

Thermophysical Properties in Combustion

Albino J.K. Leiroz
Department of Mechanical Engineering - POLI/COPPE
Federal University of Rio de Janeiro



***Escola Sul-Americana em Identificação de Propriedades
Físicas em Transferência de Calor e Massa - PROPFIS***

Rio de Janeiro
Junho, 2005

- **Information Sources - Journals**

- *Combustion and Flame*
- *Combustion Science and Technology*
- *Combustion Theory and Modeling*
- *Progress in Energy and Combustion Science*
- *Proceeding of the Combustion Institute*

- **Information Sources - Books**

- *Combustion – I. Glassman*
- *Principles of Combustion – K.K. Kuo*
- *Combustion Theory – F.A. Williams*
- *Droplets and Sprays – W.A. Sirignano*

Historical Perspective

- Development of the Modern Society
 - Pre-Historical: Heating, Cooking, Metals
 - Steam Engine
 - Industrial Revolution
 - Otto Engine (1876) and Diesel Engine(1890)
 - II World War
 - Mobility ➤ Liquid Fuels
 - Gas Turbine
 - Rocket Engine
 - Oil Crisis (1973)
- Modern Engineering
 - Environment Aspects
 - Waste Treatment
 - Alternative Fuels
 - Cogeneration

Applications

- Power Production
 - Thermoelectric Power Stations
 - Plane, Ship and Automobile Propulsion
 - Gas turbine Engines
 - Rocket Engines
- Process Industry
 - Steel, Glass, Ceramics, Cement
- Fire Prevention and Safety
- Heating – Industrial and Household
- Environment Aspects
 - Formation of Pollutants – NO_x , SO_x , CO
 - Formation of Particulates
 - Exhaust Gas Temperature Control

Motivation



Mathematical model

- ***Definitions***

- Oxidation
- Energy release
- Flame

- ***Background***

- Thermodynamics
- Chemical Kinetics
- Fluid Mechanics
- Heat and Mass Transfer
- Turbulence
- Materials Structure and Behavior

Chemical Thermodynamics

- ***Introduction***

- Thermodynamic Equilibrium
 - Mechanical + Thermal + Chemical
 - Thermodynamic properties + composition
- Nonequilibrium Thermodynamics – Rates of Change

- ***Thermodynamic Laws***

- *0th Law* – Temperature + Thermal Equilibrium
- *1th Law* – Internal Energy + Conservation of Energy
- *2th Law* – Entropy + Temperature Scale
- *3th Law* – Entropy Reference State and Value

Chemical Thermodynamics

- Criteria for Equilibrium**

TABLE 1.1 General Equilibrium Criteria for Closed Thermodynamic System¹⁵

Variables Held Constant Criteria for Thermodynamic Equilibrium in a Closed System

p	$dH - T dS = dG + S dT = 0$
V	$dU - T dS = dA + S dT = 0$
T	$d(U - TS) + p dV = dG - V dp = dA + p dV = 0$
S	$dU + p dV = dH - V dp = 0$
p, T	$dG = 0$
V, T	$dA = 0$
p, S	$dH = 0$
V, S	$dU = 0$
S, U or A, T	$dV = 0$
A, V or G, p	$dT = 0$
U, V or H, p	$dS = 0$
G, T or H, S	$dp = 0$

- Equilibrium Constants**

$$K_p \equiv \frac{P_C^c P_D^d}{P_A^a P_B^b}$$

$$\Delta G_0 = -R_u T \ln K_p$$

Chemical Thermodynamics

- Specifying Amounts**

- Mass Fraction - Y

$$Y_i = \frac{m_i}{\sum_{i=1}^N m_i}$$

- Mole Fraction - X

$$X_i = \frac{n_i}{\sum_{i=1}^N n_i}$$

- Fuel – Oxidant Ratio - F/O

$$F / O = \frac{m_{fuel}}{m_{oxidant}}$$

- Equivalence Ratio - ϕ

$$\phi = \frac{(F / O)}{(F / O) + (F / O)_{st}}$$

Chemical Thermodynamics

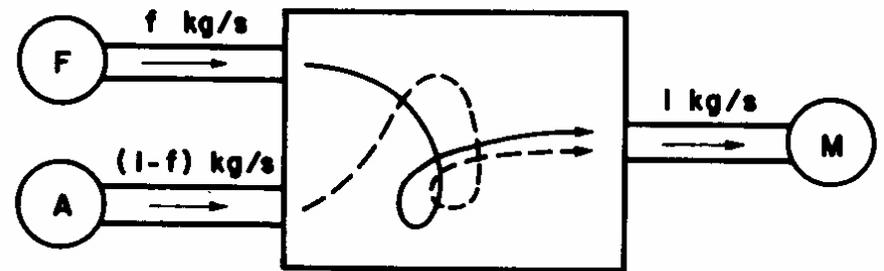
- **Specifying Amounts**

- Mixture Fraction - f

$$f\xi_F + (1-f)\xi_A = \xi_M$$

$$f = \frac{\xi_M - \xi_A}{\xi_F - \xi_A}$$

- v - Extensive Property
- Sourceless
- Y_{inert} ; $Y_F - (F/O)_{st} Y_O$;
- Complete Reaction - f_{st}



