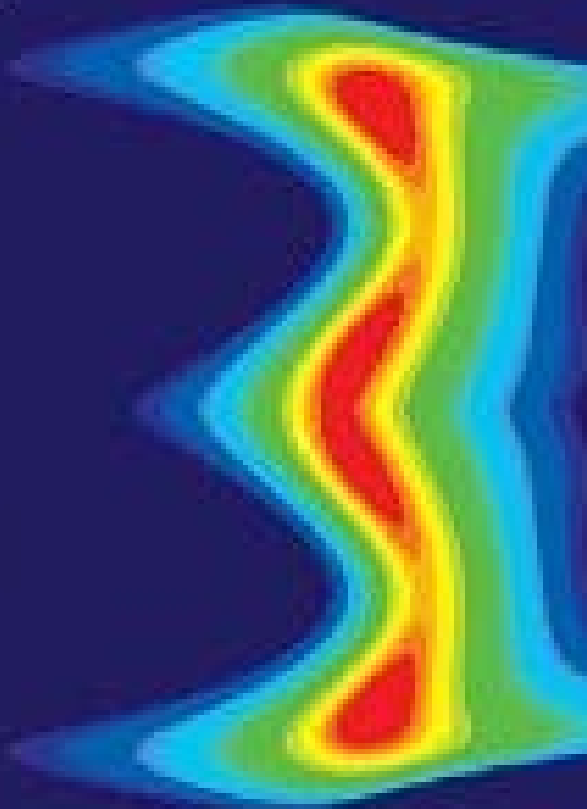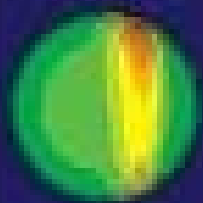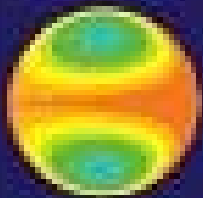William A. Sirignano

FLUID DYNAMICS AND TRANSPORT OF DROPLETS AND SPRAYS

Second Edition

Lecture Topics

Transient Droplet Vaporization
Convective Vaporization
Liquid Circulation
Transcritical Thermodynamics
Droplet Drag and Motion
Spray Computations
Turbulence Effects

Topics in Other Lectures

Droplet Groups and Array
Instability of Injected Liquid
**Liquid Fuel-Films**

Other Book Topics

Multicomponent Liquids
Buoyancy
More Details

Computational Challenges with Spray Combustion Flows

- **Combustor size -- 10 – 100 cm**

- **Computational mesh size -- 1—10 mm**

- **Droplet size -- 10—100 microns**

- **Droplet spacing -- 100—1000 microns**

- **Full resolution is not feasible; sub-grid models are required.**

- **Often vaporization is slow compared to other processes and**

- **rate controlling; so, accurate sub-grid models are required.**

- **Even when vaporization is not slow compared to other processes, the droplet trajectory and vaporization rate controls the mixture ratio distribution in the combustor. So, again, accurate modelling is vital.**

Isolated Spherically Symmetric Burning Fuel Droplet
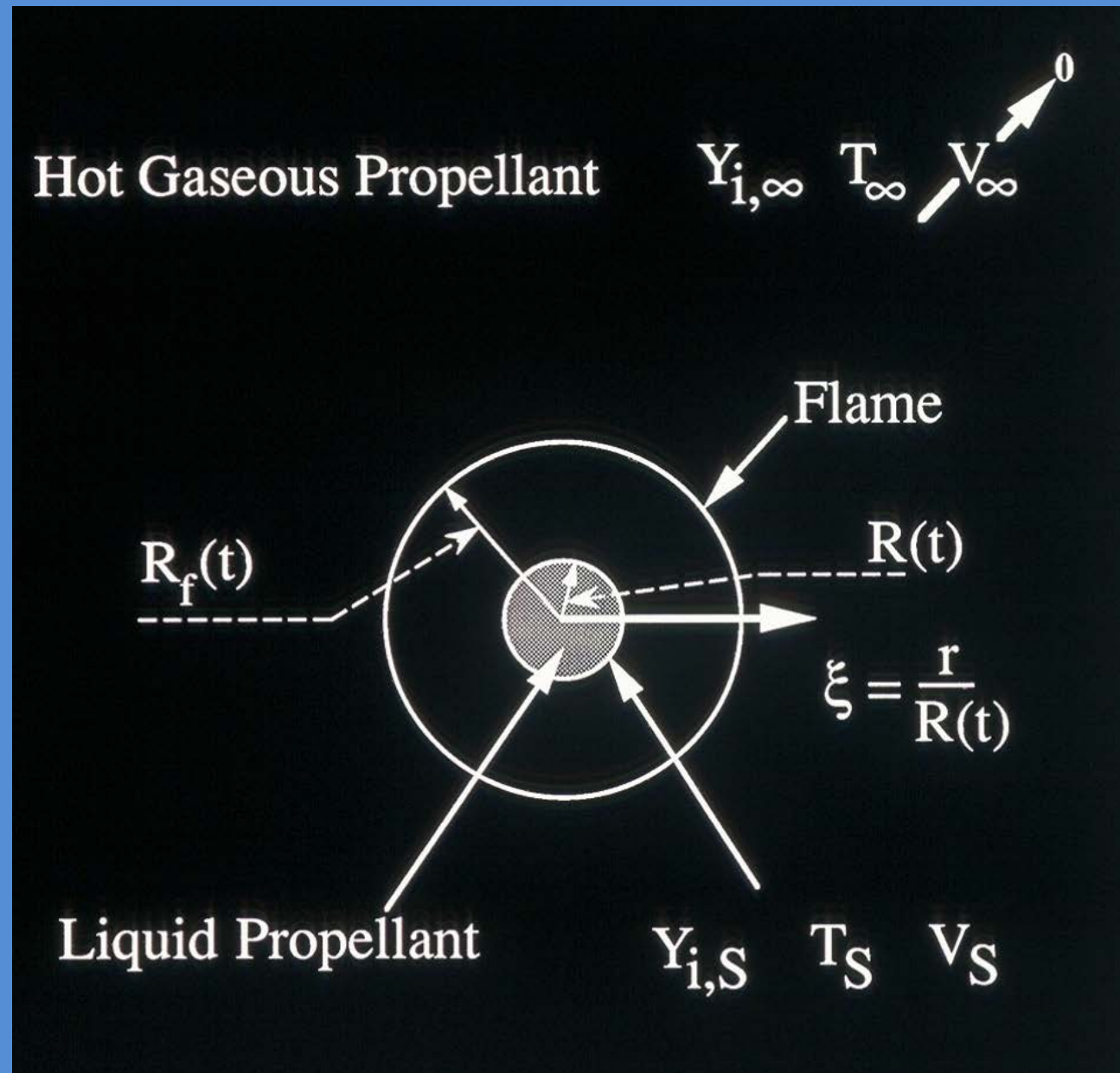
SPHERICALLY SYMMETRIC VAPORIZATION MODEL

Gas-Phase Equations:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2}\frac{\partial(\rho u r^2)}{\partial r} = 0$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{1}{r^2}\frac{\partial}{\partial r}(\rho u r^2 Y_i) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho r^2 \mathcal{D}\frac{\partial Y_i}{\partial r}\right) + S_{Y_i}$$

$$\frac{\partial}{\partial t}(\rho C_p T) + \frac{1}{r^2}\frac{\partial}{\partial r}(\rho u r^2 C_p T) =$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(k r^2 \frac{\partial T}{\partial r}\right) + T\left[\frac{\partial}{\partial t}(\rho C_p) + \frac{1}{r^2}\frac{\partial}{\partial r}(\rho u r^2 C_p)\right] + S_T$$

Liquid-Phase Equations:

$$\frac{\partial T}{\partial t} = \frac{1}{\rho C_p r^2}\frac{\partial}{\partial r}\left(k r^2 \frac{\partial T}{\partial r}\right)$$

$$\frac{\partial}{\partial t}(\rho Y_i) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho \mathcal{D} r^2 \frac{\partial Y_i}{\partial r}\right)$$

Non-dimensional Parameters and Vaporization Rate
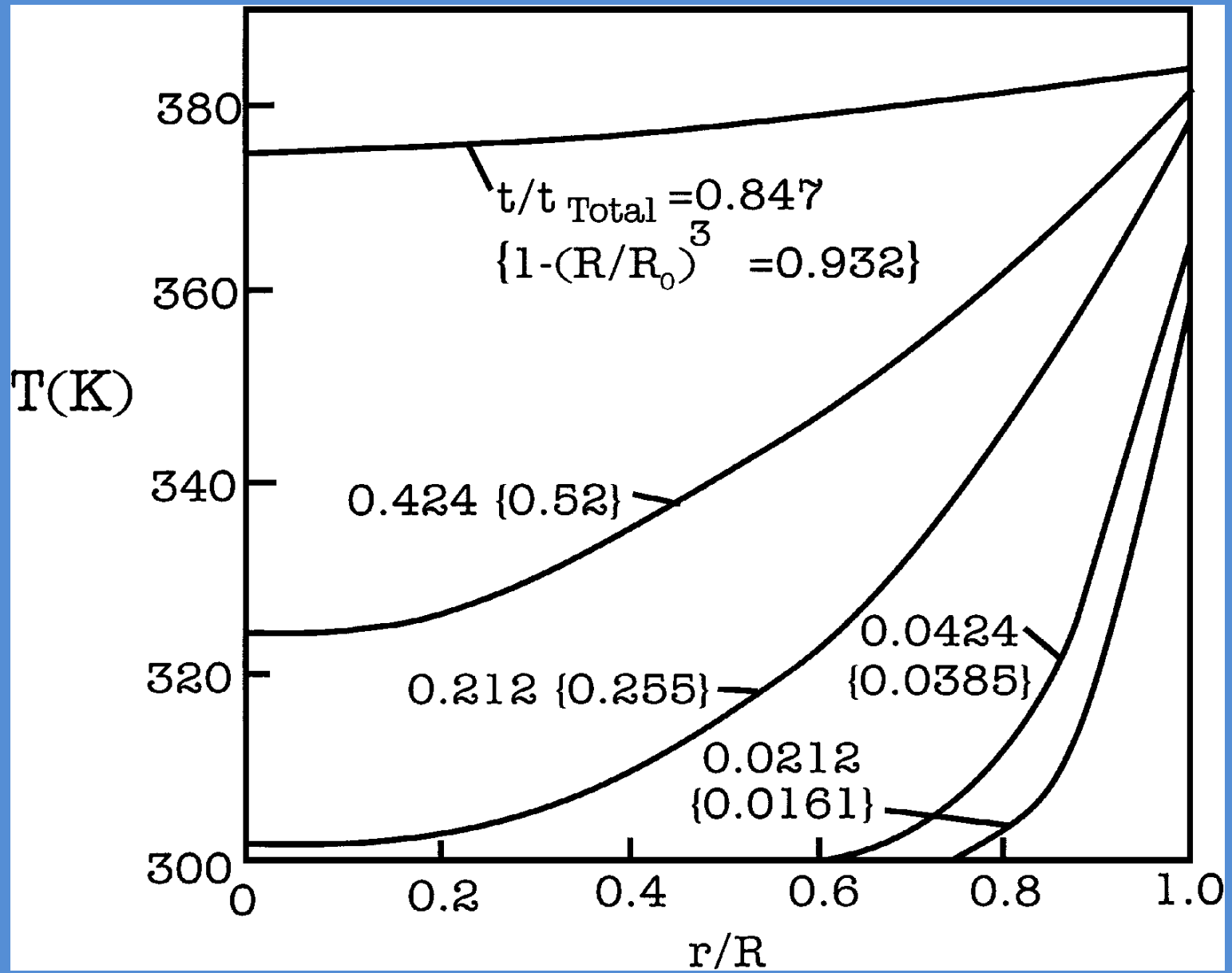
$$\mathrm{Nu} \;=\; 2\frac{\log(1 + B_H)}{B_H}$$

$$\mathrm{Sh} \;=\; 2\frac{\log(1 + B_M)}{B_M}$$

$$\dot{m} \;=\; 4\pi\frac{\lambda R}{c_{pF}}\log(1 + B_H) = \; 4\pi\rho DR\log(1 + B_M)$$
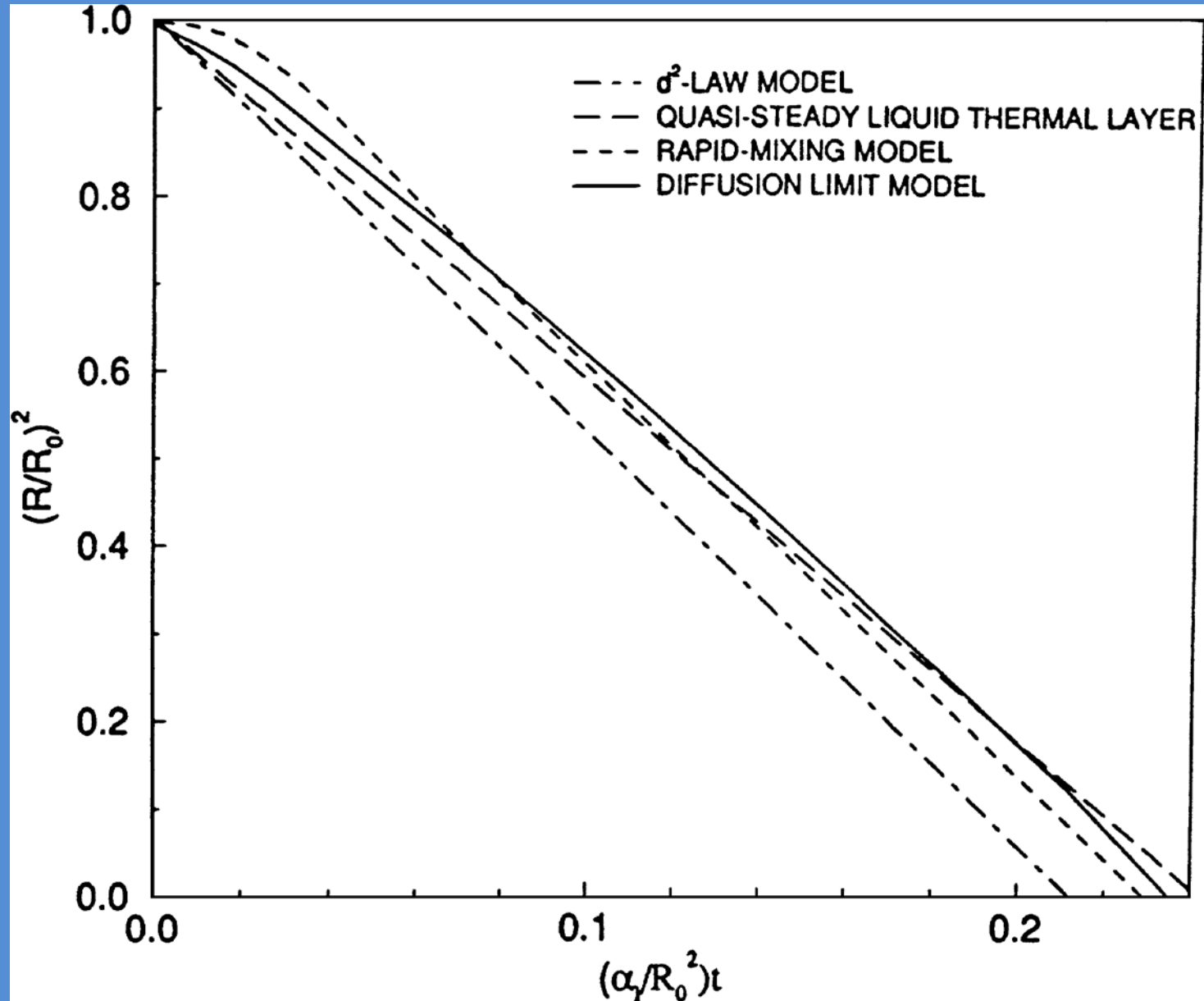
$$B_H = \frac{h_e - h_s}{L_{\mathrm{eff}}}, \qquad B_M = \frac{Y_{Fs} - Y_{F\infty}}{1 - Y_{Fs}},$$

