}\tilde{u}_j\tilde{P}_{sgs}(\underline{\psi})}{\partial x_j}-\boxed{\frac{\overline{\rho}\dot{m}(\underline{\psi})}{\rho(\underline{\psi})}\tilde{P}_{sgs}(\underline{\psi})}+\sum_{\alpha=1}^{N_s}\boxed{\frac{\partial}{\partial \psi_\alpha}\left[\overline{\rho}\dot{\omega}_\alpha(\underline{\psi})\tilde{P}_{sgs}(\underline{\psi})\right]}$$
$$+\boxed{\sum_{\alpha=1}^{N_s}\frac{\partial}{\partial \psi_\alpha}\left[\frac{\overline{\rho}\left(\dot{m}_\alpha(\underline{\psi})-\dot{m}(\underline{\psi})\psi_\alpha\right)}{\rho(\underline{\psi})}\tilde{P}_{sgs}(\underline{\psi})\right]}$$
$$=\boxed{-\frac{\partial}{\partial x_i}\left[\left(\overline{\rho u_i}-\overline{\rho}\tilde{u}_i|\underline{\phi}=\underline{\psi}\right)\tilde{P}_{sgs}(\underline{\psi})\right]}$$
$$-\boxed{\sum_{\alpha=1}^{N_s}\sum_{\beta=1}^{N_s}\frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta}\left[\left(\overline{\frac{\mu}{\sigma}\frac{\partial \phi_\alpha}{\partial x_i}\frac{\partial \phi_\beta}{\partial x_i}}\Big|\underline{\phi}=\underline{\psi}\right)\tilde{P}_{sgs}(\underline{\psi})\right]}$$

Transport in composition space due to **chemical reactions**

Spray Evaporation Contribution

Jones, W. P., Marquis, A. J. & Vogiatzaki, K. Large-eddy simulation of spray combustion in a gas turbine combustor. *Combust. Flame* 161, 222–239 (2014).

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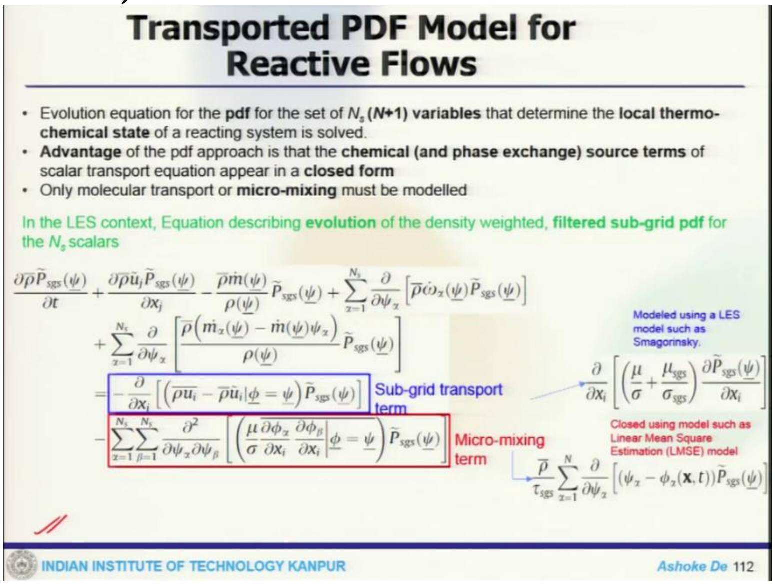

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- **Advantage** of the pdf approach is that the **chemical (and phase exchange) source terms** of scalar transport equation appear in a **closed form**
- Only molecular transport or **micro-mixing** must be modelled

In the LES context, Equation describing **evolution** of the density weighted, **filtered sub-grid pdf** for the N_s scalars

$$\frac{\partial \bar{\rho}\tilde{P}_{sgs}(\underline{\psi})}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{P}_{sgs}(\underline{\psi})}{\partial x_j}-\frac{\bar{\rho}\dot{m}(\underline{\psi})}{\rho(\underline{\psi})}\tilde{P}_{sgs}(\underline{\psi})+\sum_{\alpha=1}^{N_s}\frac{\partial}{\partial \psi_\alpha}\left[\bar{\rho}\dot{\omega}_\alpha(\underline{\psi})\tilde{P}_{sgs}(\underline{\psi})\right]$$

$$+\sum_{\alpha=1}^{N_s}\frac{\partial}{\partial \psi_\alpha}\left[\frac{\bar{\rho}\left(\dot{m}_\alpha(\underline{\psi})-\dot{m}(\underline{\psi})\psi_\alpha\right)}{\rho(\underline{\psi})}\tilde{P}_{sgs}(\underline{\psi})\right]$$

$$=\boxed{-\frac{\partial}{\partial x_i}\left[\left(\overline{\rho u_i}-\bar{\rho}\tilde{u}_i|\underline{\phi}=\underline{\psi}\right)\tilde{P}_{sgs}(\underline{\psi})\right]}$$