Chemical Thermodynamics

- **Standard Heat of Formation**

- Amount of energy (heat) absorbed or released when a substance is formed from its elements in the reference state (298.15K – 1 atm).
- Stable elements in the standard state have *zero heat of formation*.

- **Heat of Reaction**

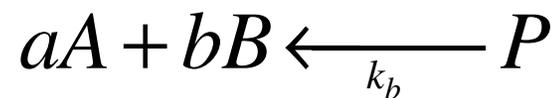
- Amount of energy (heat) absorbed or released during a reaction occurring at a given T and p .

- **Adiabatic Flame Temperature**

- Temperature of the products when the combustion process occurs adiabatically, with no work interactions, changes in kinetic or potential energy.
- Maximum temperature for the given conditions.

Chemical Kinetics

- Reaction Rates - Arrhenius**



$$\left. \frac{dC_A}{dt} \right|_f = -ak_f C_A^a C_B^b = -a\beta_f C_A^a C_B^b \exp\left(-\frac{E_{a,f}}{R_u T}\right)$$

$$\left. \frac{dC_A}{dt} \right|_r = +ak_r C_A^a C_B^b = +a\beta_r C_A^a C_B^b \exp\left(-\frac{E_{a,r}}{R_u T}\right)$$

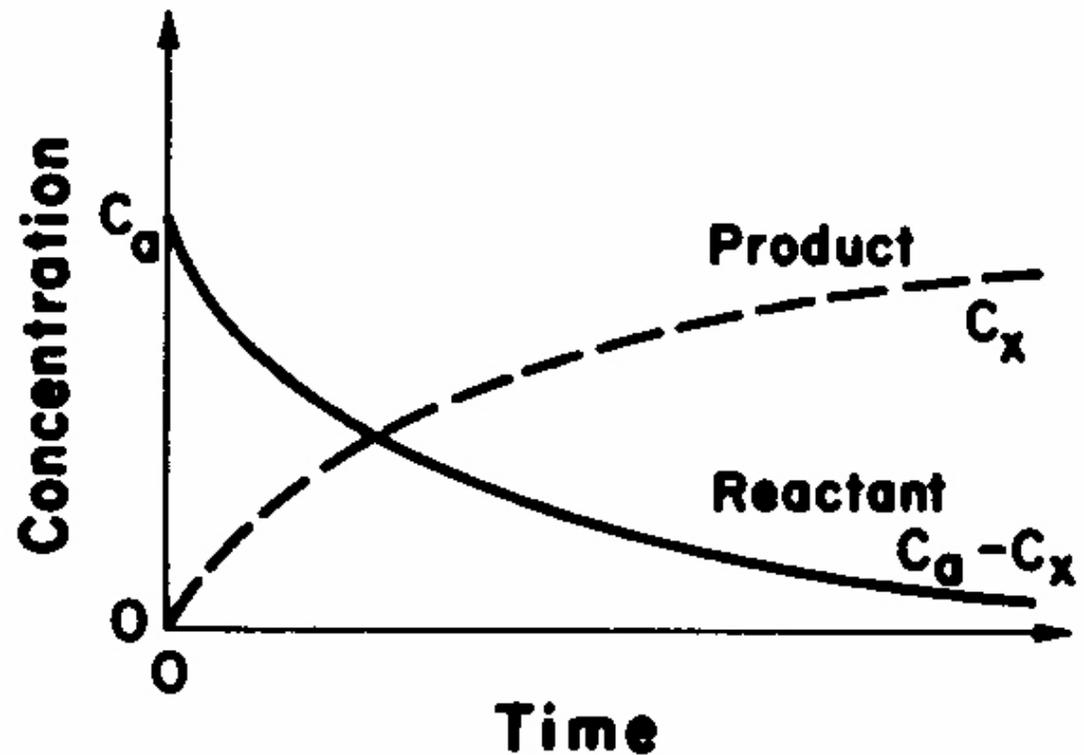
Chemical Kinetics

- Equilibrium**

$$\left. \frac{dC_A}{dt} \right|_f = \left. \frac{dC_A}{dt} \right|_r$$

$$\left. \frac{dC_B}{dt} \right|_f = \left. \frac{dC_B}{dt} \right|_r$$

$$\left. \frac{dC_P}{dt} \right|_f = \left. \frac{dC_P}{dt} \right|_r$$



Conservation Equations

- Continuity**

Rectangular coordinates (x, y, z) :

