Gas-Liquid Flows Involving Multicomponent Fuel Evaporating Spray

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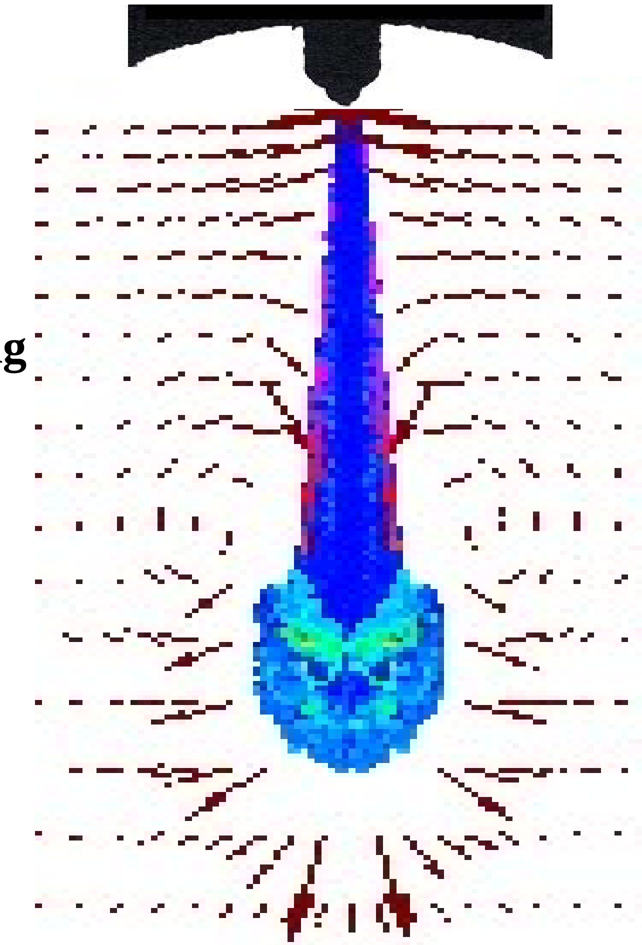

Morgantown WV
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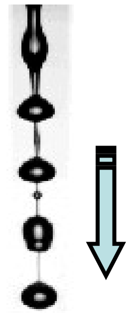
Introduction

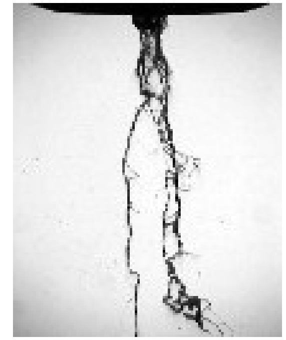
- Liquid Spray devices are widely used in many industrial processes.

Paint Spray



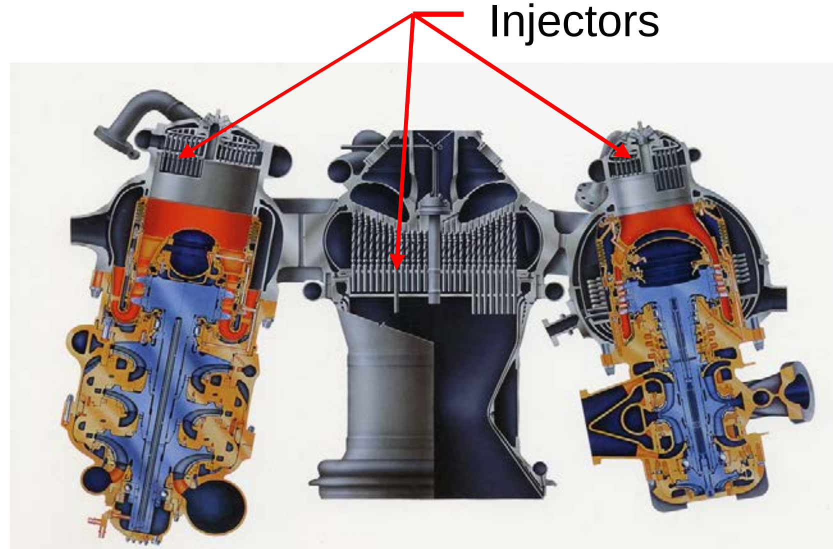
Simulated Ink Jet

Melted Metal Spray



Polymer solution Spray

- For the combustion system, the combustion efficiency and behavior are dependent on the effectiveness of the liquid fuel breaking up into droplets.
  - Finer drop size would enhance performance,
  - A rapid mixing and combustion due to generating fine propellant drops may cause the injector overheating.