Note that when $\mathrm{Pr} = \mathrm{Sc}$, we have $B_M = B_H$.
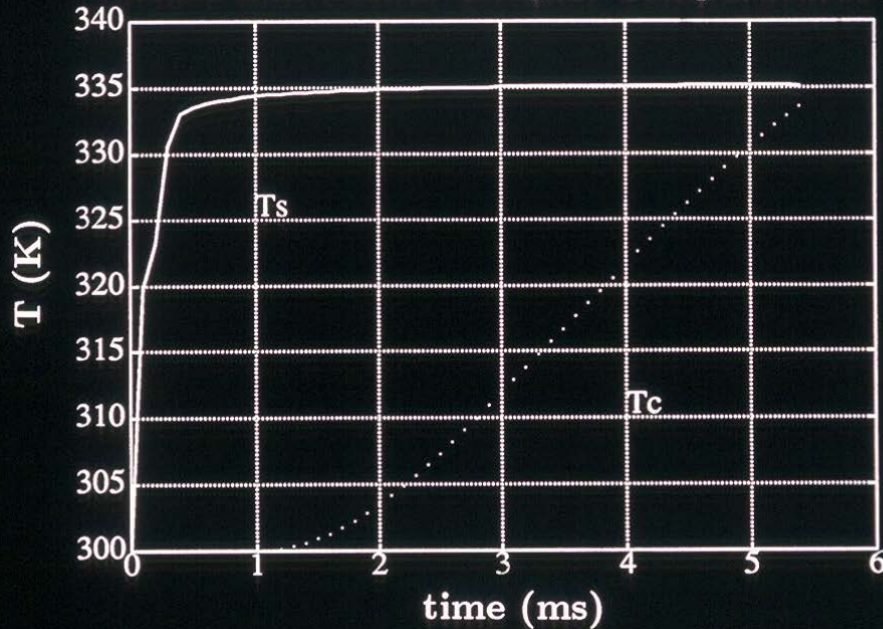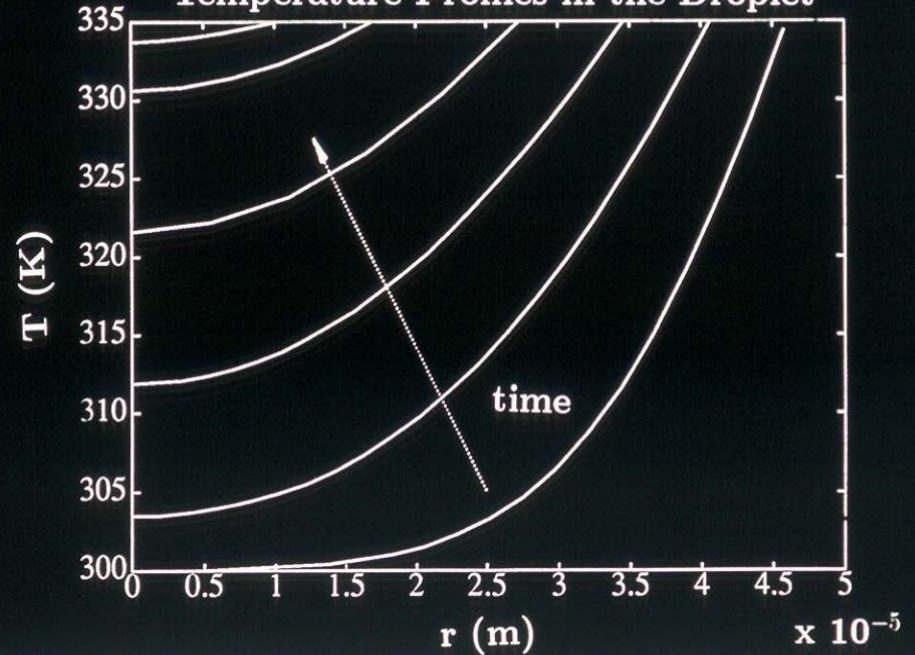
Transient Liquid Temperature
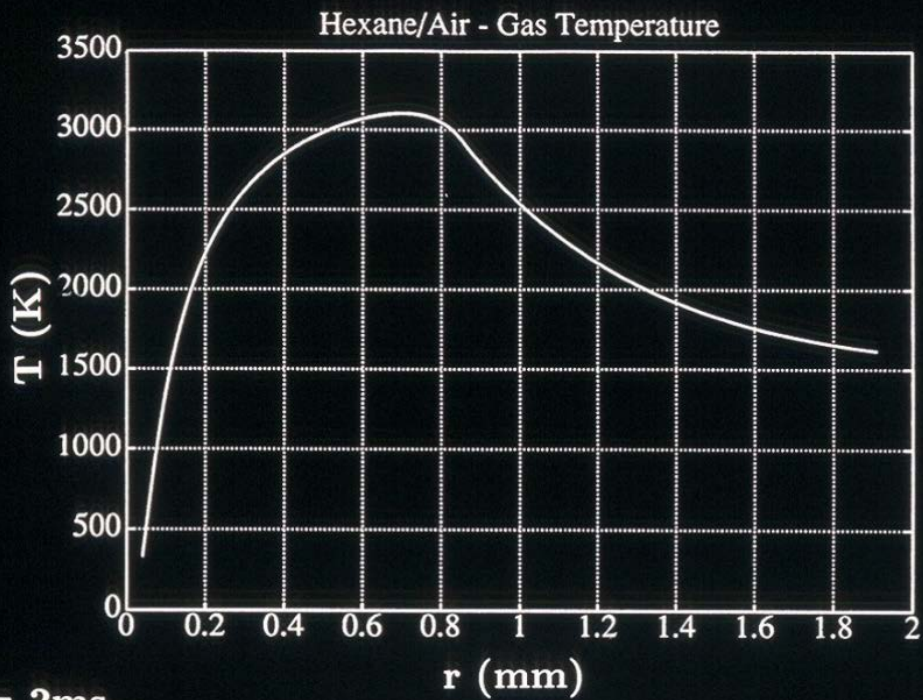
Droplet Radius vs. Time

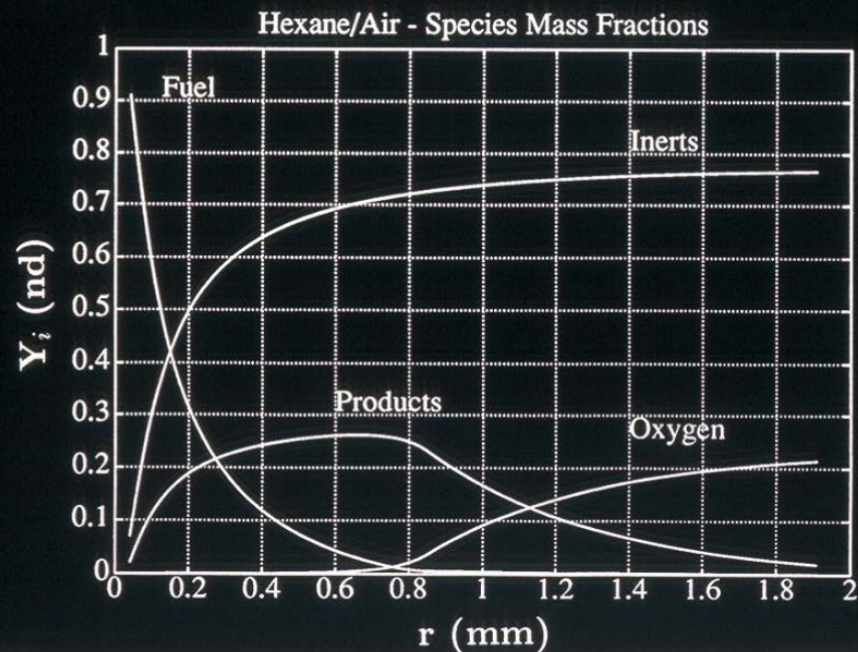**For rapid vaporization, delay in liquid heating becomes significant. A uniform-temperature assumption is poor.**
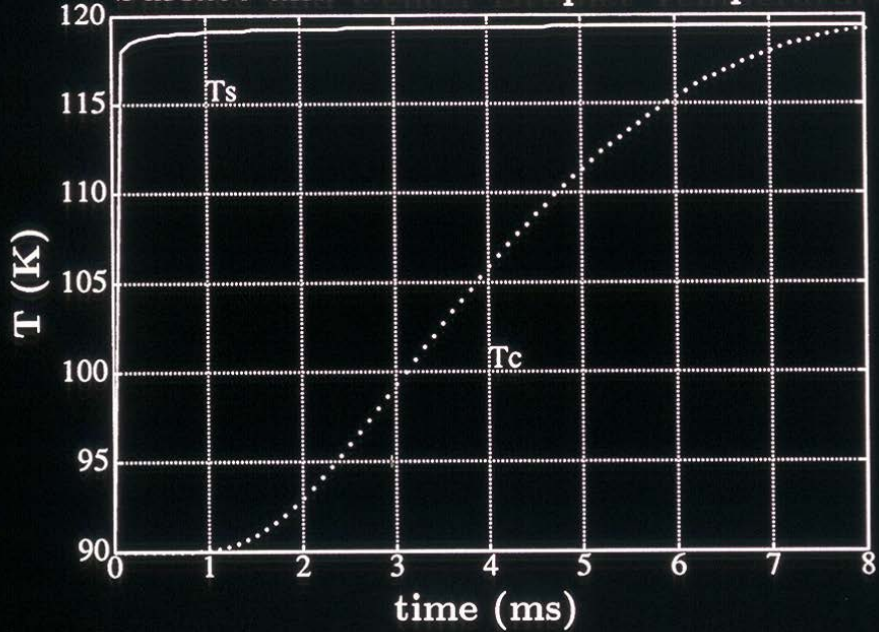
Hexane/Air - Gas Temperature

$t = 2ms$

Gas thermal and mass diffusivities are large. Thus, gas has a quasi-steady behavior. However, continual adjustment to liquid conditions occurs.
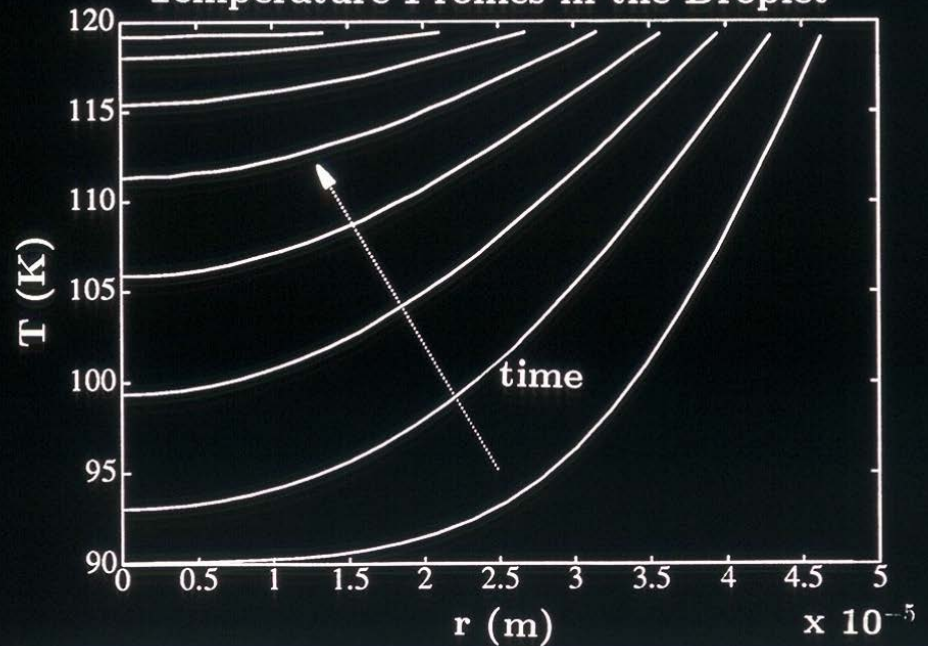

Hexane/Air - Species Mass Fractions

LOX Droplet in Hydrogen
Surface and Center Droplet Temperatures

Temperature Profiles in the Droplet

For H$_2$ / O$_2$ propellants, the oxygen droplet vaporizes more slowly.