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u_x) + \frac{\partial}{\partial y}(\rho u_y) + \frac{\partial}{\partial z}(\rho u_z) = 0 \quad (\text{A})$$

Cylindrical coordinates (r, θ, z) :^a

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r}(\rho r u_r) + \frac{1}{r} \frac{\partial}{\partial \theta}(\rho u_\theta) + \frac{\partial}{\partial z}(\rho u_z) = 0 \quad (\text{B})$$

Spherical coordinates (r, θ, ϕ) :^b

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r}(\rho r^2 u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta}(\rho u_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}(\rho u_\phi) = 0 \quad (\text{C})$$

^a $r \geq 0, 2\pi \geq \theta \geq 0$.

^b $r \geq 0, 2\pi > \phi \geq 0, \pi \geq \theta \geq 0$.

Conservation Equations

- Species**

$$\rho \left(\frac{\partial Y_i}{\partial t} + u_x \frac{\partial Y_i}{\partial x} + u_y \frac{\partial Y_i}{\partial y} + u_z \frac{\partial Y_i}{\partial z} \right) + \frac{\partial}{\partial x} (\rho Y_i V_{ix}) + \frac{\partial}{\partial y} (\rho Y_i V_{iy}) + \frac{\partial}{\partial z} (\rho Y_i V_{iz}) = \omega_i$$

[where

$$V_{ix} = -\frac{\mathcal{D}}{Y_i} \frac{\partial Y_i}{\partial x}, \quad V_{iy} = -\frac{\mathcal{D}}{Y_i} \frac{\partial Y_i}{\partial y}, \quad \text{and} \quad V_{iz} = -\frac{\mathcal{D}}{Y_i} \frac{\partial Y_i}{\partial z}$$

- Momentum**

Conservation Equations

- Energy**

$$\begin{aligned}
 & \rho C_p \left(\frac{\partial T}{\partial t} + u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z} \right) - \left(\frac{\partial p}{\partial t} + u_x \frac{\partial p}{\partial x} + u_y \frac{\partial p}{\partial y} + u_z \frac{\partial p}{\partial z} \right) \\
 &= \lambda \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) - \sum_{i=1}^N \omega_i \Delta h_{f,i} \\
 & - \left[\frac{\partial}{\partial x} \left(\rho T \sum_{i=1}^N C_{pi} Y_i V_{ix} \right) + \frac{\partial}{\partial y} \left(\rho T \sum_{i=1}^N C_{pi} Y_i V_{iy} \right) + \frac{\partial}{\partial z} \left(\rho T \sum_{i=1}^N C_{pi} Y_i V_{iz} \right) \right] \\
 & + \mu \left\{ 2 \left[\left(\frac{\partial u_x}{\partial x} \right)^2 + \left(\frac{\partial u_y}{\partial y} \right)^2 + \left(\frac{\partial u_z}{\partial z} \right)^2 \right] + \left[\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right]^2 \right. \\
 & \quad \left. + \left[\frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z} \right]^2 + \left[\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right]^2 - \frac{2}{3} \left[\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right]^2 \right\} \\
 & + \rho \sum_{i=1}^N Y_i (f_{ix} V_{ix} + f_{iy} V_{iy} + f_{iz} V_{iz}) \tag{A}
 \end{aligned}$$

Conservation Equations

- **Source Term**

$$\omega_i = W_i \sum_{k=1}^M (v''_{i,k} - v'_{i,k}) B_k T^\alpha \exp\left[-\frac{E_{ak}}{R_u T}\right] \prod_{j=1}^N \left(\frac{X_j P}{R_u T}\right)^{v'_{i,k}}$$

- Coupling
- M – Total number of chemical reactions
- N – Total number of chemical species

- **Equation of State**

Conservation Equations

- **Unknowns**

$$Y_1, Y_2, Y_3, \dots, Y_N, \rho, T, p, u, v, w$$

- **Equations**

- 1 overall mass continuity equation
- 3 momentum equations
- 1 energy equation
- $N - 1$ species equation
- 1 equation of state
- 1 equation relating all Y_i