Sub-grid transport term

$$-\boxed{\sum_{\alpha=1}^{N_s}\sum_{\beta=1}^{N_s}\frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta}\left[\left(\overline{\frac{\mu}{\sigma}\frac{\partial \phi_\alpha}{\partial x_i}\frac{\partial \phi_\beta}{\partial x_i}}\bigg|\underline{\phi}=\underline{\psi}\right)\tilde{P}_{sgs}(\underline{\psi})\right]}$$

Micro-mixing term

Modeled using a LES model such as Smagorinsky.

$$\frac{\partial}{\partial x_i}\left[\left(\frac{\mu}{\sigma}+\frac{\mu_{sgs}}{\sigma_{sgs}}\right)\frac{\partial \tilde{P}_{sgs}(\underline{\psi})}{\partial x_i}\right]$$

Closed using model such as Linear Mean Square Estimation (LMSE) model

$$\frac{\bar{\rho}}{\tau_{sgs}}\sum_{\alpha=1}^{N}\frac{\partial}{\partial \psi_\alpha}\left[\left(\psi_\alpha-\phi_\alpha(\mathbf{x},t)\right)\tilde{P}_{sgs}(\underline{\psi})\right]$$

So, I will show you some of the images that how you can, this is the non-reactive case, this is the reactive case and this is the fuel.

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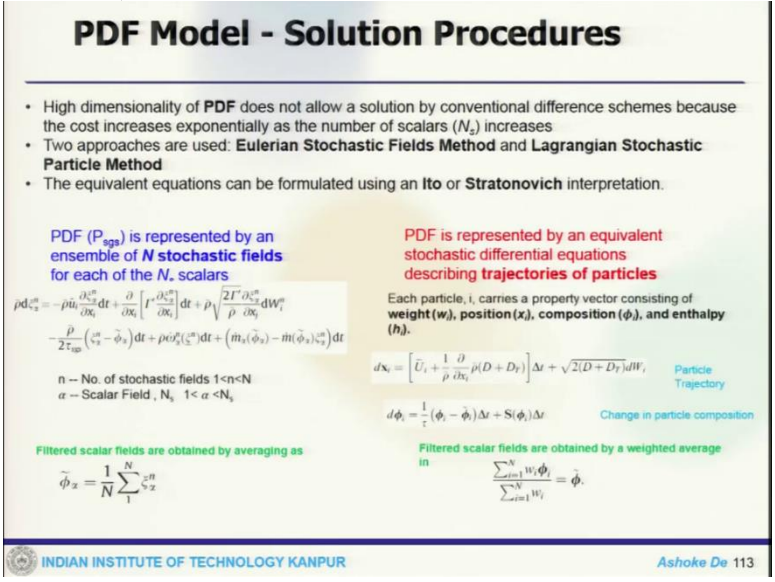

PDF Model - Solution Procedures

- High dimensionality of **PDF** does not allow a solution by conventional difference schemes because the cost increases exponentially as the number of scalars (N_s) increases
- Two approaches are used: **Eulerian Stochastic Fields Method** and **Lagrangian Stochastic Particle Method**
- The equivalent equations can be formulated using an **Ito** or **Stratonovich** interpretation.

PDF (P_{sgs}) is represented by an ensemble of ***N* stochastic fields** for each of the N_s scalars

$$\bar{\rho}d\xi_\alpha^n=-\bar{\rho}\tilde{u}_i\frac{\partial \xi_\alpha^n}{\partial x_i}dt+\frac{\partial}{\partial x_i}\left[\Gamma^*\frac{\partial \xi_\alpha^n}{\partial x_i}\right]dt+\bar{\rho}\sqrt{\frac{2\Gamma^*}{\bar{\rho}}}\frac{\partial \xi_\alpha^n}{\partial x_i}dW_i^n$$
$$-\frac{\bar{\rho}}{2\tau_{sgs}}\left(\xi_\alpha^n-\tilde{\phi}_\alpha\right)dt+\bar{\rho}\dot{\omega}_\alpha^n(\xi^n)dt+\left(\dot{m}_\alpha(\tilde{\phi}_\alpha)-\dot{m}(\tilde{\phi}_\alpha)\xi_\alpha^n\right)dt$$