Relative Gas-droplet Motion:
Convection and Advection

Gas-Phase Equations:

$$\mathbf{L}^\diamond[\rho] = 0$$

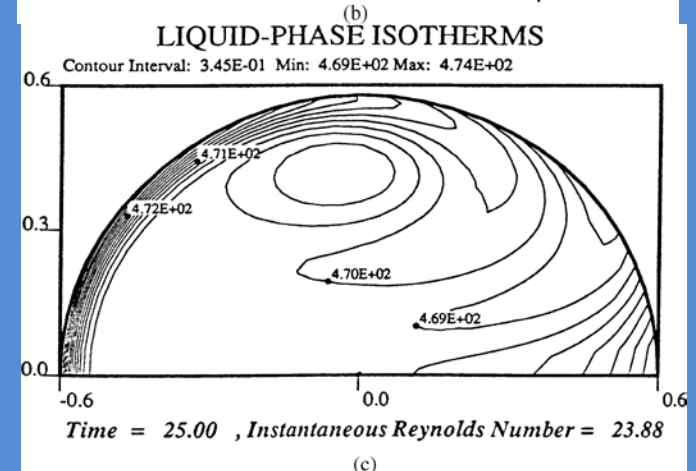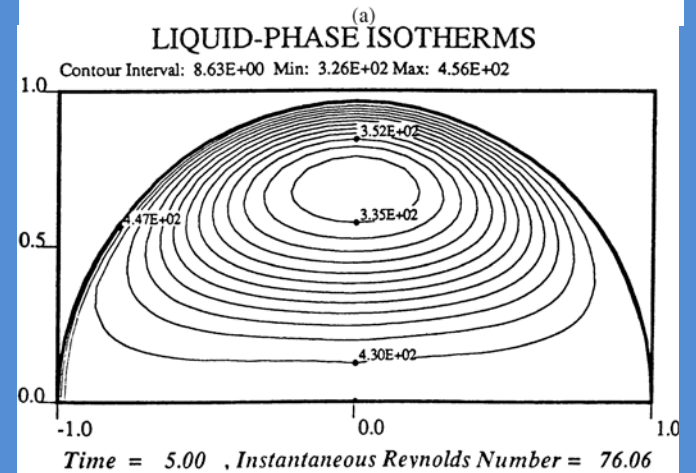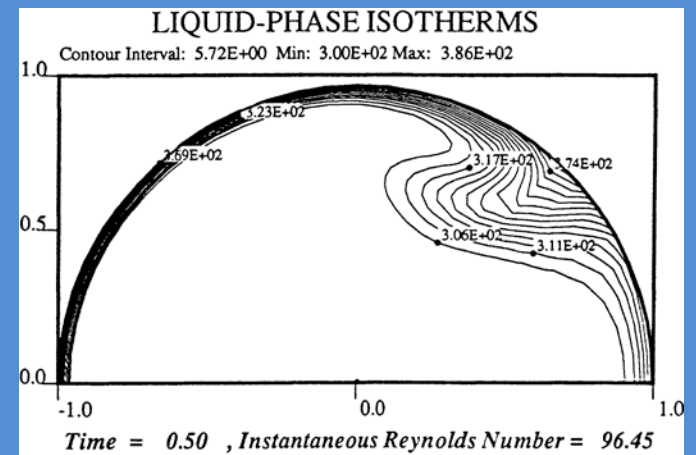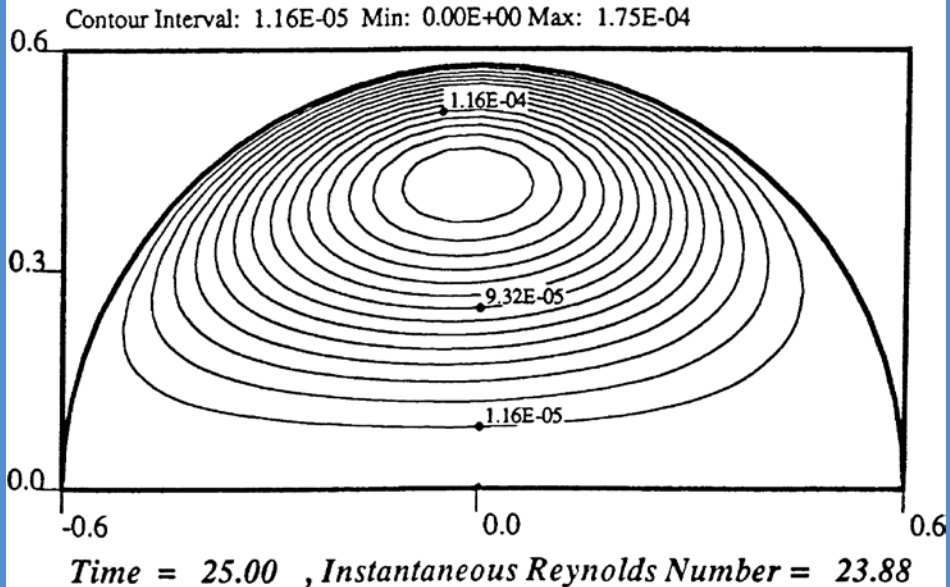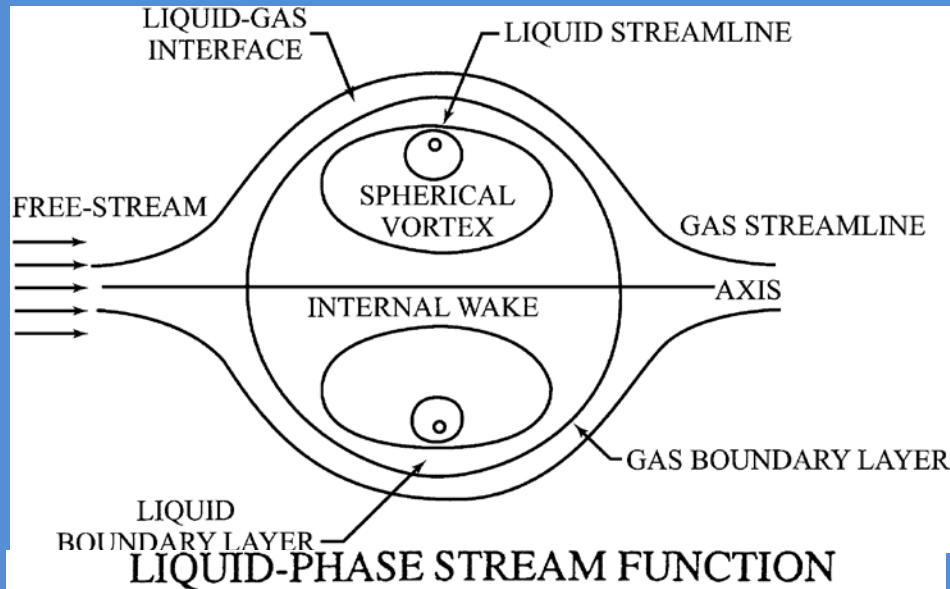$$\mathbf{L}^\diamond[\rho Y_i] = \nabla.(\rho\mathcal{D}\nabla Y_i) + S_{Y_i}$$

$$\mathbf{L}^\diamond[\rho C_p T] = \nabla.(k\nabla T) + \rho T\frac{DC_p}{Dt} + S_T$$

$$\mathbf{L}^\diamond[\ ] = \frac{\partial()}{\partial t} + (\nabla.()\mathbf{v}) \qquad \frac{D}{Dt}[\ ] = \frac{\partial()}{\partial t} + \mathbf{v}.(\nabla())$$

**Liquid-Phase Equations:**

$$\rho C_p\frac{DT}{Dt} = \nabla.(k\nabla T)$$

Internal circulation of the liquid is important: convection.

LIQUID-GAS INTERFACE — LIQUID STREAMLINE

FREE-STREAM

SPHERICAL VORTEX

GAS STREAMLINE

AXIS

INTERNAL WAKE

GAS BOUNDARY LAYER

LIQUID BOUNDARY LAYER

LIQUID-PHASE STREAM FUNCTION

Contour Interval: 1.16E-05 Min: 0.00E+00 Max: 1.75E-04

1.16E-04

9.32E-05

1.16E-05

Time = 25.00 , Instantaneous Reynolds Number = 23.88

LIQUID-PHASE ISOTHERMS

Contour Interval: 5.72E+00 Min: 3.00E+02 Max: 3.86E+02

3.23E+02

2.69E+02

3.17E+02   3.74E+02

3.06E+02   3.11E+02

Time = 0.50 , Instantaneous Reynolds Number = 96.45

(a)

LIQUID-PHASE ISOTHERMS

Contour Interval: 8.63E+00 Min: 3.26E+02 Max: 4.56E+02

3.52E+02

3.47E+02   3.35E+02

4.30E+02

Time = 5.00 , Instantaneous Reynolds Number = 76.06

(b)

LIQUID-PHASE ISOTHERMS

Contour Interval: 3.45E-01 Min: 4.69E+02 Max: 4.74E+02

4.71E+02

4.72E+02

4.70E+02

4.69E+02

Time = 25.00 , Instantaneous Reynolds Number = 23.88

(c)

"Rapid Mixing" does not produce a uniform temperature. However, characteristic liquid heating length and time are reduced considerably.
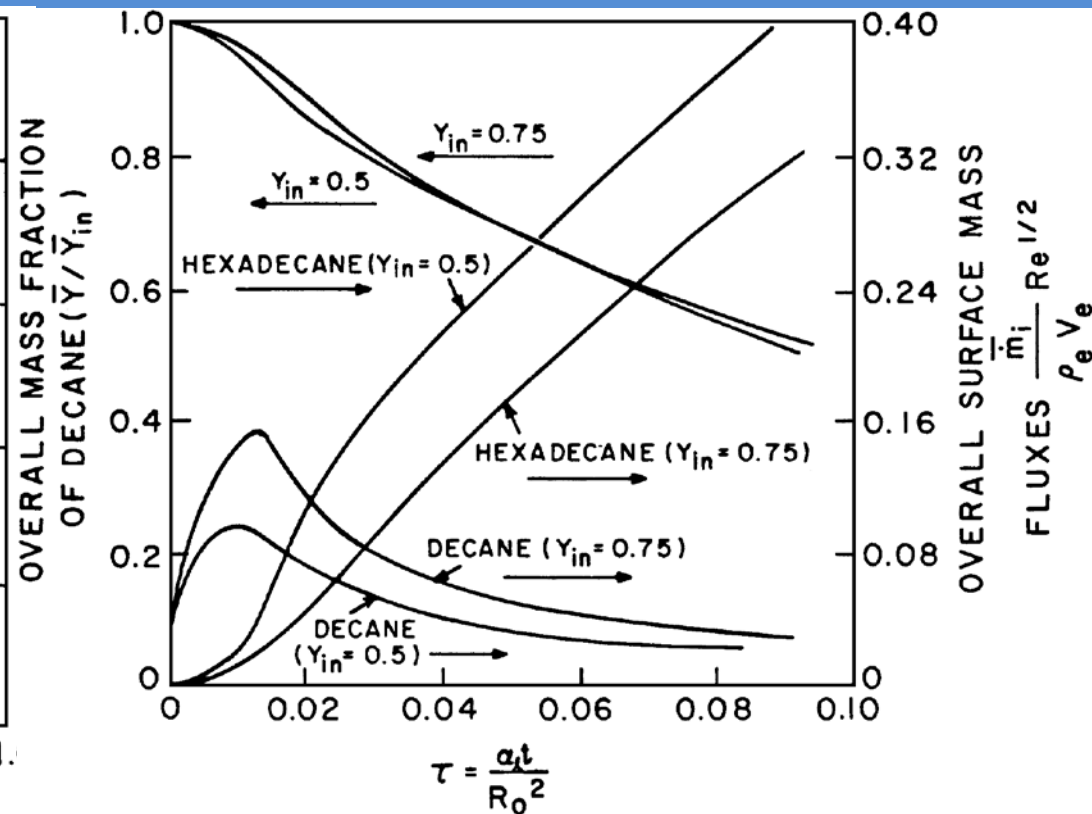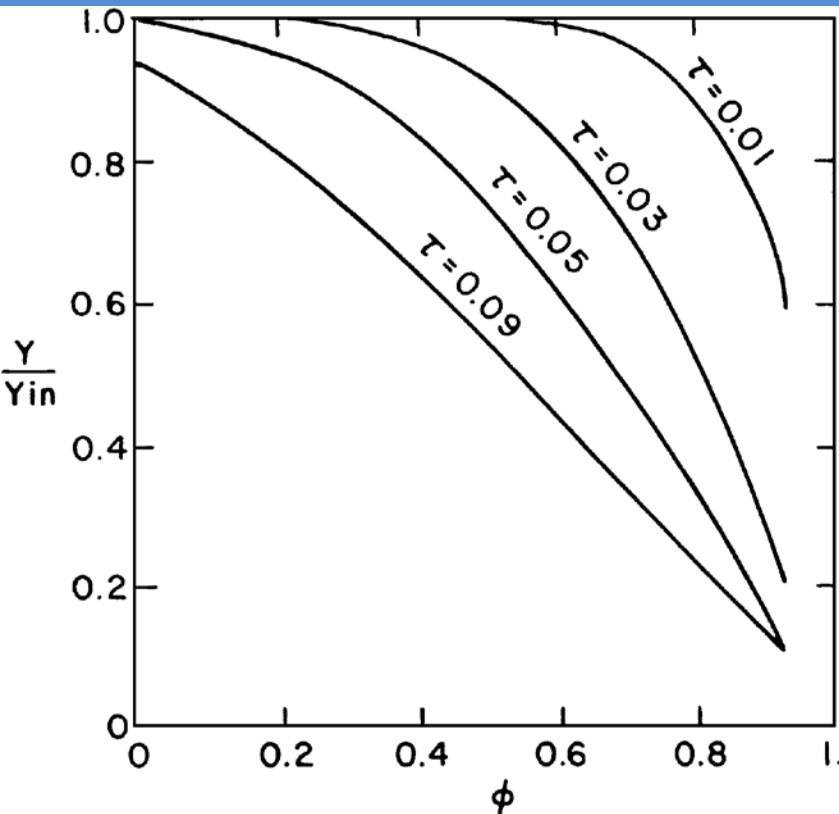
CURRENT PHILOSOPHY

SIMPLIFIED MODELS -	PROVIDE NECESSARY COMPUTATIONAL SIMPLICITY TO PREDICT DROPLET VAPORIZATION IN SPRAY COMBUSTOR (A VERY LARGE SCALE INTEGRATED SYSTEM).
EXACT MODELS -	PREDICT DRAG COEFFICIENTS, NUSSELT & SHERWOOD NUMBERS FOR SIMPLIFIED MODELS. PROVIDE DETAILED INSIGHTS. STUDY DROPLET INTERACTIONS.
INFINITE-CONDUCTIVITY -	USEFUL HISTORICAL STEP. USEFUL IN CODE DEVELOPMENT. NOT RECOMMENDED FOR SPRAY CALCULATION.
FINITE-CONDUCTIVITY	ZERO REYNOLDS NUMBER LIMIT OF SIMPLIFIED MODELS.
CONSTANT LIQUID TEMPERATURE -	REVERENCE TO THE FOUNDERS. NOT RECOMMENDED FOR SPRAY CALCULATIONS.