Space Shuttle Main Engine

Presentation Outline

- **Introduction**
- **New Atomization and Evaporation Models**
  - **T-Blob/T-TAB, Two-temperature evaporation model**
  - **A Hybrid Model**

    Primary breakup (T-Blob)/Secondary breakup (T-TAB)
- **Multi-component Droplet Heat/Mass Transfer**
- **Concluding Remarks**

Stages of Liquid Jet Atomization

Primary **jet breakup**:

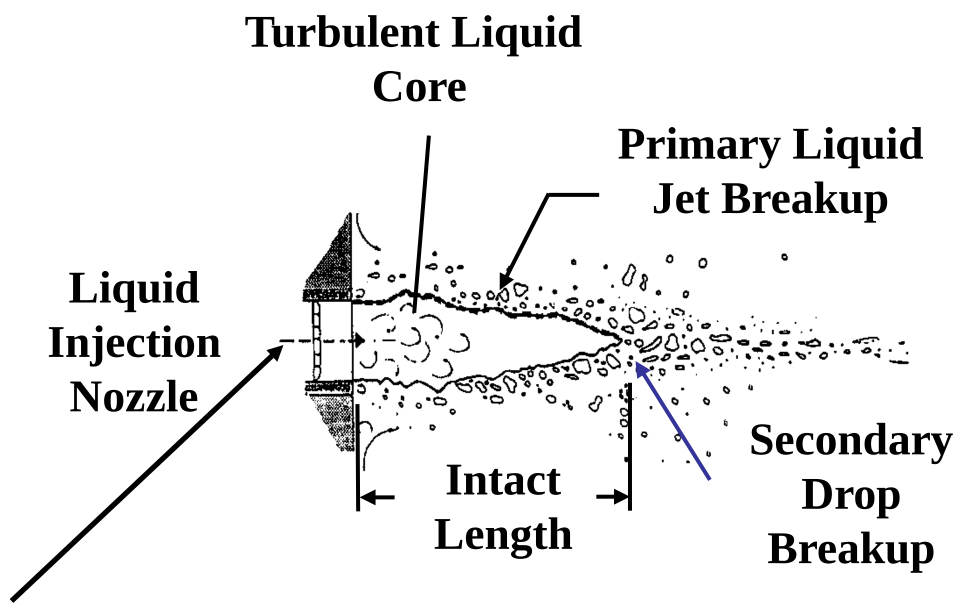
A disintegration process of the liquid jet is subject to cohesive and disruptive forces acting on the jet

Secondary **drop breakup**:

Liquid drops continue breaking into smaller drop sizes as they when traveling downstream

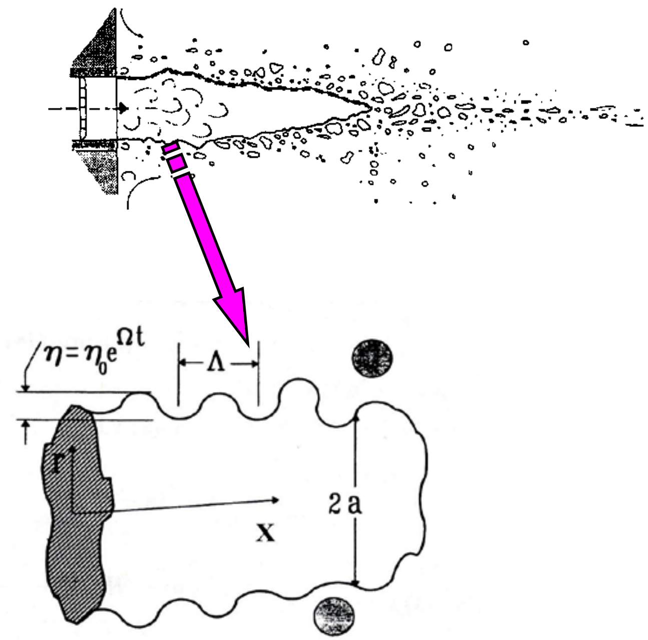
- **In atomization…. "surprising findings…..long accepted theories of primary breakup were NOT effective", Faeth et. al (1994)**

- **"….Sauter Mean Diameter vs. Stream-wise distance could be correlated using surface tension and liquid turbulence alone…"**



Classical Kevin-Helmholtz (KH) Model: Primary Atomization

- Derived based on the linear surface wave stability analysis of a liquid jet.
- The fastest wave growth rate and corresponding wave length responsible for the jet breakup.
- Liquid jet in a form of “blob” parcels containing liquid spherical drops with their size equal to the injection orifice diameter.



Liquid jet represented by “blob” parcels

Fastest Wave Growth Rate →
$$\Omega\left[\frac{\rho_l a^3}{\sigma}\right]^{0.5} = \frac{\left(0.34+0.38We_g^{1.5}\right)}{(1+Z)\left(1+1.4T^{0.6}\right)}$$

Corresponding Wave length →
$$\frac{\Lambda}{a} = 9.02\frac{\left(1+0.45Z^{0.5}\right)\left(1+0.4T^{0.7}\right)}{\left(1+0.87We_g^{1.67}\right)^{0.6}}$$

Rate of Parent Drop Size Change →
$$\frac{da}{dt} = -\left[\frac{a}{\tau} - C_a\frac{L_w}{\tau_w}\right]$$

$$\tau = 3.726 B_1 a / \Lambda\Omega \qquad C_a = \frac{B_0}{3.726 B_1}$$

Time Scale →
$$\tau_w = a/\Lambda\Omega$$

Z : Ohnesorge number
T : Taylor parameter
We : Weber number $\left(\rho_g U^2 r_p/\sigma\right)$
Re : Reynolds number

T-Blob Primary Breakup Model

- Include surface wave phenomenon and turbulence behavior on the primary breakup
- Breakup process described by characteristic length and time scales of individual physical phenomena
- Motion due to a larger kinetic energy having a stronger influence in the liquid jet breakup
- Account for the initial turbulence of the liquid jet as well as the effects of the injector design