n -- No. of stochastic fields 1<n<N
α -- Scalar Field , N_s $1<\alpha<N_s$

Filtered scalar fields are obtained by averaging as

$$\tilde{\phi}_\alpha=\frac{1}{N}\sum_{1}^{N}\xi_\alpha^n$$

PDF is represented by an equivalent stochastic differential equations describing **trajectories of particles**

Each particle, i, carries a property vector consisting of **weight (w_i), position (x_i), composition (ϕ_i), and enthalpy (h_i).**

$$d\mathbf{x}_i=\left[\tilde{U}_i+\frac{1}{\bar{\rho}}\frac{\partial}{\partial x_i}\bar{\rho}(D+D_T)\right]\Delta t+\sqrt{2(D+D_T)}dW_i$$

Particle Trajectory

$$d\phi_i=\frac{1}{\tau}(\phi_i-\tilde{\phi}_i)\Delta t+S(\phi_i)\Delta t$$

Change in particle composition

Filtered scalar fields are obtained by a weighted average in

$$\frac{\sum_{i=1}^{N}w_i\phi_i}{\sum_{i=1}^{N}w_i}=\tilde{\phi}.$$

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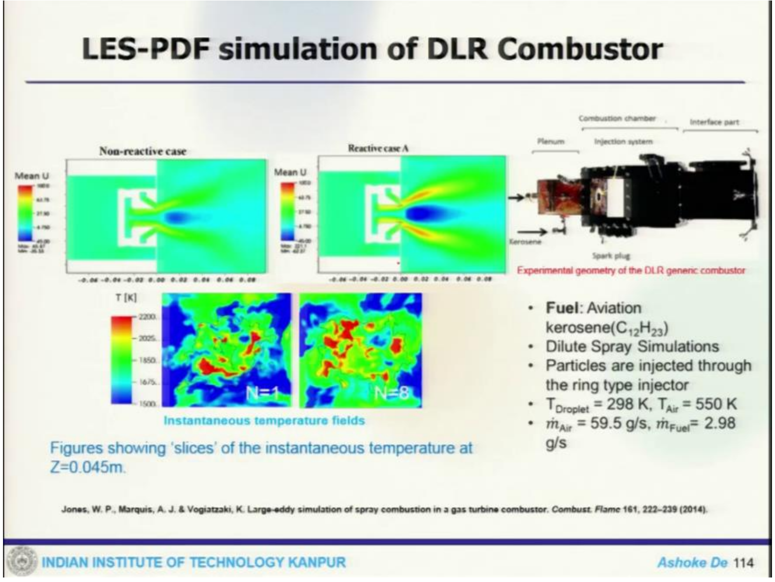

LES-PDF simulation of DLR Combustor

Experimental geometry of the DLR generic combustor

Instantaneous temperature fields

Figures showing 'slices' of the instantaneous temperature at Z=0.045m.

- **Fuel**: Aviation kerosene($C_{12}H_{23}$)
- Dilute Spray Simulations
- Particles are injected through the ring type injector
- $T_{Droplet} = 298$ K, $T_{Air} = 550$ K
- $\dot{m}_{Air} = 59.5$ g/s, $\dot{m}_{Fuel} = 2.98$ g/s

Jones, W. P., Marquis, A. J. & Vogiatzaki, K. Large-eddy simulation of spray combustion in a gas turbine combustor. *Combust. Flame* 161, 222–239 (2014).