Gas Film Model

Abramzon-Sirignano Convective Droplet Heating and Vaporization Model:
Gas Film Model and Effective Liquid Diffusivity Model

$$\text{Nu} = 2\frac{\log(1+B_H)}{B_H}\left[1 + \frac{k}{2}\frac{\text{Pr}^{1/3}\text{Re}^{1/2}}{F(B_H)}\right]$$

$$\text{Sh} = 2\frac{\log(1+B_M)}{B_M}\left[1 + \frac{k}{2}\frac{\text{Sc}^{1/3}\text{Re}^{1/2}}{F(B_M)}\right],$$

$$\dot{m} = 4\pi\frac{\lambda R}{c_{pF}}\log(1+B_H)\left[1 + \frac{k}{2}\frac{\text{Pr}^{1/3}\text{Re}^{1/2}}{F(B_H)}\right]$$

$$= 4\pi\rho DR\log(1+B_M)\left[1 + \frac{k}{2}\frac{\text{Sc}^{1/3}\text{Re}^{1/2}}{F(B_M)}\right]$$

Note that when $\text{Pr} = \text{Sc}$, we have $B_M = B_H$. Otherwise,

$$B_H = (1+B_M)^a - 1$$

$$F(B) = (1+B)^{0.7}\frac{\ln(1+B)}{B}$$

$$a \equiv \frac{c_{pF}}{c_p}\frac{1}{\text{Le}}\frac{1 + \frac{k}{2}\frac{\text{Sc}^{1/3}\text{Re}^{1/2}}{F(B_M)}}{1 + \frac{k}{2}\frac{\text{Pr}^{1/3}\text{Re}^{1/2}}{F(B_H)}}.$$

$$B_H = \frac{h_e - h_s}{L_{\text{eff}}}, \qquad B_M = \frac{Y_{Fs} - Y_{F\infty}}{1 - Y_{Fs}},$$

Effective Diffusivity Model for Liquid Phase

$$\alpha_{l\,\text{eff}} = \chi\alpha_l, \qquad \chi = 1.86 + 0.86\tanh[2.225\log_{10}(\text{Pe}_l/30)].$$

$$\frac{\partial T_l}{\partial t} = \frac{\alpha_{l\,\text{eff}}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T_l}{\partial r}\right) = \alpha_{l\,\text{eff}}\left(\frac{\partial^2 T_l}{\partial r^2} + \frac{2}{r}\frac{\partial T_l}{\partial r}\right).$$

$$\zeta = \frac{r}{R(t)}, \qquad \tau = \frac{\alpha_l t}{R_0^2}, \qquad r_s(\tau) = \frac{R(t)}{R_0}, \qquad \frac{\partial z}{\partial \zeta}(0,\tau) = 0.$$

$$z = \frac{T_l - T_{l0}}{T_{l0}}, \qquad \beta = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\tau}(r_s^2),$$

$$r_s^2\frac{\partial z}{\partial \tau} - \beta\zeta\frac{\partial z}{\partial \zeta} = \frac{\chi}{\zeta^2}\frac{\partial}{\partial \zeta}\left(\zeta^2\frac{\partial z}{\partial \zeta}\right). \qquad \beta = -\dot{m}/4\pi\rho_l\alpha_l R.$$

$$\frac{\partial z}{\partial \zeta}(1,\tau) = \frac{\lambda}{\lambda_l}\left(\frac{T_\infty - T_s}{2T_{l0}}\right)\text{Nu} - \frac{\dot{m}L}{4\pi R\lambda_l T_{l0}}. \qquad \beta = -\frac{\lambda}{\lambda_l}\frac{c_l}{c_{pF}}\log(1+B_H)\left[1 + \frac{k}{2}\frac{\text{Pr}^{1/3}\text{Re}^{1/2}}{F(B_H)}\right].$$

$$\frac{\partial z}{\partial \zeta}(1,\tau) = \log(1+B_H)\left[1 + \frac{k}{2}\frac{\text{Pr}^{1/3}\text{Re}^{1/2}}{F(B_H)}\right]\frac{\lambda}{\lambda_l}\left(\frac{T_\infty - T_s}{T_0 B_H} - \frac{L}{c_p T_0}\right).$$

Reynolds number and Peclet number can become large. This will tend to make stream surfaces closer to isotherms. The characteristic length and characteristic time for liquid-phase conduction are reduced significantly.
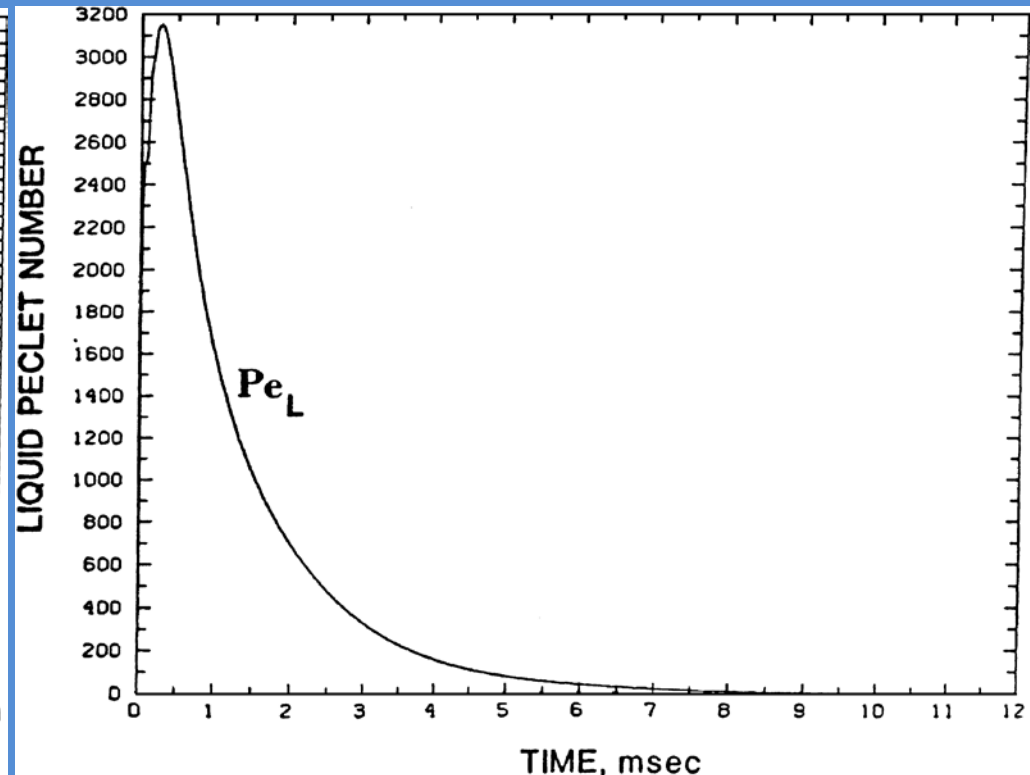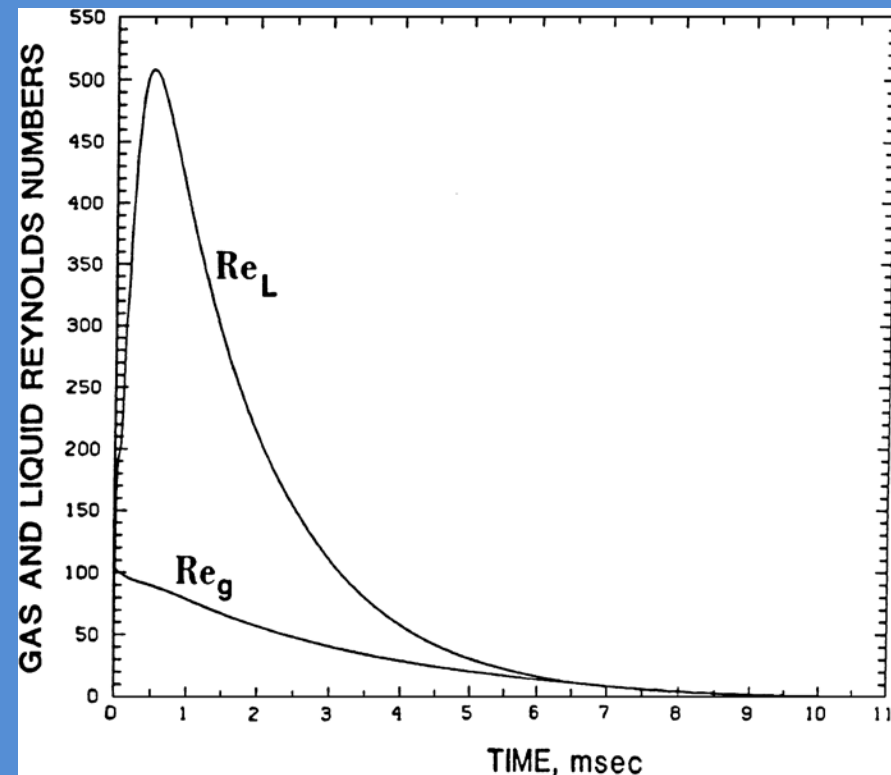
Comparisons

1) **Exact Numerical Solution**
2) **Infinite Conductivity (Rapid Mixing)**
3) **Finite Conductivity**
4) **Effective Conductivity, clearly the most successful match with the benchmark.**
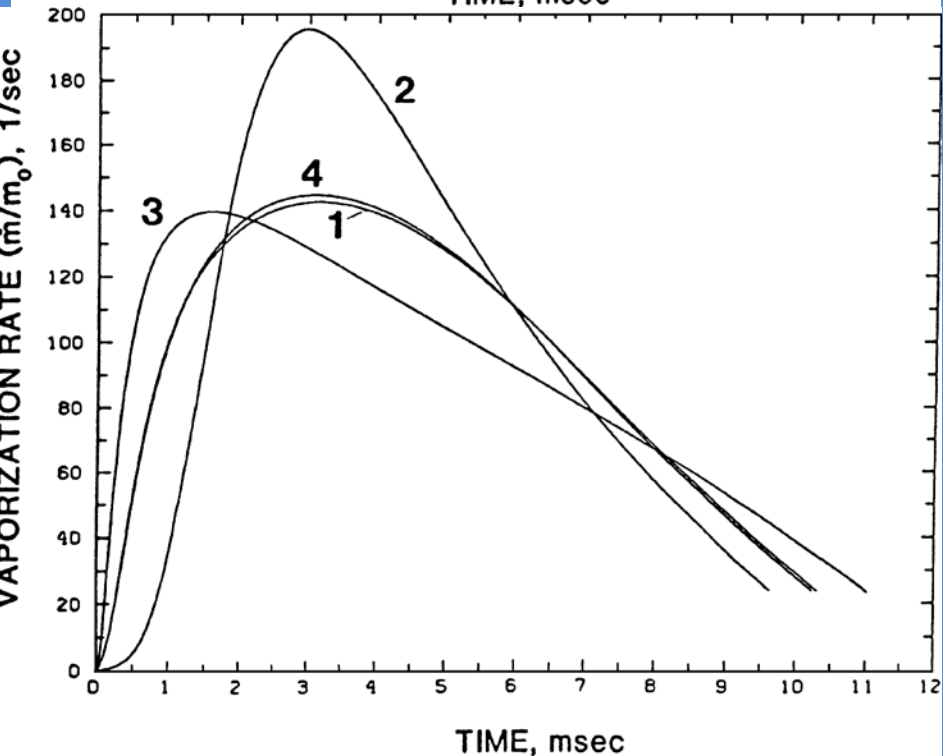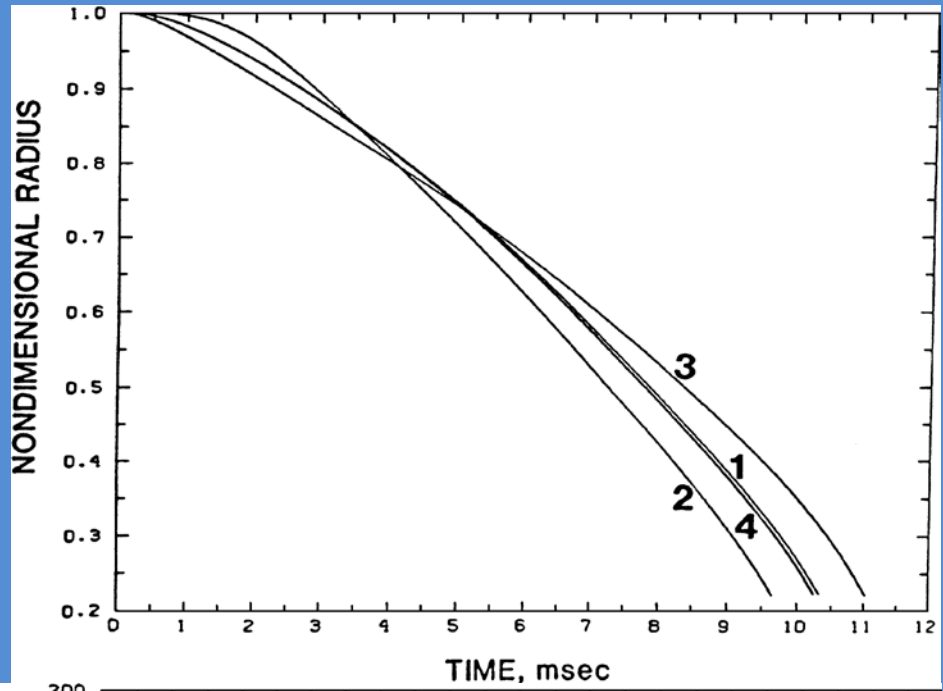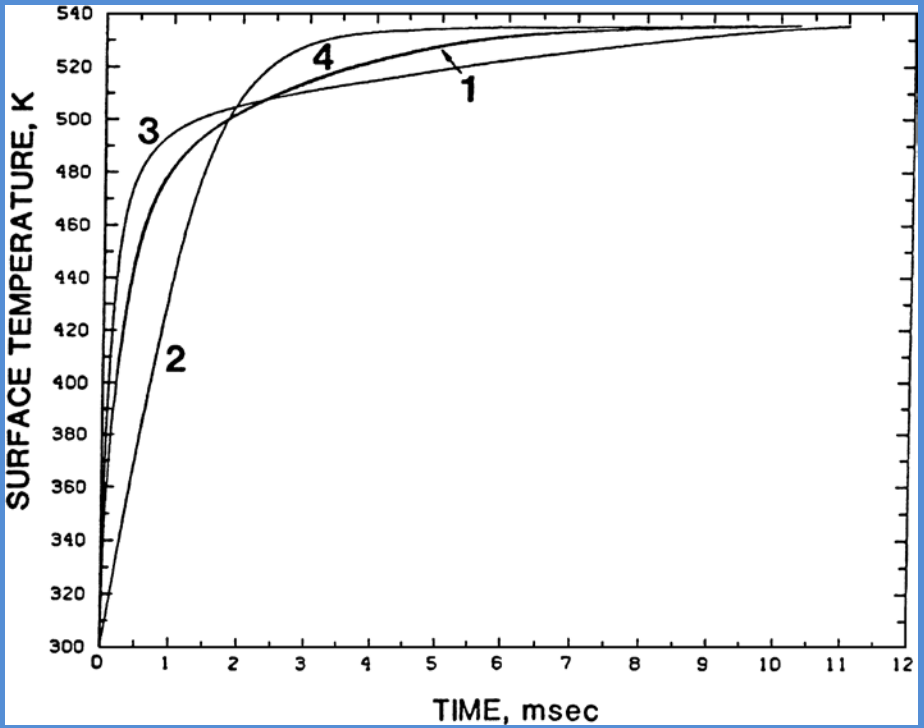
Near-Critical and Transcritical Thermodynamic Behavior