New Term

Rate of Parent Drop Size Change →

$$\frac{da}{dt} = -\left[\frac{a}{\tau} - C_a\left(\frac{L_w}{\tau_w} - \frac{L_t}{\tau_t}\right)\right]$$

Turbulent time scale: $\tau_t = \tau_0 + 0.0828t$

Turbulent length scale: $L_t = L_t^0\left(1 + \frac{0.0828t}{\tau_t^0}\right)^{0.457}$

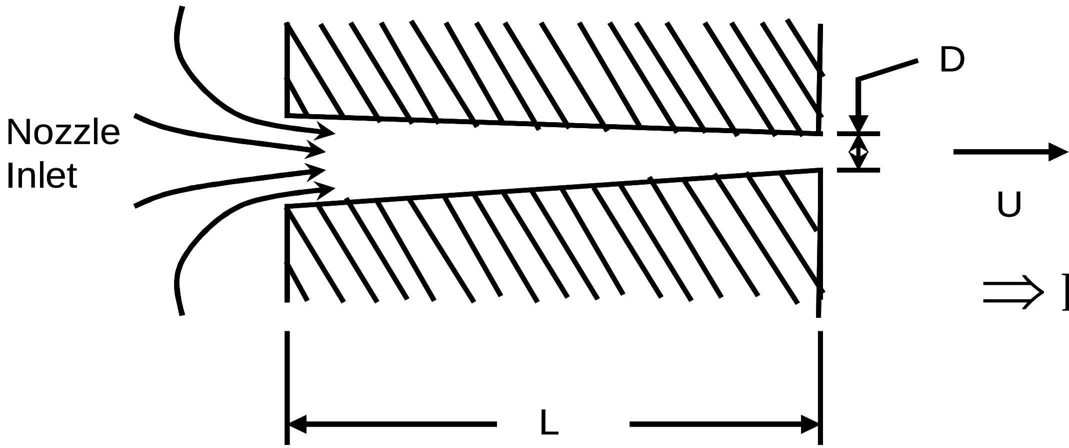
The initial turbulence and injector geometry represented by

τ_t^o and L_t^o

Trinh, H. P., and Chen, C. P., "Modeling of Turbulence Effects on Liquid Jet Atomization & Breakup", *Atomization and Spray*, Vol. 16, pp. 907-932, 2006.

Estimation of Initial Turbulence Quantities

- Total Pressure drop across the injection nozzle



$$\Rightarrow k_t^0 = u'^2 = \frac{U^2}{8L/D}\left[\frac{1}{C_d^2} - Kc - \left(1 - s^2\right)\right]$$

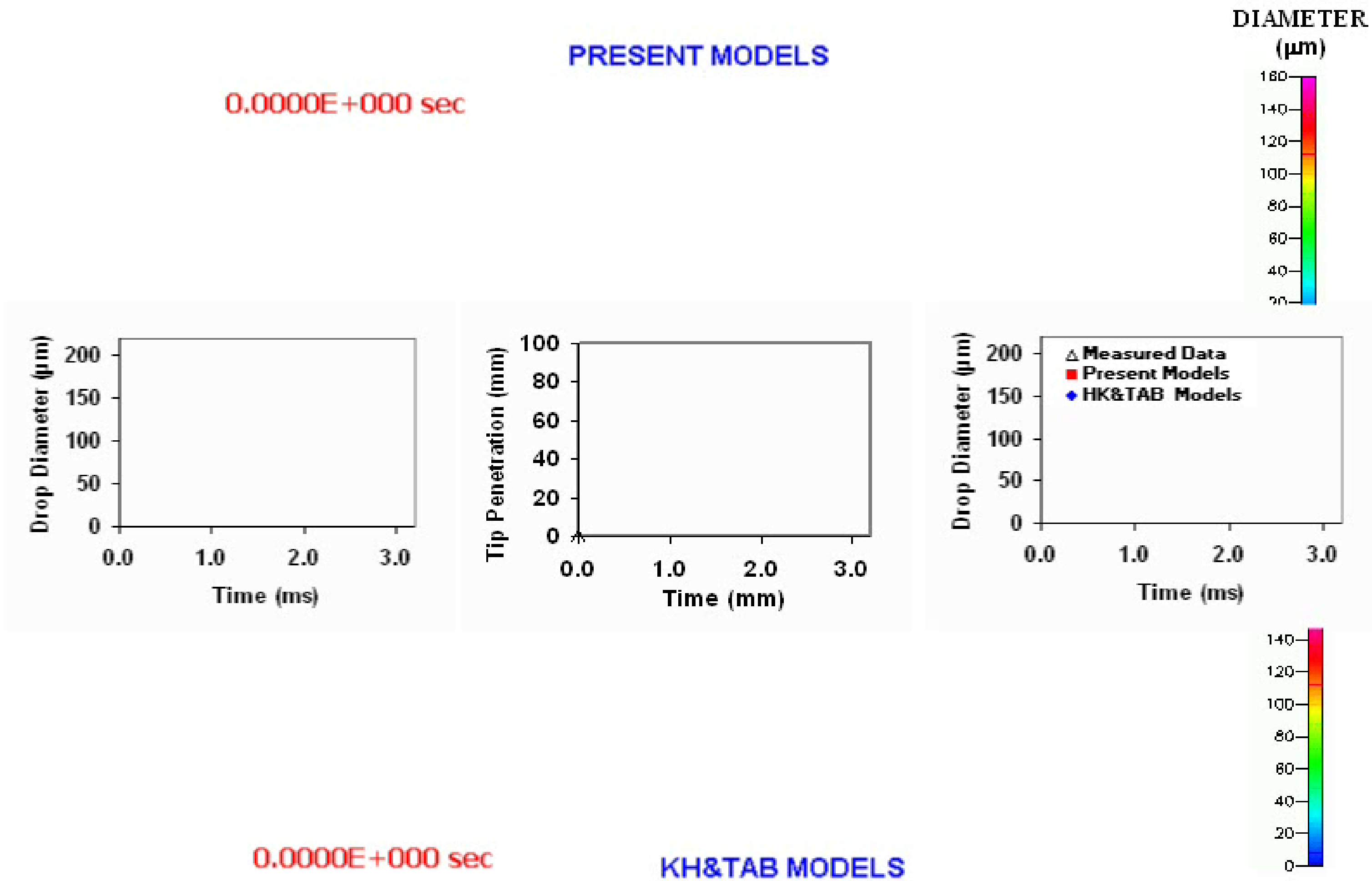
$$\Rightarrow \varepsilon_t^o = K_\varepsilon \frac{U^3}{2L}\left[\frac{1}{C_d^2} - Kc - \left(1 - s^2\right)\right]$$