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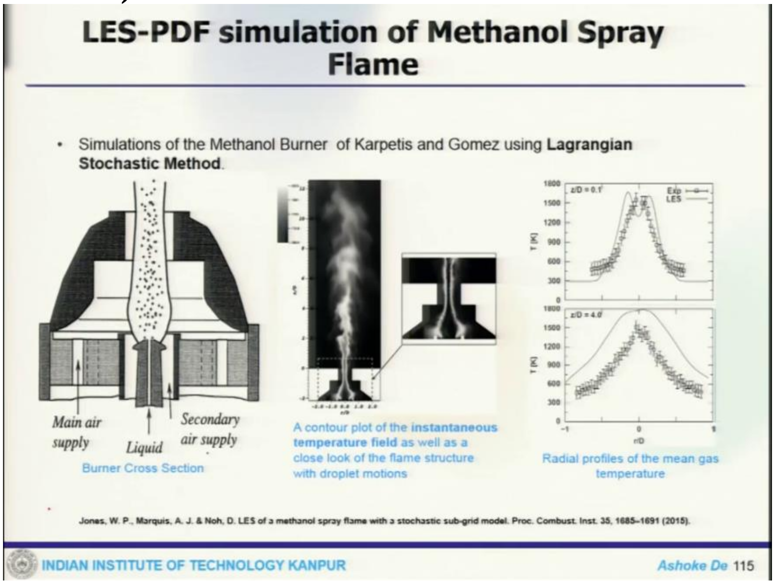

LES-PDF simulation of Methanol Spray Flame

- Simulations of the Methanol Burner of Karpetis and Gomez using **Lagrangian Stochastic Method**.

Burner Cross Section

A contour plot of the **instantaneous temperature field** as well as a close look of the flame structure with droplet motions

Radial profiles of the mean gas temperature

Jones, W. P., Marquis, A. J. & Noh, D. LES of a methanol spray flame with a stochastic sub-grid model. Proc. Combust. Inst. 35, 1685–1691 (2015).

You can see those images from there.

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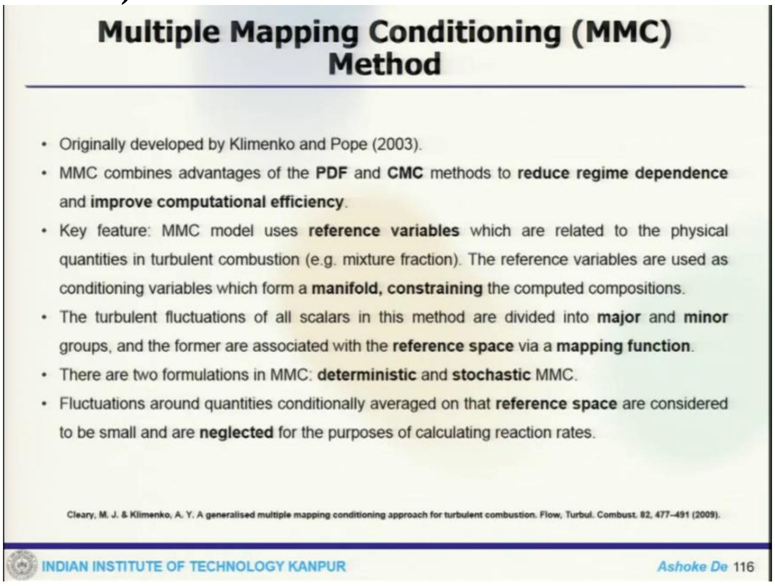

Multiple Mapping Conditioning (MMC) Method

- Originally developed by Klimenko and Pope (2003).
- MMC combines advantages of the **PDF** and **CMC** methods to **reduce regime dependence** and **improve computational efficiency**.
- Key feature: MMC model uses **reference variables** which are related to the physical quantities in turbulent combustion (e.g. mixture fraction). The reference variables are used as conditioning variables which form a **manifold, constraining** the computed compositions.
- The turbulent fluctuations of all scalars in this method are divided into **major** and **minor** groups, and the former are associated with the **reference space** via a **mapping function**.
- There are two formulations in MMC: **deterministic** and **stochastic** MMC.
- Fluctuations around quantities conditionally averaged on that **reference space** are considered to be small and are **neglected** for the purposes of calculating reaction rates.

Cleary, M. J. & Klimenko, A. Y. A generalised multiple mapping conditioning approach for turbulent combustion. Flow, Turbul. Combust. 82, 477–491 (2009).

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Now, there is another approach which got more attention is the multiple mapping closure. So, this has been they are using, I mean the advantage or combines the effect of PDF approach, I mean the transported PDF approach and the CMC.