Consider a droplet with an initial sub-critical temperature in an ambience that is supercritical. Initially, composition is discontinuous across the interface as described by phase equilibrium. $t_3 > t_c > t_1$. With time, droplet radius decreases; the critical temperature surface moves towards the phase interface; once those two surfaces merge, phase distinction disappears.
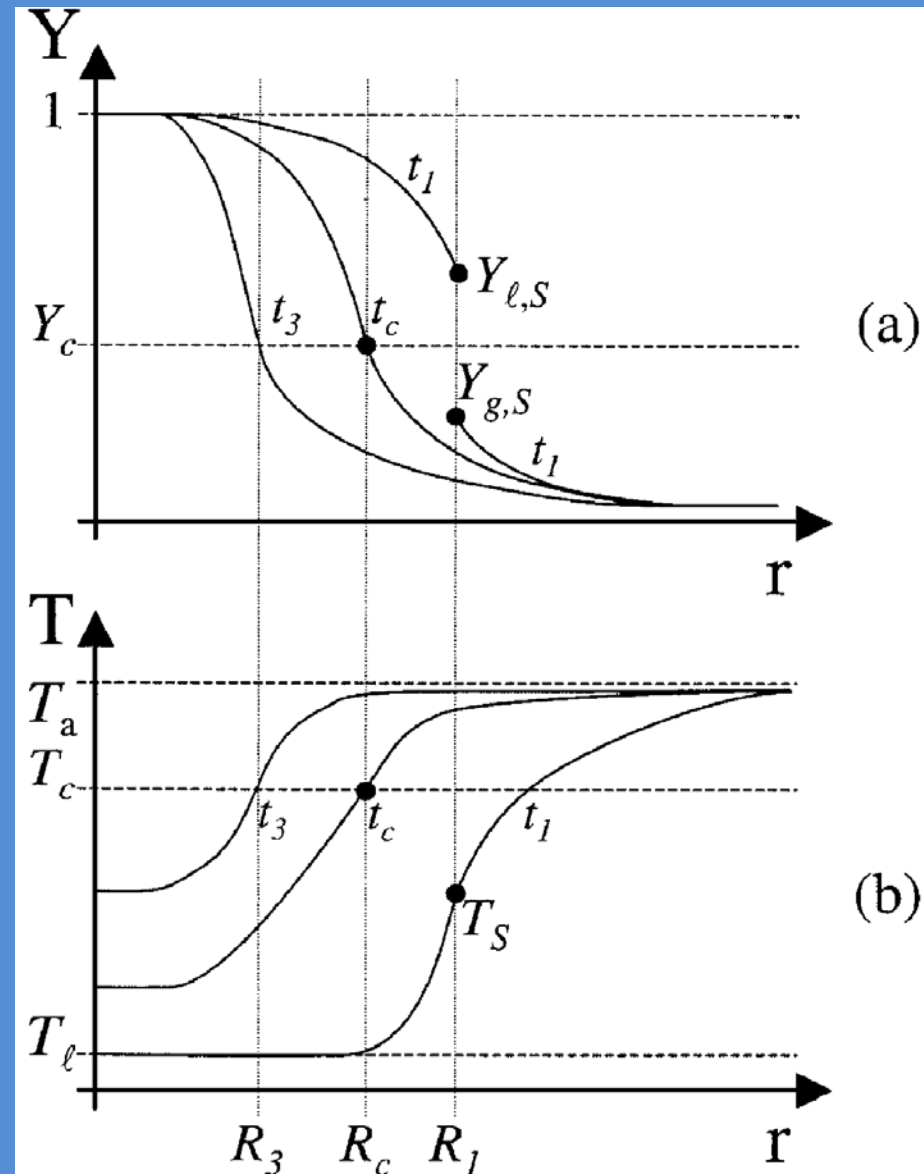
At near-critical conditions, ambient gas components can dissolve in the liquid. The liquid therefore is not a pure substance.
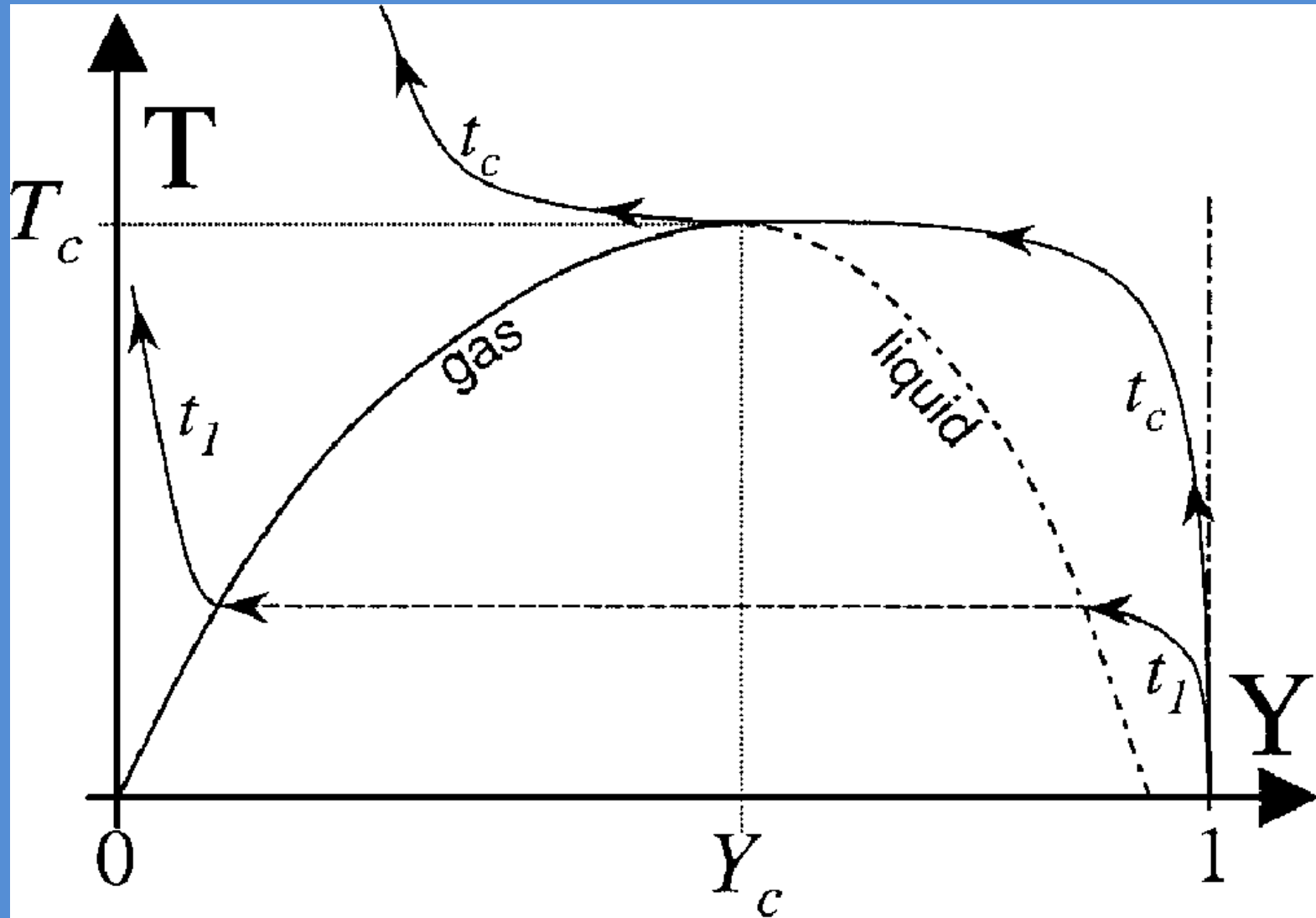
Profiles for Oxygen Droplet in Hydrogen Gas
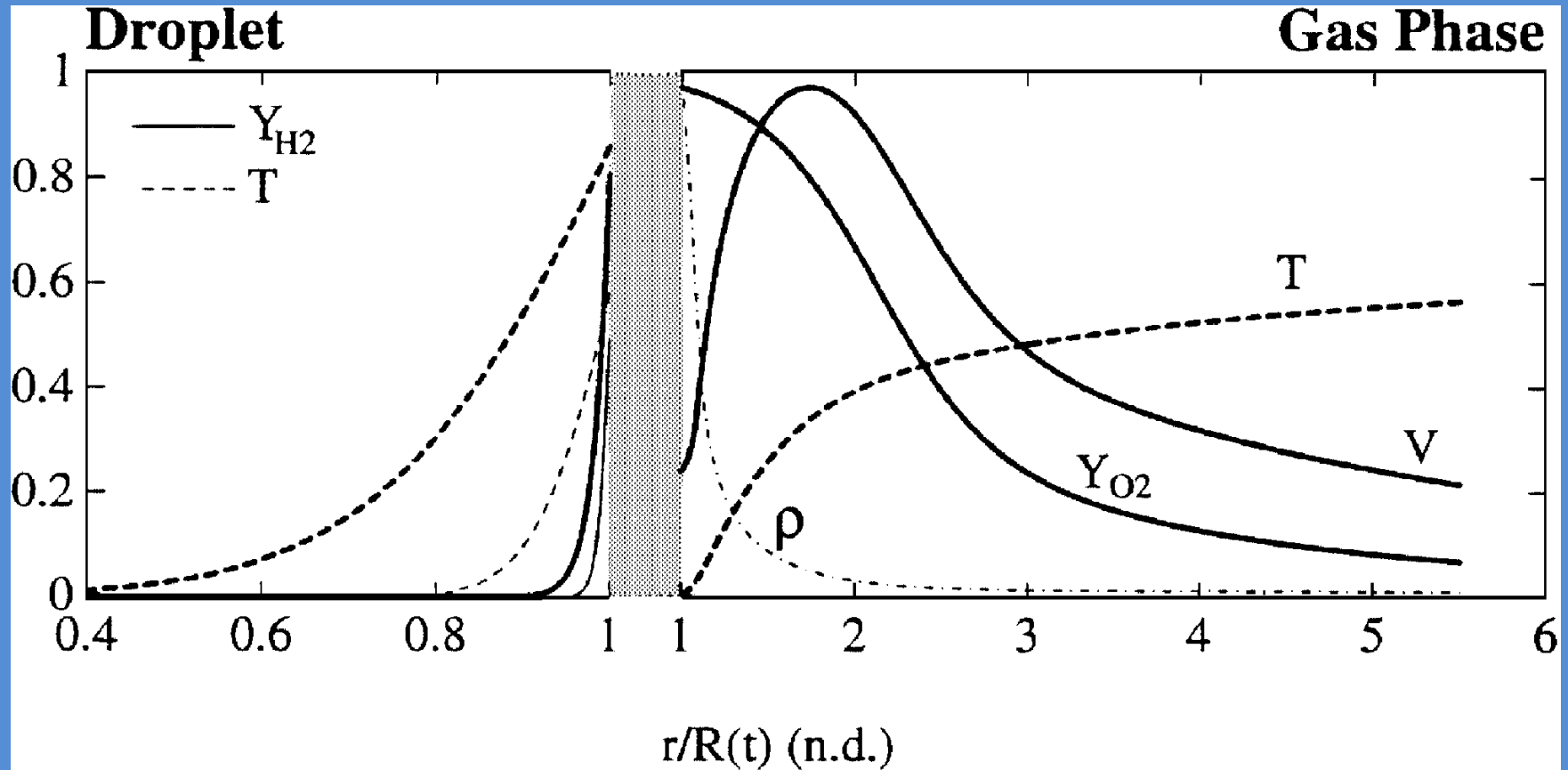
# High-Pressure Phase Equilibrium
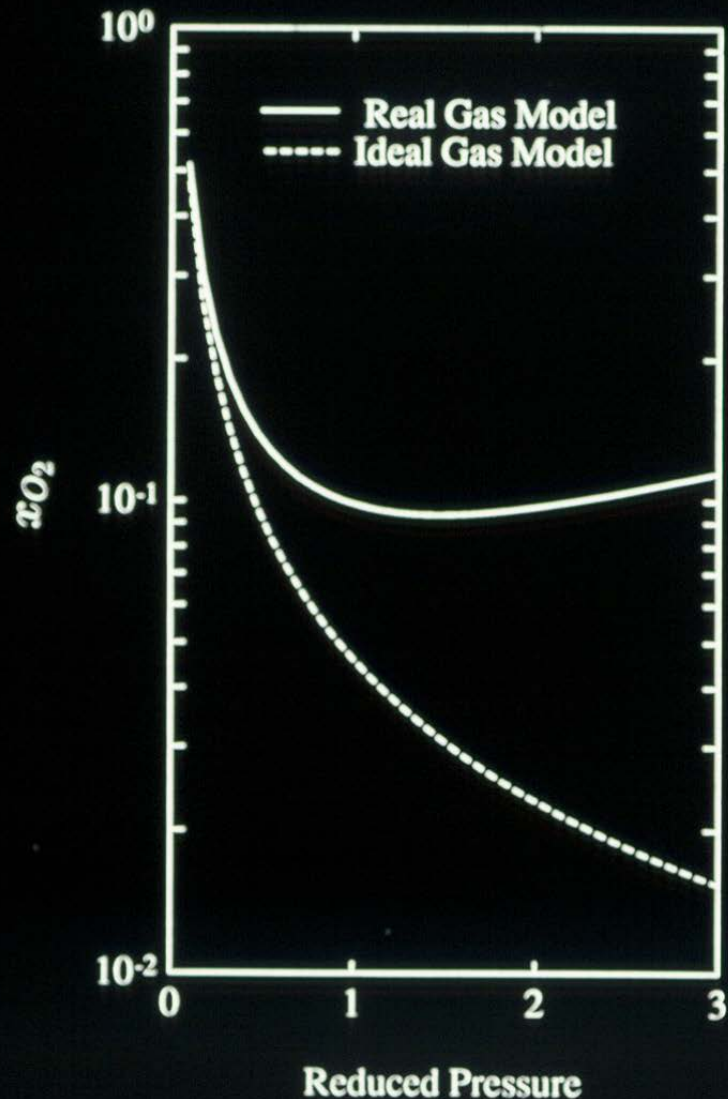
- Unsteady effects in the gas phase are particularly significant for a LOX droplet vaporizing in hydrogen and cannot be neglected.