s: Nozzle contraction area ratio

Kc: Loss coefficient due to nozzle inlet geometry

Cd: Discharge coefficient

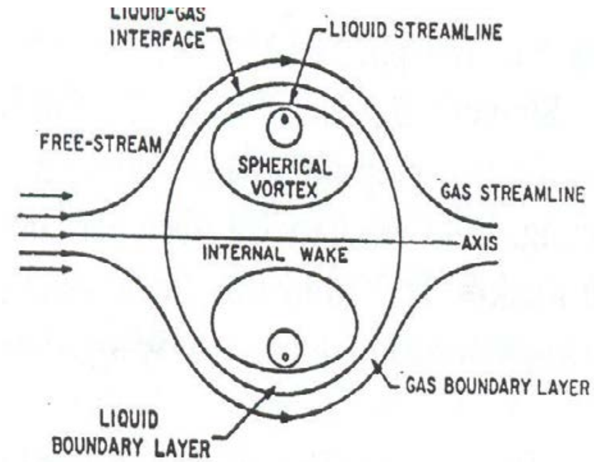
The T-Blob/T-TAB Model



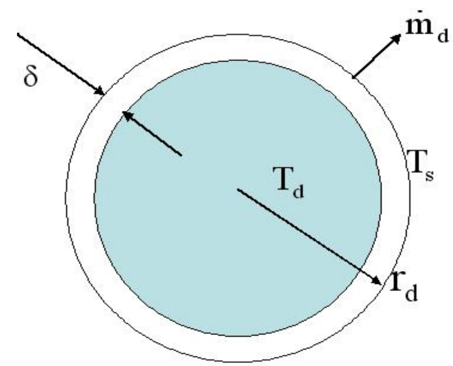
Trinh, Huu P., Chen, C. P. and Balasubramanyan, M. S., ***J. Engineering for Gas Turbines and Power***, Vol. 129, pp. 920-928, **2007**.

Extension to Evaporating Spray

- **“..years of studies show that evaporation *CANNOT* be simplified by rapid-mixing (uniform temperature)… or purely diffusion….” Amsden et al. (2003)**
- **Fully resolution using Differential Equations within each droplet is CPU expensive**



•The T-Blob/T-TAB model can supply phenomenological “structure”
•Current approach based on ‘film theory’ and Two-Temperature formulation
•Mass & heat transfer, takes place inside a thin film surrounding the droplet core
•Film (boundary layer) thickness estimated from the T-Blob/T-TAB



Turbulent Finite Conductivity Model (Cont.)