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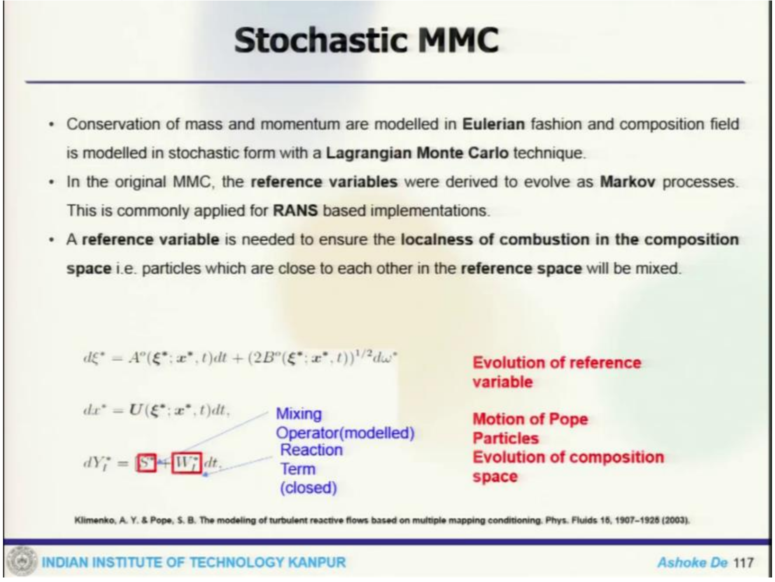

Stochastic MMC

- Conservation of mass and momentum are modelled in **Eulerian** fashion and composition field is modelled in stochastic form with a **Lagrangian Monte Carlo** technique.
- In the original MMC, the **reference variables** were derived to evolve as **Markov** processes. This is commonly applied for **RANS** based implementations.
- A **reference variable** is needed to ensure the **localness of combustion in the composition space** i.e. particles which are close to each other in the **reference space** will be mixed.

$$d\xi^* = A^o(\boldsymbol{\xi}^*;\boldsymbol{x}^*,t)dt + (2B^o(\boldsymbol{\xi}^*;\boldsymbol{x}^*,t))^{1/2}d\omega^*$$ Evolution of reference variable

$$dx^* = \boldsymbol{U}(\boldsymbol{\xi}^*;\boldsymbol{x}^*,t)dt,$$ Motion of Pope Particles

$$dY_I^* = \boxed{S^*} + \boxed{W_I^*}dt,$$ Evolution of composition space

Mixing Operator(modelled)

Reaction Term (closed)

Klimenko, A. Y. & Pope, S. B. The modeling of turbulent reactive flows based on multiple mapping conditioning. Phys. Fluids 15, 1907–1925 (2003).

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So combining this, so one can have stochastic MMC or deterministic MMC and one can look at this recent articles where you can see the details of these things.

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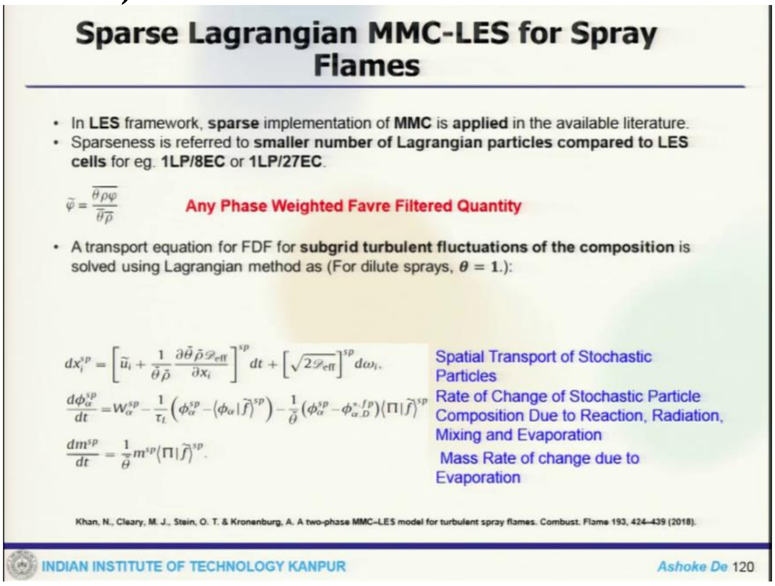

Sparse Lagrangian MMC-LES for Spray Flames

- In **LES** framework, **sparse** implementation of **MMC** is **applied** in the available literature.
- Sparseness is referred to **smaller number of Lagrangian particles compared to LES cells** for eg. **1LP/8EC** or **1LP/27EC**.

$$\tilde{\varphi} = \frac{\overline{\theta \rho \varphi}}{\bar{\theta} \bar{\rho}}$$