- The quasi-steady film theory must be corrected to take unsteadiness into account.

- At near- and super-critical pressures, gas solubility in the liquid must be considered.

- Under super-critical pressures, the droplet surface temperature reaches the critical mixture value.

- Supercritical combustion must be modeled under such conditions.
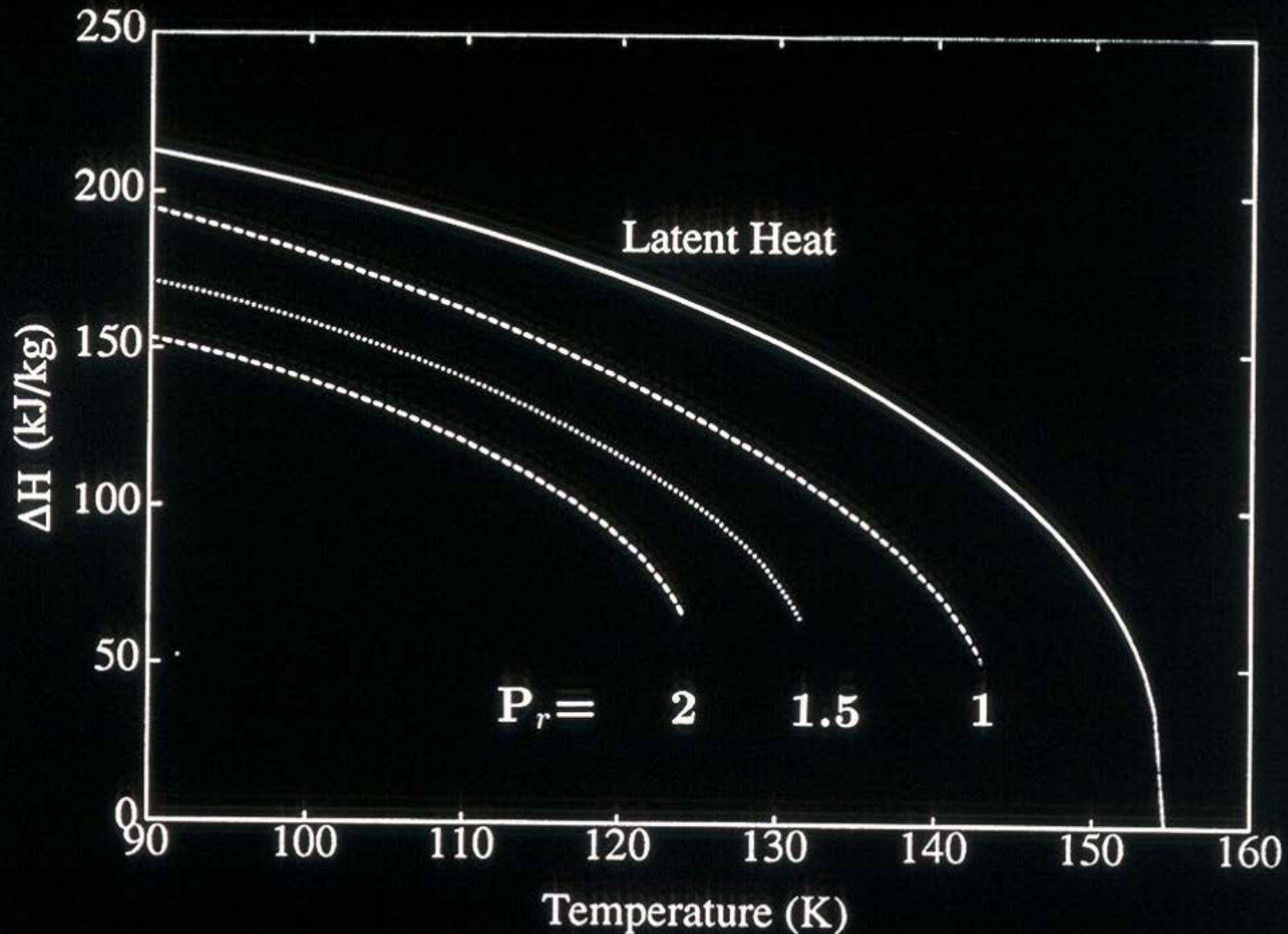
Molecular Dynamics calculations require only a description of the attractive / repulsive forces between the molecules. No apriori description of phase is required. However, only sub-micron-size droplets can be analyzed due to computational limitations. (There are more than a billion molecules in a cubic micron of water or oil.)

- ● droplet molecule
- ● vapor molecule
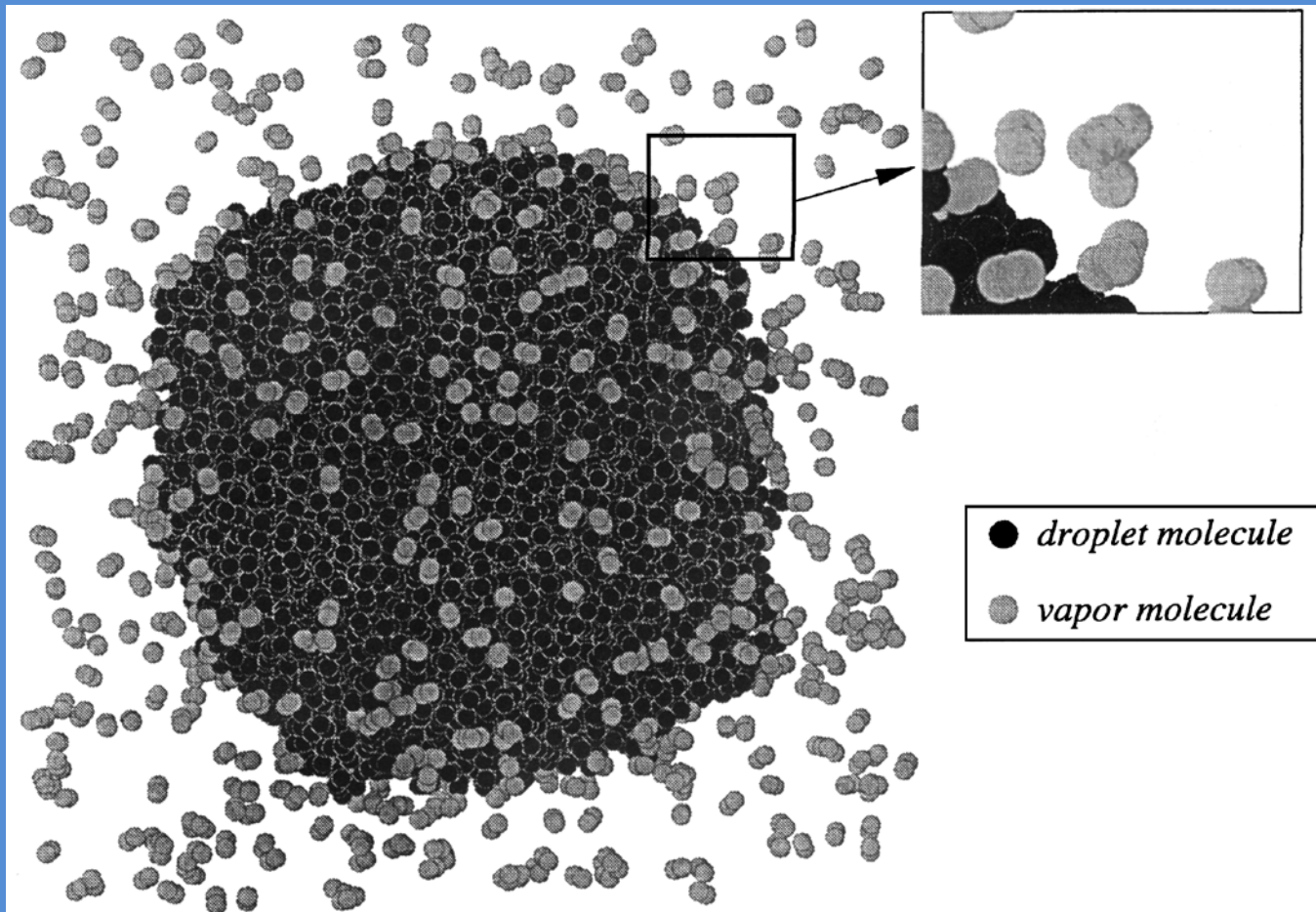
SPRAY COMBUSTION

EXCHANGE OF MASS, MOMENTUM, AND ENERGY

VAPORIZATION - RATE - CONTROLLING

INITIAL DROPLET SIZE DISTRIBUTION
    ATOMIZATION

DROPLET TRAJECTORIES
    DRAG COEFFICIENT

DROPLET HEATING
    CONVECTIVE BOUNDARY LAYERS
    LIQUID-PHASE HEAT DIFFUSION
    INTERNAL CIRCULATION

VAPORIZATION
    STEFAN FLOW
    LIQUID-PHASE MASS DIFFUSION

TWO-WAY COUPLING BETWEEN PHASES
    SOURCE TERMS IN GAS-PHASE MODEL
    LOCAL AMBIENT CONDITIONS FOR DROPLET

DROPLET-DROPLET INTERACTIONS
    MODIFICATION TO LOCAL AMBIENT CONDITIONS
    GEOMETRICAL CONFIGURATION
    COLLISIONS

TURBULENCE-DROPLET INTERACTIONS
    LARGE EDDIES
    SMALL EDDITES

Approaches to Spray Computations

- **Two-continua models: the properties are an average over a neighborhood so that both liquid and gas properties exist at each point in a continuous fashion.**

- **Discrete-particle models: a Lagrangian approach is taken for droplets and an Eulerian approach for the gas. The Lagrangian equations are equivalent to a characteristics method for the continuous droplet equation in the first method.**

- **Probability density function: this can be useful when resolution is desired to be smaller than droplet spacing and a probabilistic behavior exists. For more coarse resolution, the pdf is a distribution function.**
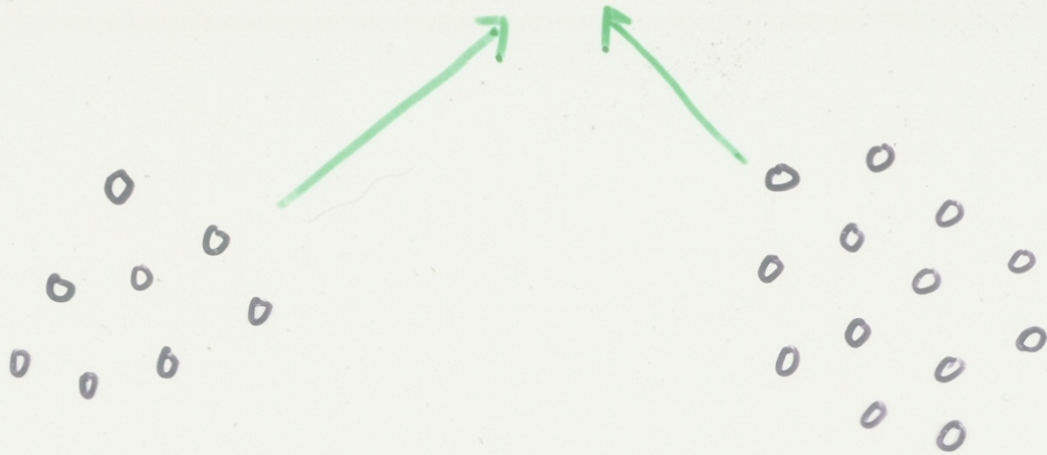
Intersection of Two Moving
Clouds of Droplets

Negligible Collision Rate if:

Droplet Spacing >>> Droplet Size

Characteristic Lines and Eulerian-Lagrangian Method

Droplet Path or Characteristic

Eulerian Mesh Point
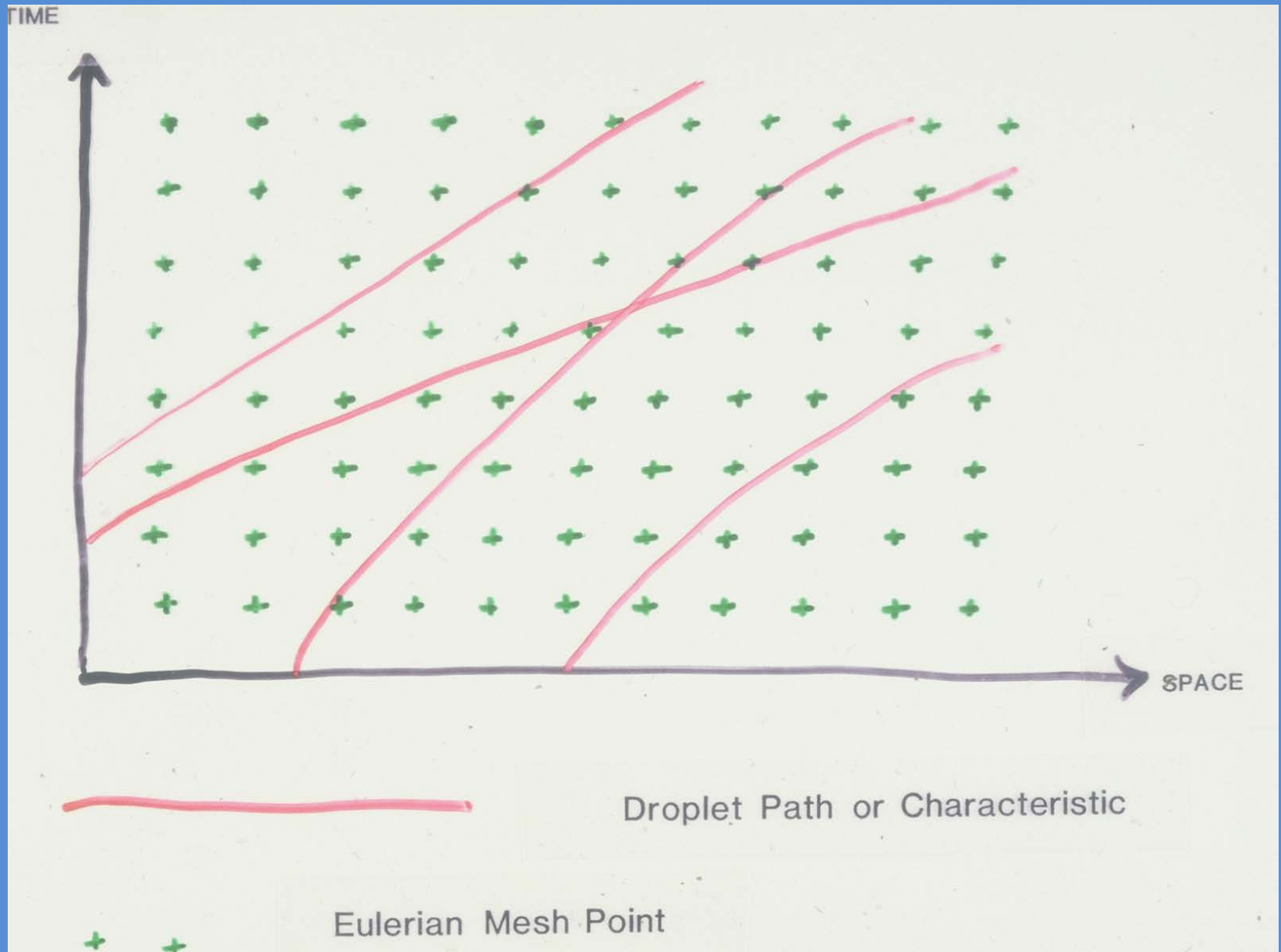
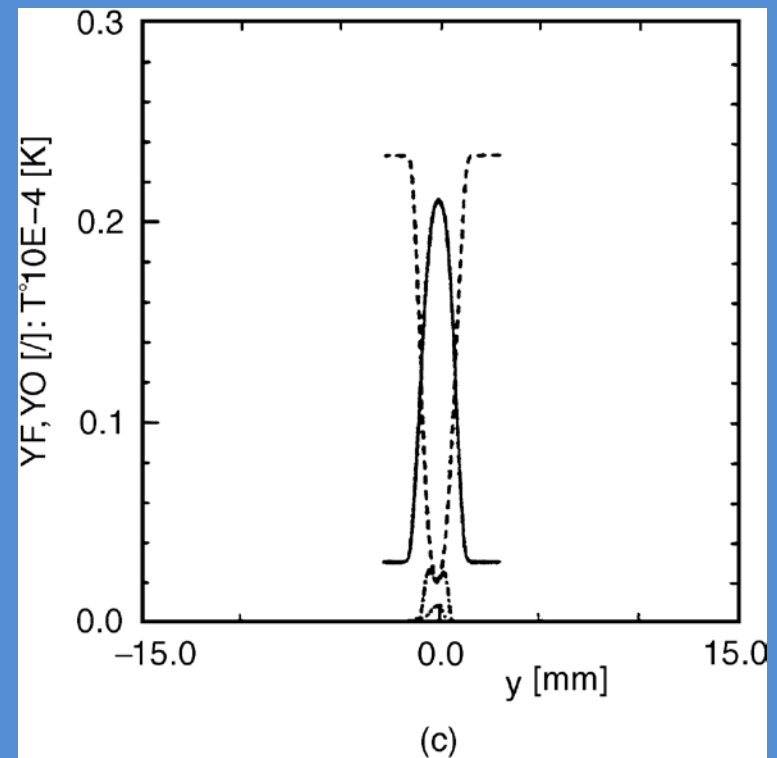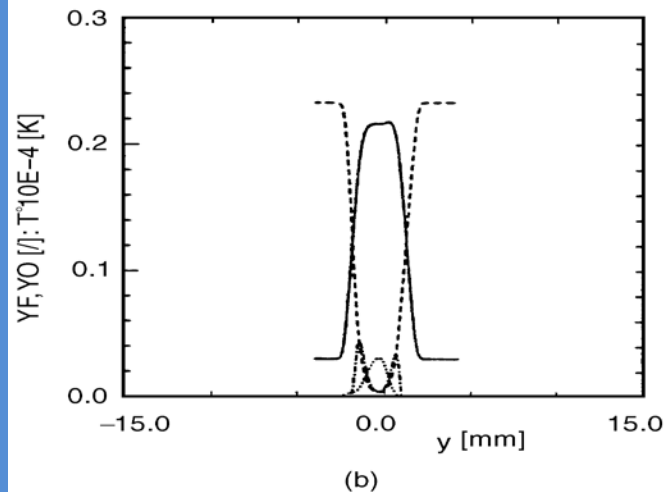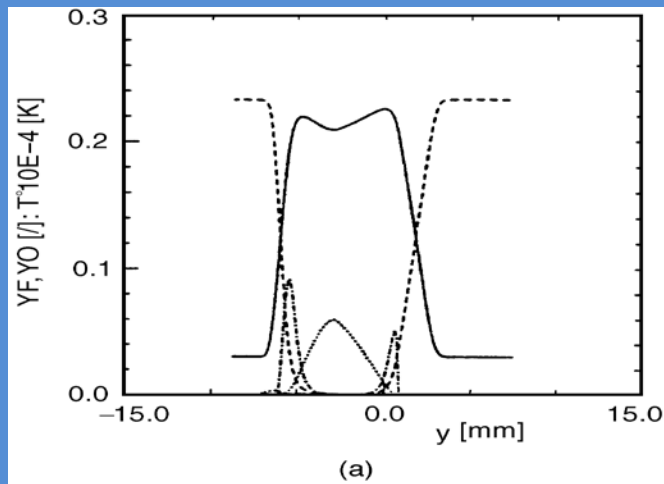# Ignition Problem:
droplets near a hot wall

Ignition delay can be minimized depending on droplet size and distance from hot wall.

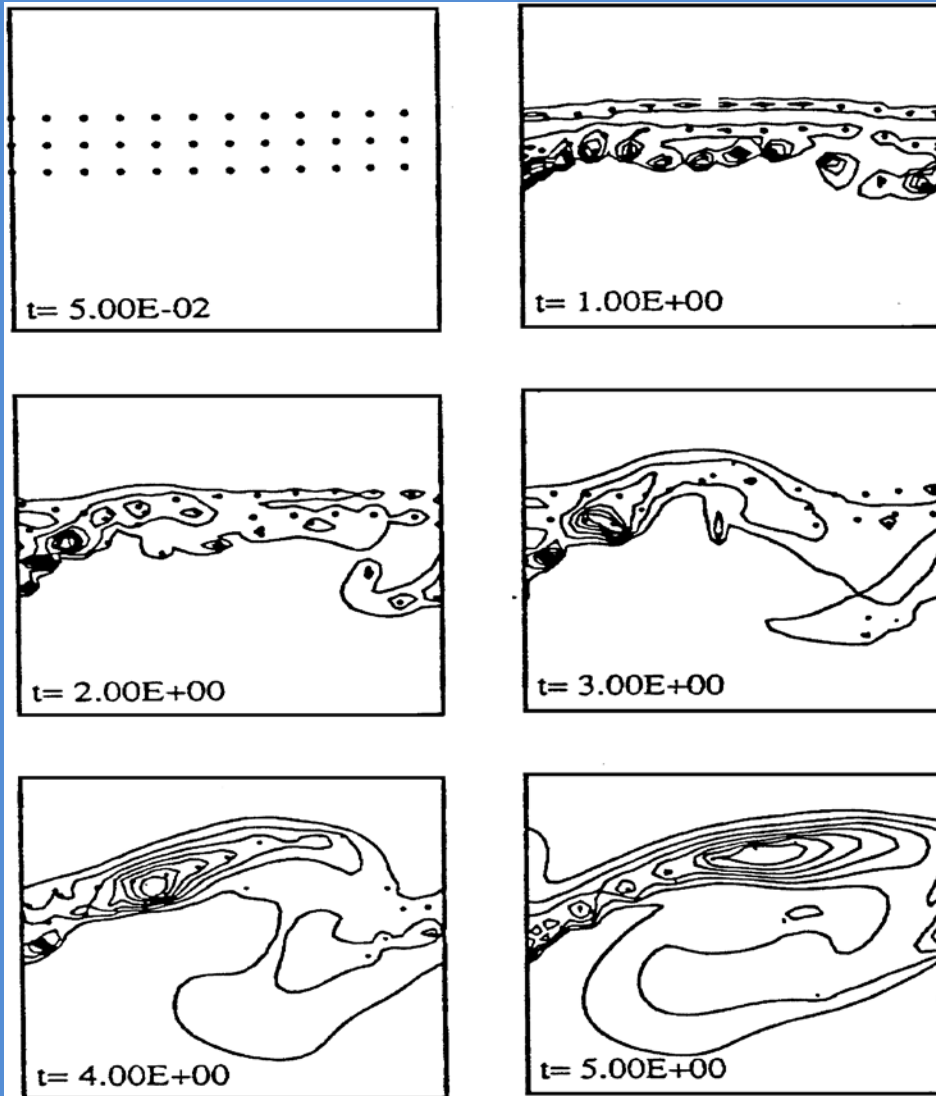**d_{20} is a better average droplet diameter than d_{32} for ignition predictions; i.e., surface area is critical.**
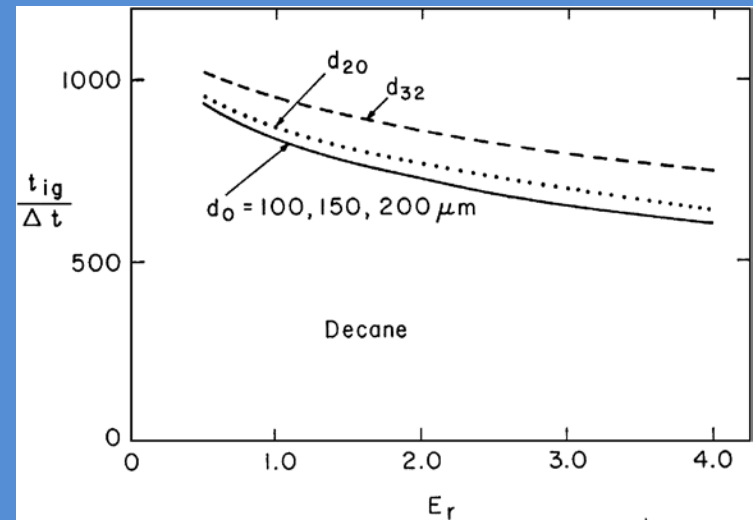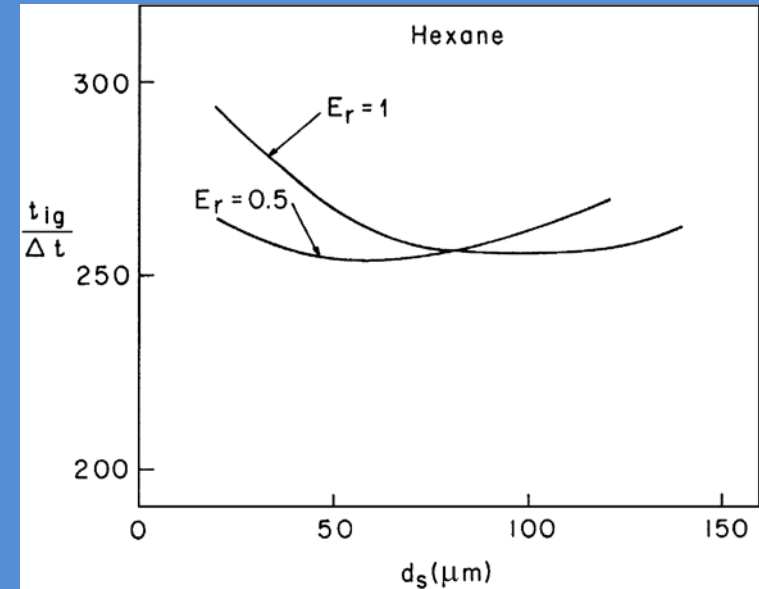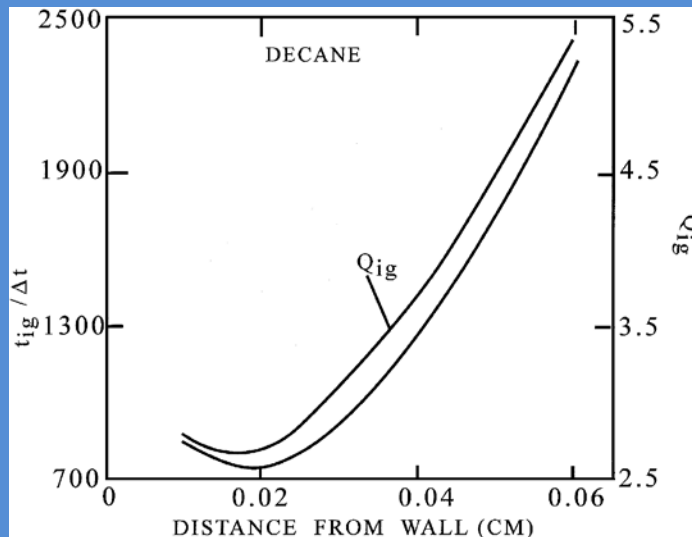
Counterflow Flames

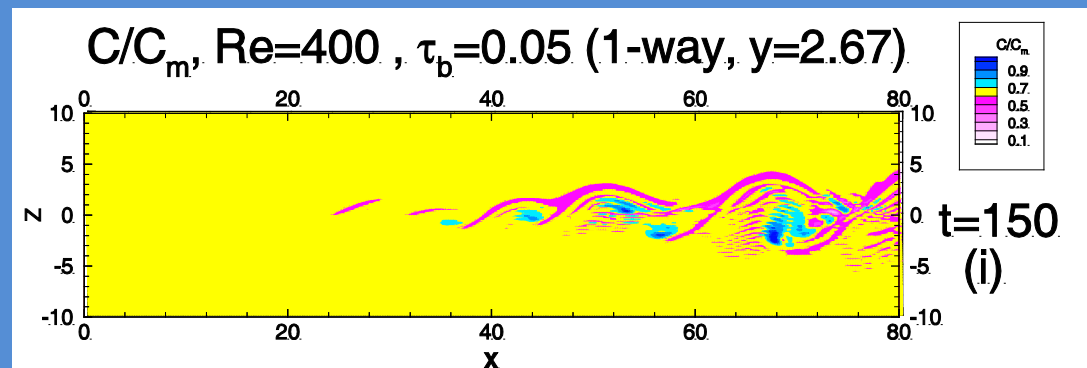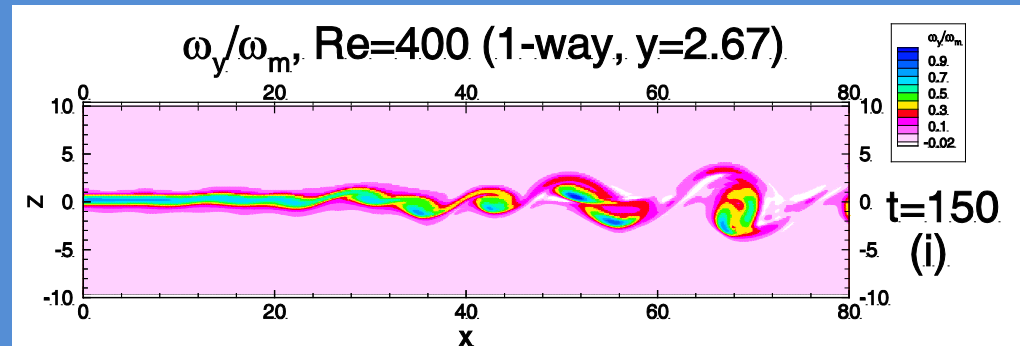**Two diffusion flames can occur even if droplets enter only from one side.**