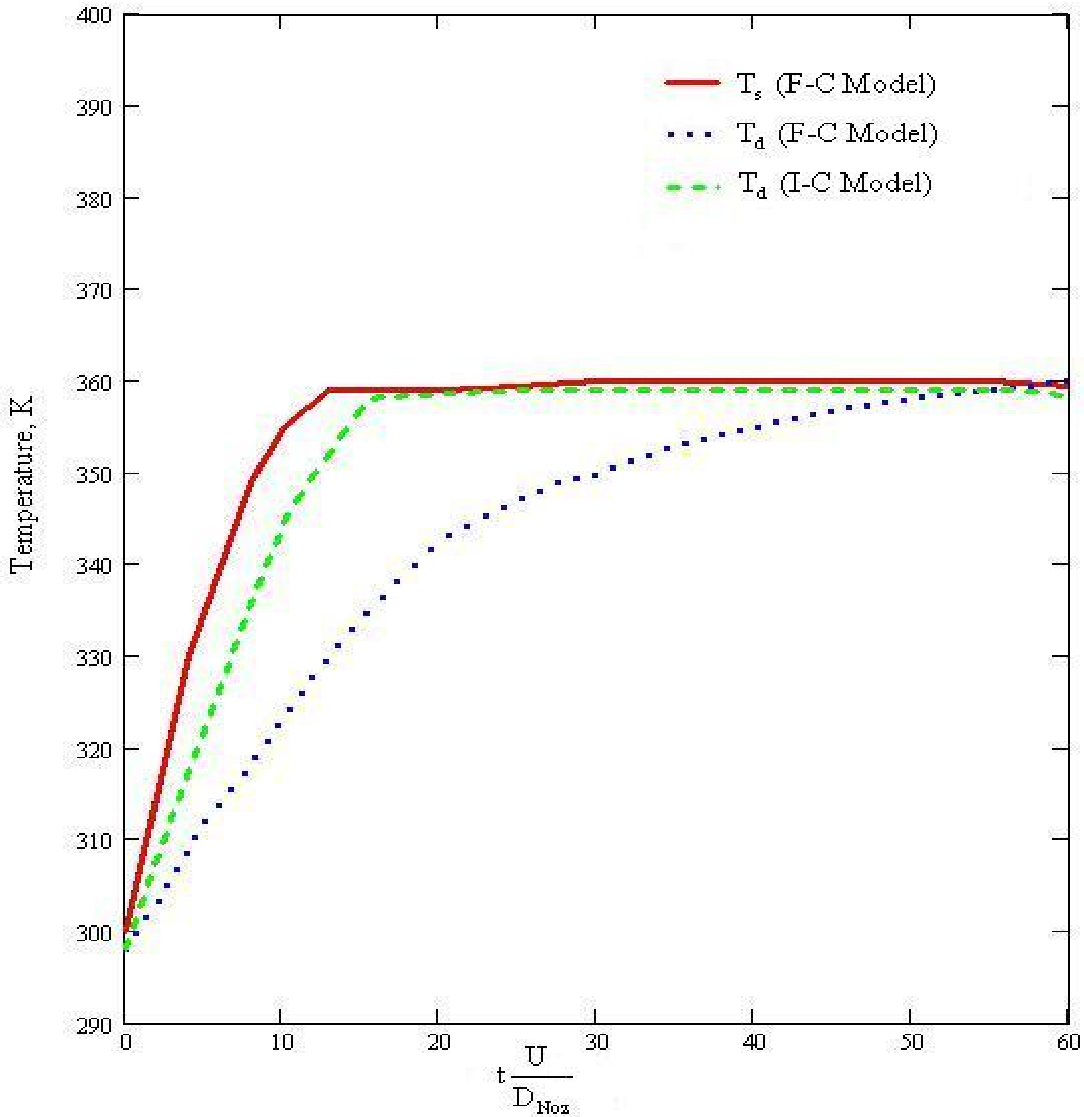
- **Temporal change of the droplet temperature** $$\frac{dT_d}{dt} = \frac{h_l (T_s - T_d) A_d}{\rho_l C_{P,l} V_d}$$
- **HTC - formulated through turbulence characteristics supplied from the T-blob model**
- **The HTC inside droplet determined from the ratio,** $$h_l = \frac{k_l}{\delta_e}$$
- **δ_e , an equivalent thermal boundary layer film thickness,** $$\delta_e = \sqrt{\pi \alpha_{eff} t}$$

$$\alpha_{eff} = \alpha_{lam} + \alpha_{turb}$$

$$\alpha_{lam} = \frac{k_l}{\rho_l C_{P,l}} \qquad \alpha_{turb} = \frac{C_\mu}{Pr_{turb}} \frac{k_l^2}{\varepsilon_l}$$

- **The liquid droplet turbulence quantities k_l and ε_l are obtained from the T-blob spray model**

Variation of the T_s and T_d (one-way results)



- **Study variation of T_S and T_d for the turbulent F-C model**
- **U_d - 102 m/s**
- **Ambient environment - quiescent nitrogen at 600 K**

Mass Transfer Formulation

- Conservation of species "i" across the droplet surface requires:

$$\dot{m}_i = \dot{m} Y_i^{l,s} + J_i^{l,s}(Y_i^l - Y_i^{l,s}) = \dot{m} Y_i^{g,s} + J_i^{g,s}(Y_i^{g,s} - Y_i^{\infty})$$

- The mass transfer rate between the surface and inside of the droplet is modeled by:

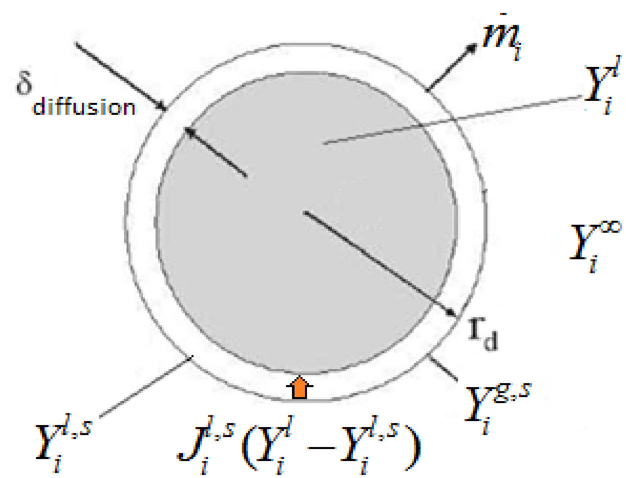
$$J_i^{l,s} = \rho^l \frac{D_{eff}}{\delta_{diffusion}}$$