Any Phase Weighted Favre Filtered Quantity

- A transport equation for FDF for **subgrid turbulent fluctuations of the composition** is solved using Lagrangian method as (For dilute sprays, $\boldsymbol{\theta = 1}$.):

$$dx_i^{sp} = \left[\tilde{u}_i + \frac{1}{\bar{\theta}\bar{\rho}} \frac{\partial \bar{\theta} \bar{\rho} \mathscr{D}_{\text{eff}}}{\partial x_i}\right]^{sp} dt + \left[\sqrt{2\mathscr{D}_{\text{eff}}}\right]^{sp} d\omega_i.$$

Spatial Transport of Stochastic Particles

$$\frac{d\phi_\alpha^{sp}}{dt} = W_\alpha^{sp} - \frac{1}{\tau_L}\left(\phi_\alpha^{sp} - \langle \phi_\alpha | \tilde{f} \rangle^{sp}\right) - \frac{1}{\bar{\theta}}\left(\phi_\alpha^{sp} - \phi_{\alpha,D}^{*,fp}\right)\langle \Pi | \tilde{f} \rangle^{sp}$$

Rate of Change of Stochastic Particle Composition Due to Reaction, Radiation, Mixing and Evaporation

$$\frac{dm^{sp}}{dt} = \frac{1}{\bar{\theta}} m^{sp} \langle \Pi | \tilde{f} \rangle^{sp}.$$

Mass Rate of change due to Evaporation

Khan, N., Cleary, M. J., Stein, O. T. & Kronenburg, A. A two-phase MMC–LES model for turbulent spray flames. Combust. Flame 193, 424–439 (2018).

And these are the equation systems which are essentially solving the particle phase and the gas phase is mixed with the gas phase. And these are some of the calculations what you can see they are using these advanced MMC structure.

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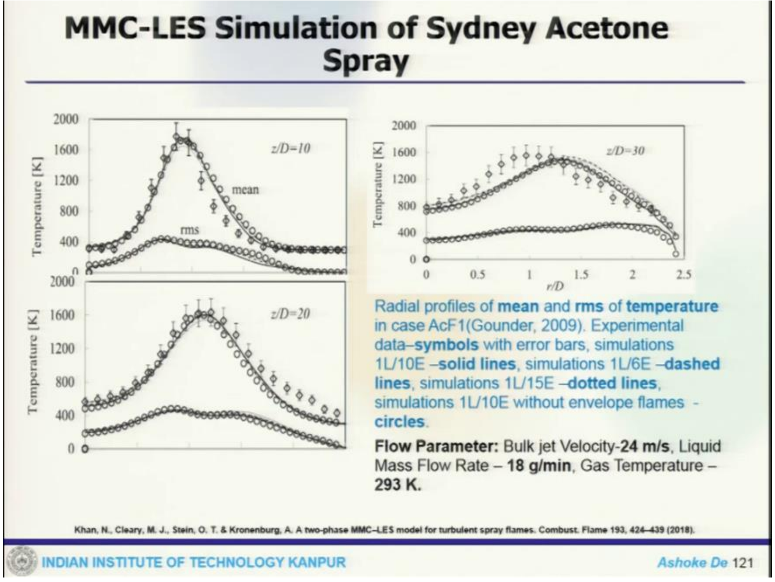

MMC-LES Simulation of Sydney Acetone Spray

Radial profiles of **mean** and **rms** of **temperature** in case AcF1(Gounder, 2009). Experimental data–**symbols** with error bars, simulations 1L/10E –**solid lines**, simulations 1L/6E –**dashed lines**, simulations 1L/15E –**dotted lines**, simulations 1L/10E without envelope flames - **circles**.

Flow Parameter: Bulk jet Velocity-**24 m/s**, Liquid Mass Flow Rate – **18 g/min**, Gas Temperature – **293 K.**

Khan, N., Cleary, M. J., Stein, O. T. & Kronenburg, A. A two-phase MMC–LES model for turbulent spray flames. Combust. Flame 193, 424–439 (2018).

So, that pretty much gives you an idea what you can do and what are the models you have in the handling the multi-phase system. So, you have all the gas phase models, which you have discussed that are required on top of that when you go to multi-phase system. You have all these sources from which are arising due to the droplet and the droplet combustion itself is complicated. On top of that, the droplet is formed through the automation process and all these.

So that will give you a fair amount of idea how the multiple systems are handled. And I hope this will give you a good fair amount of idea about this turbulence combustion modelling and their recent advances. And I hope you have enjoyed the course and we will take it forward. Thank you very much!