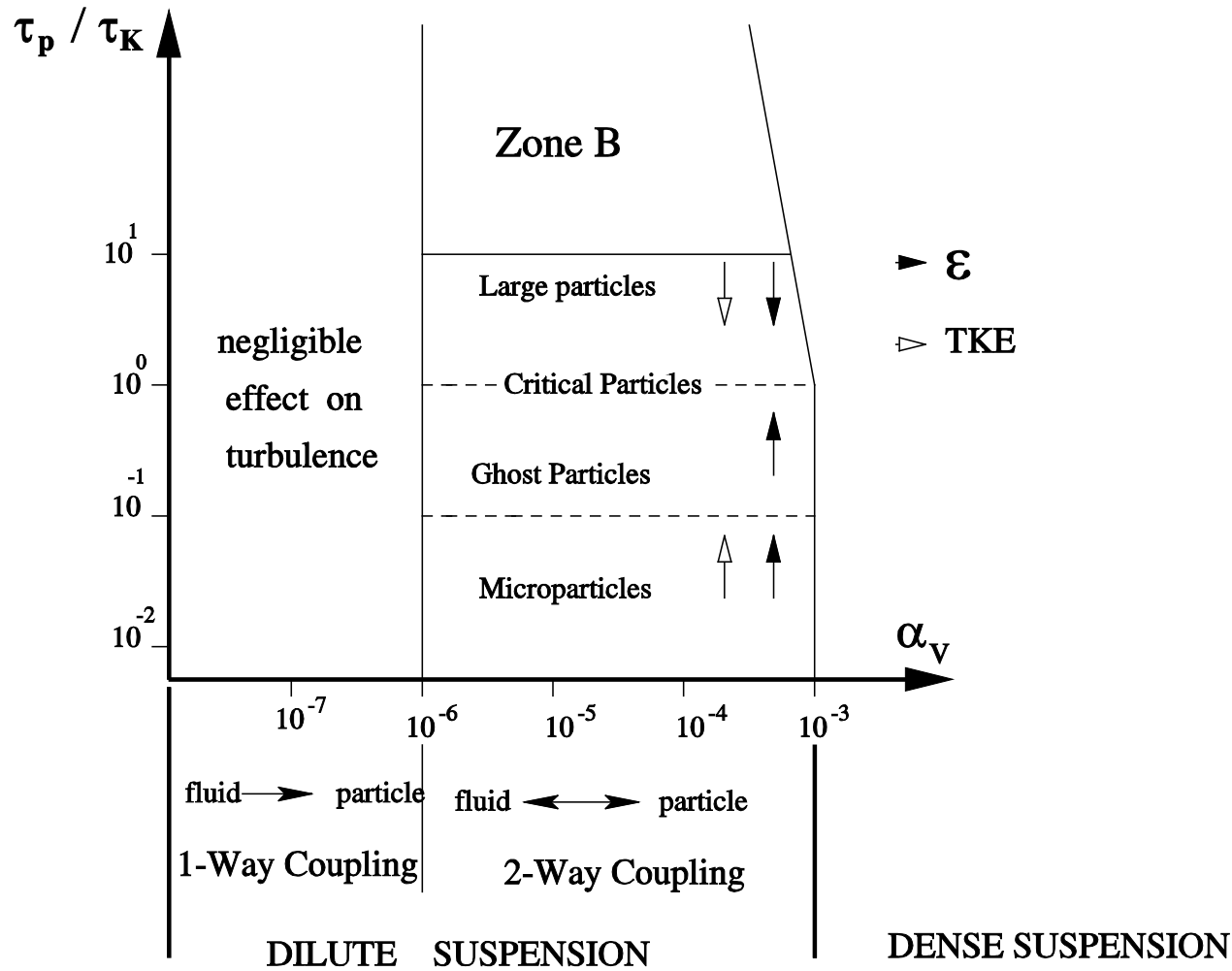# *Droplet Streams interacting with Vortex Structures in Mixing Layer*

t= 5.00E-02

t= 1.00E+00

t= 2.00E+00

t= 3.00E+00

t= 4.00E+00

t= 5.00E+00

Droplet number density variation is affected by strain of vortex field.

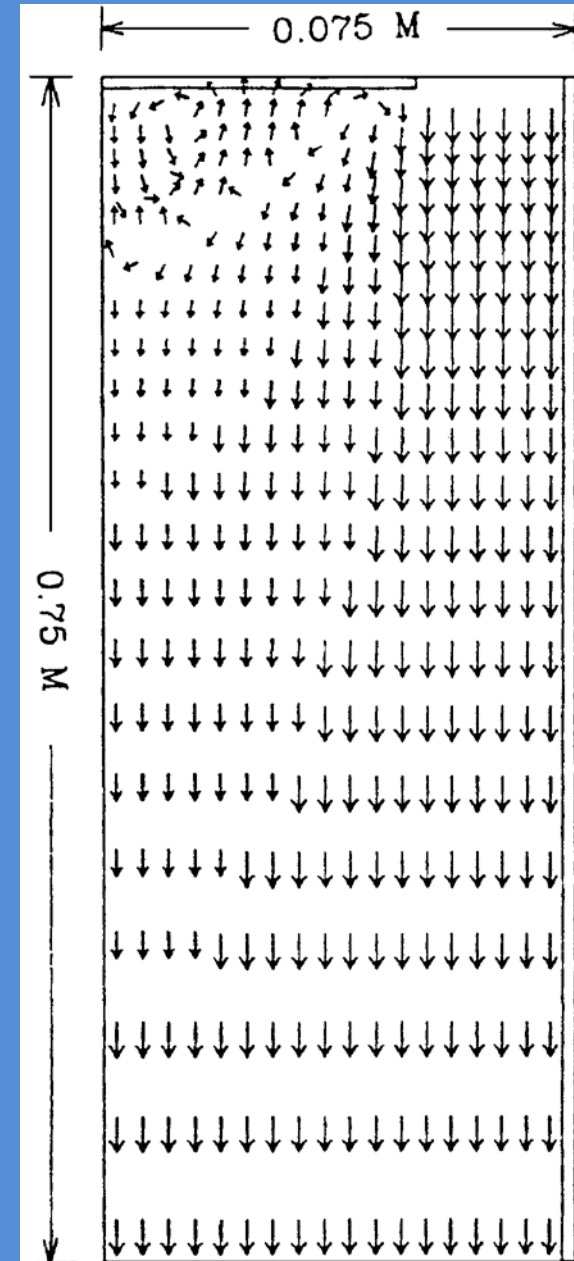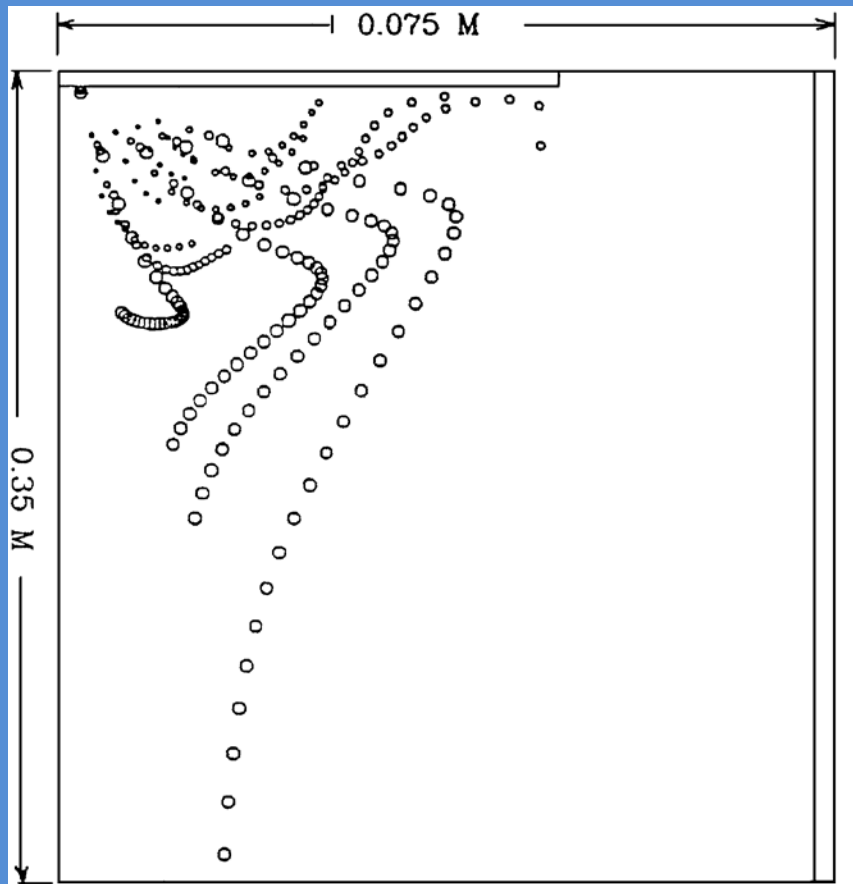**Larger droplets have greater inertia.**

3D mixing-layer solutions for bubble-laden flows

Turbulent Domains for Particle-laden Flows
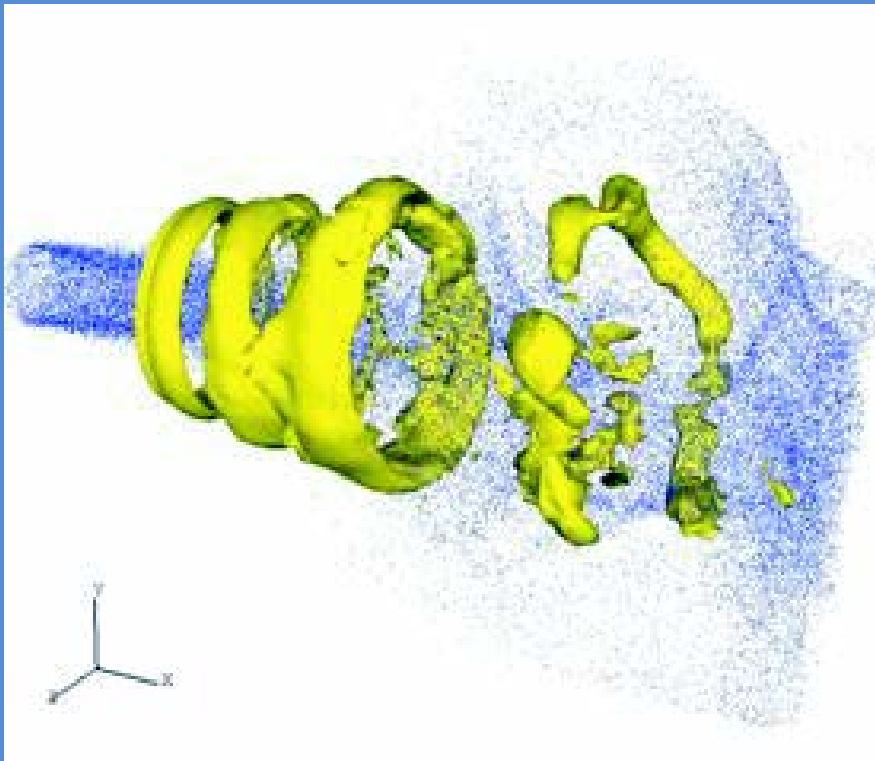
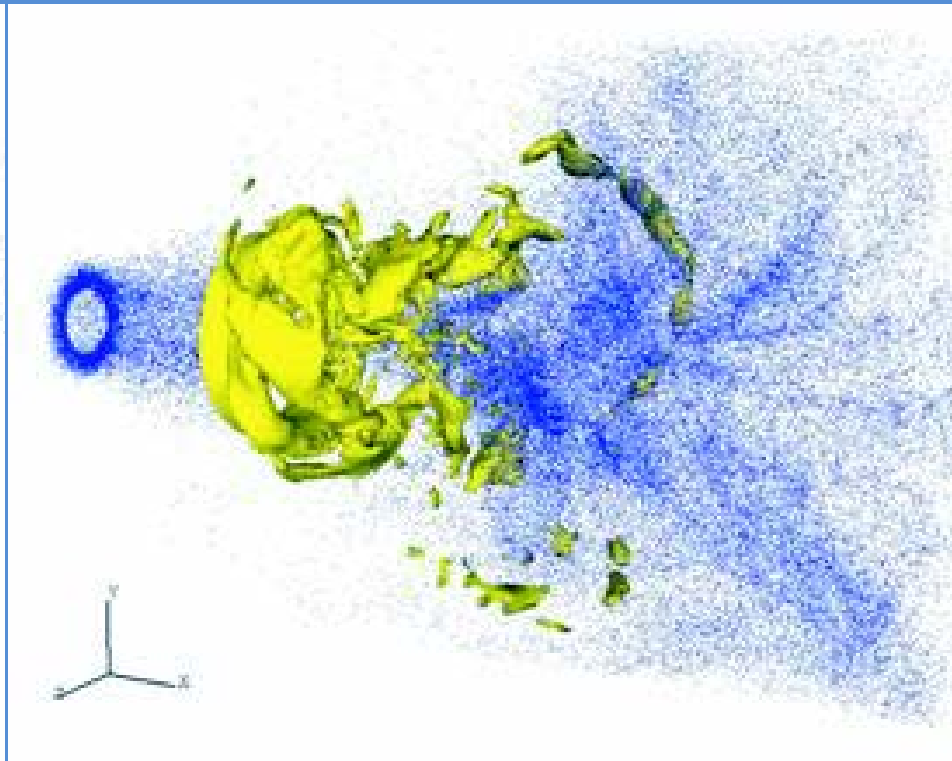# Axisymmetric Centerbody Injection, Vaporization, and Combustion

3D Large-Eddy Simulation
Vorticity and Droplet Position

Low swirl rate　　　　　　　　　　　**High swirl rate**

Thank You