where:

$$D_{eff} = D^l + D^t$$

$$D^t = C_\mu \frac{(\kappa^t)^2}{\varepsilon^t Sc^t}$$

$$\delta_{diffusion} = \sqrt{\pi D_{eff} t}$$



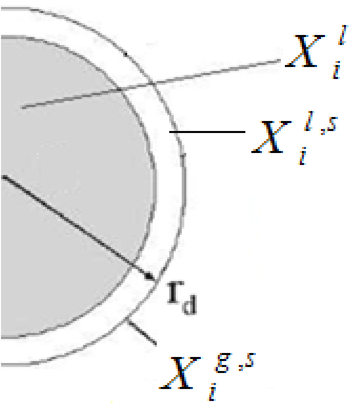
Vapor-Liquid phase Equilibrium

- At high pressure, The vapor-liquid equilibrium at the droplet surface is expressed by the equality of chemical potential of each species in the liquid and vapor phases, and can be written as:

$$X_i^{g,s}\phi_i^{g,s} = X_i^{L,s}\phi_i^{L,s}$$

Where

$$\ln\phi_i = \frac{b_i}{b}(Z-1) - \ln(Z-B) + \frac{A}{2\sqrt{2}B}\left(\frac{b_i}{b} - \delta_i\right)\ln\left(\frac{Z+2.414B}{Z-0.414B}\right)$$



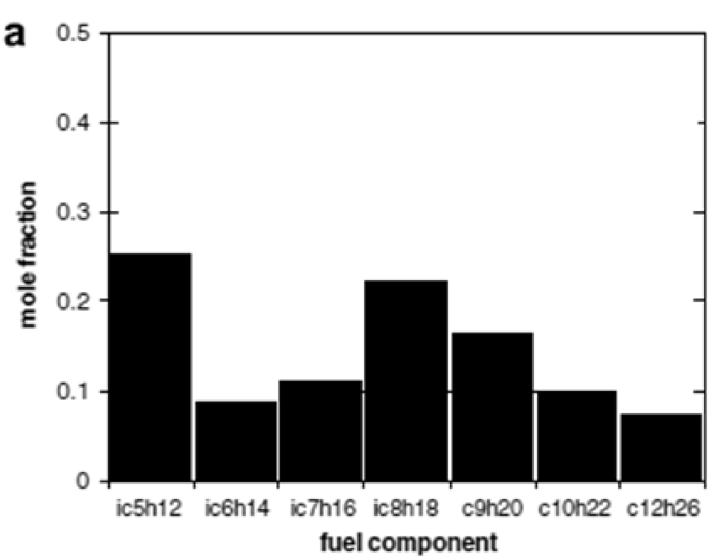
- And compressibility factor:

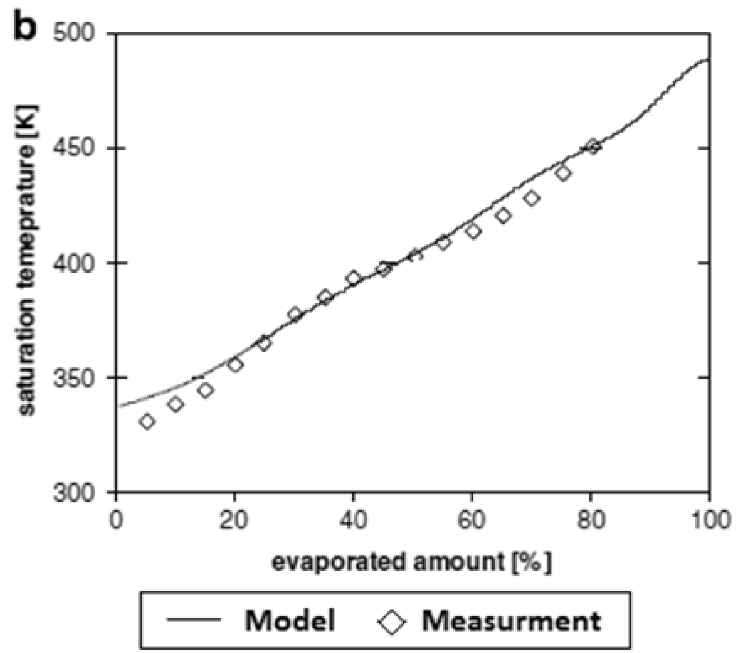
$$Z^3 - (1-B)Z^2 + (A - 3B^2 - 2B)Z - (A\times B - B^2 - B^3) = 0$$