- **Premixed \times Diffusion Flames**

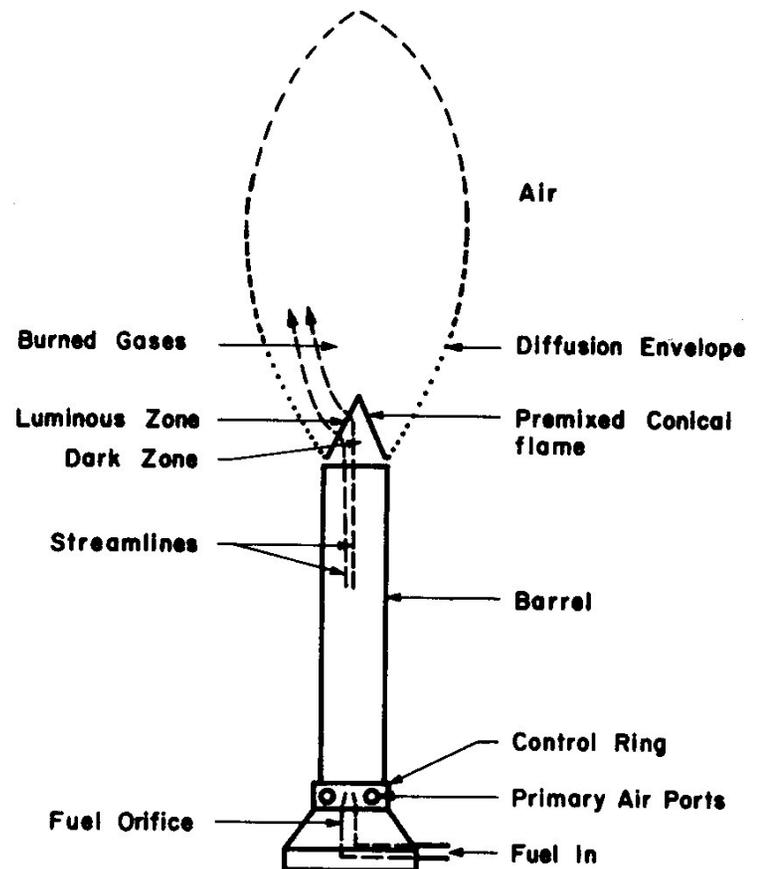
Premixed Flames

- **Deflagration Waves**

- Subsonic
- Propagated by Energy Release from Chemical Reaction

- **Experiment**

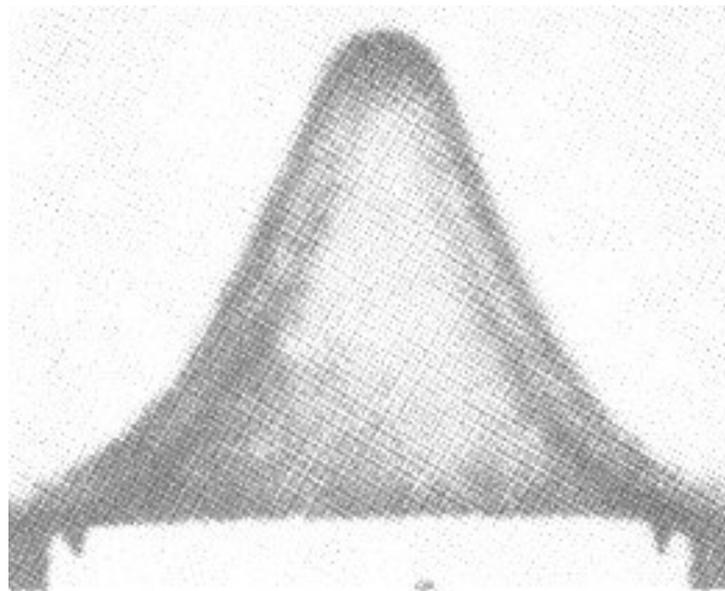
- Bunsen, 1855
- Gaseous fuel
- Entrainment of Primary Air
- Anchored Flame



Premixed Flames

- ***Experiment (cont.)***

- Luminous Conical Region
 - 1mm thick
 - Color – Fuel/Air Ratio
- Reaction and Heat release
- Nonstationary
- Nonplanar
- Find Laminar Flame Speed