- Partial molar enthalpy:

$$h_i - h_i^0 = -RT^2\frac{\partial}{\partial T}(\ln\phi_i)$$

Diesel Cases - Fuel Surrogate Model





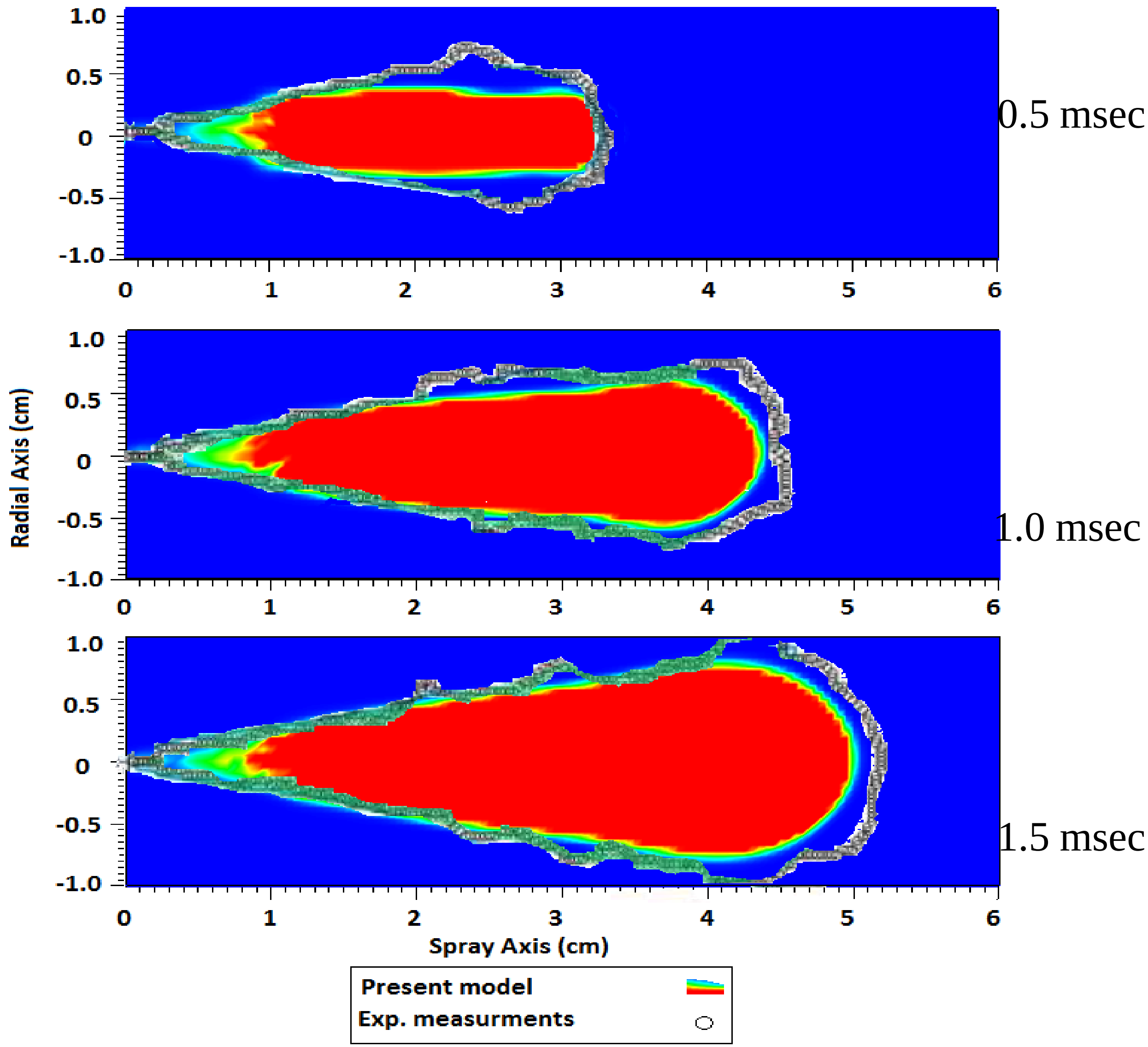
The diesel fuel surrogate mixture :

Matching Distillation Curve

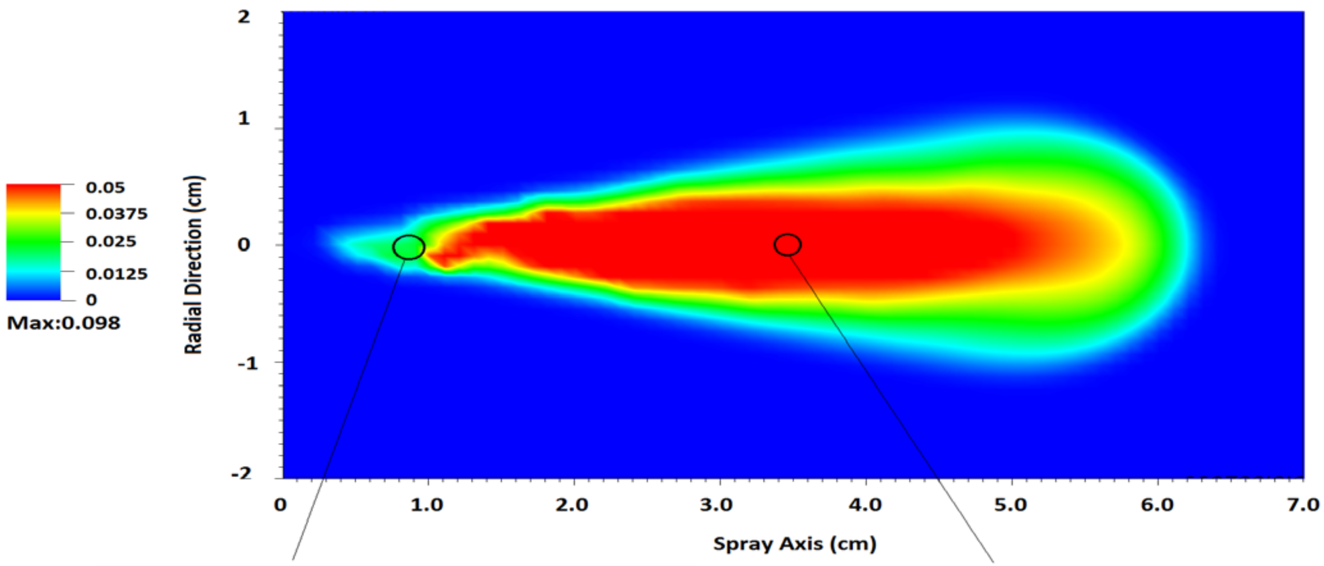
toluene (0.22), decane (0.14), dodecane (0.15), tetradecane (0.23), hexadecane (0.13) octadecane (0.13)

Jet (vapor) penetration at different times

Sandia Lab Spray A Experimental Data - Validations

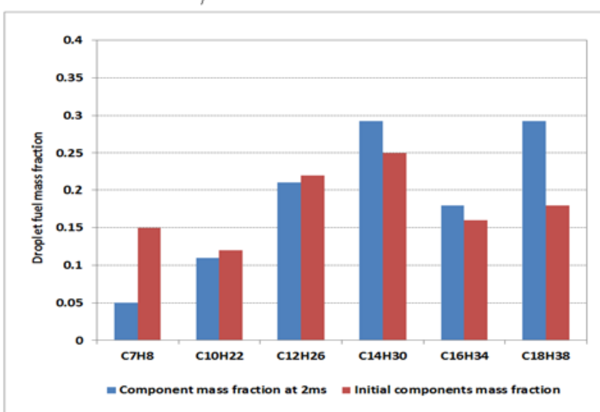


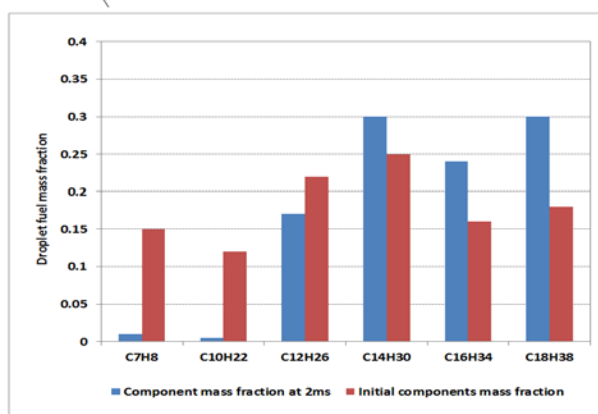
Fuel Vapour mass fraction and Droplet fuel component distributions



KIVA 3V code used

At 2.0 msec





Red bars show initial droplet mass fraction

Summaries

- **Sub-grid Phenomenological models, providing useful predictions for practical engineering applications having similar flow conditions**
- **Development, implementation and validation of T-Blob/T-TAB model**
- **A phenomenological model was formulated to account for finite heat/mass transfer and liquid turbulence within droplet for multi-component fuels.**
- **Due to low diffusivities, transient behavior is present during the entire droplet lifetime.**
- **Two-Way coupled CFD (KIVA-3V, rel. 2) results for diesel evaporating spray show good predictive capability.**

Thank You

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Backup Charts

Sandia Lab Spray A Experimental Data - Validations

Injector dimensions at Sandia National Laboratory experiments (Engine combustion network exp. data archive., 2012).

Injector Type	Bosch common-rail, 2nd generation
Nozzle	Single-hole, KS1.5/86, mini-sac
Nozzle hole exit diameter, D_{exit}	90 μm
Nozzle length	1.0 *mm*
KS factor $(D_{inlet}-D_{exit})/10\ \mu m$	1.5
Max discharge coefficient	0.86
Injection pressure	1500 bar
Injection duration	1.5 ms
Total mass injected	3.5 mg

Operating conditions at Sandia National Laboratory experiments, (Engine Combustion Network exp. data archive., 2012).

Ambient gas temperature	900 K
Ambient gas pressure	Near 6 MPa (Simulation: 5.8 MPa)
Ambient gas density	22.8 kg/m^3
Ambient gas velocity	Near-quiescent, less than 1 m/s

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Summaries -II

- A phenomenological model was formulated to account for **finite heat/mass transfer** and **liquid turbulence** within droplet for multi-component fuels.

- Due to low diffusivities, **transient behavior** is present during the entire droplet lifetime.

- The surface mass fraction of the light component is high during the early period of the heat-up /evaporation **(swelling possible);** light component trapped within droplet may cause **micro-explosion**

- By increasing turbulent Schmidt/Prandtl number, the rate of mass transfer/Heat transfer will be decreased inside of the droplet.; has the capability for tuning **liquid turbulent Schmidt** number for each component to get varied vapor mass fraction history at gas side.

- Two-Way coupled CFD (KIVA-3V) results for diesel evaporating spray show good predictive capability