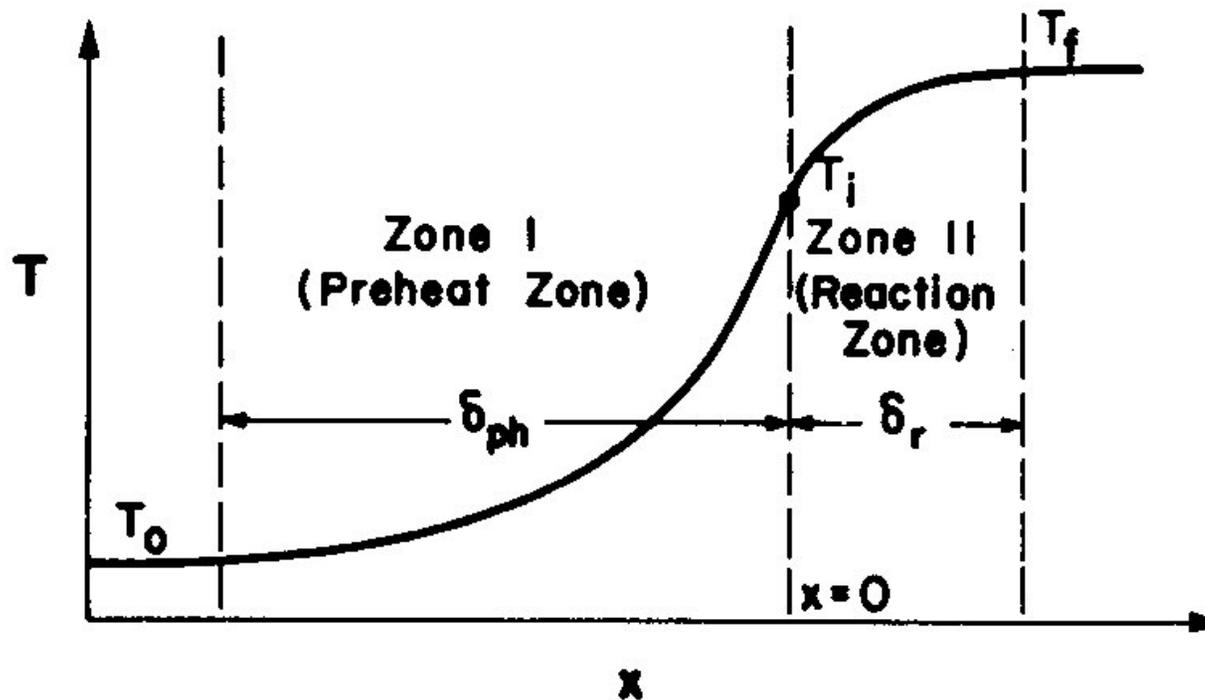
Inner and Outer Cones

Premixed Flames

- Thermal Theory**

$$S_L = C_I \sqrt{\alpha \cdot RR}$$

- Mallard and Le Chatelier

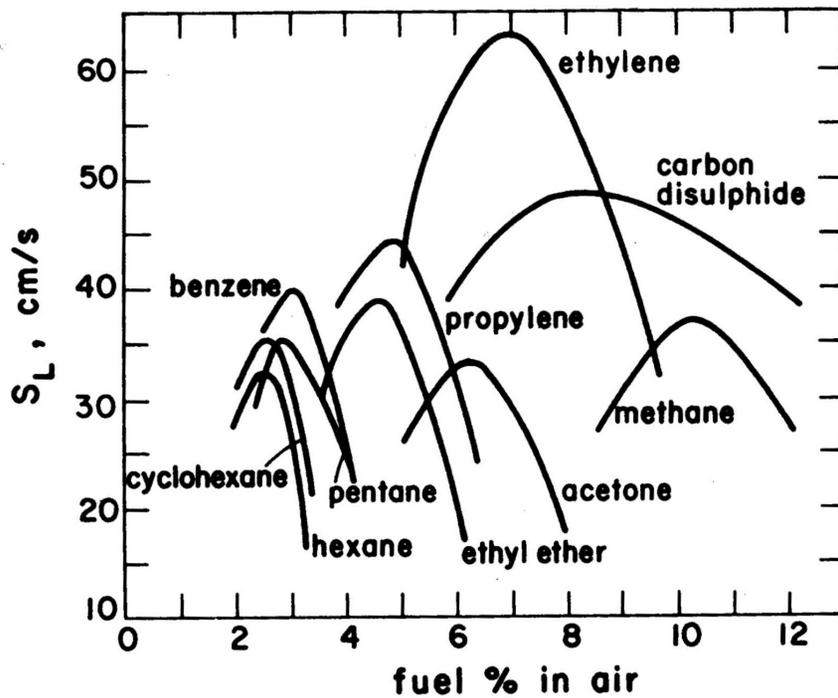


Typical Temperature Variation

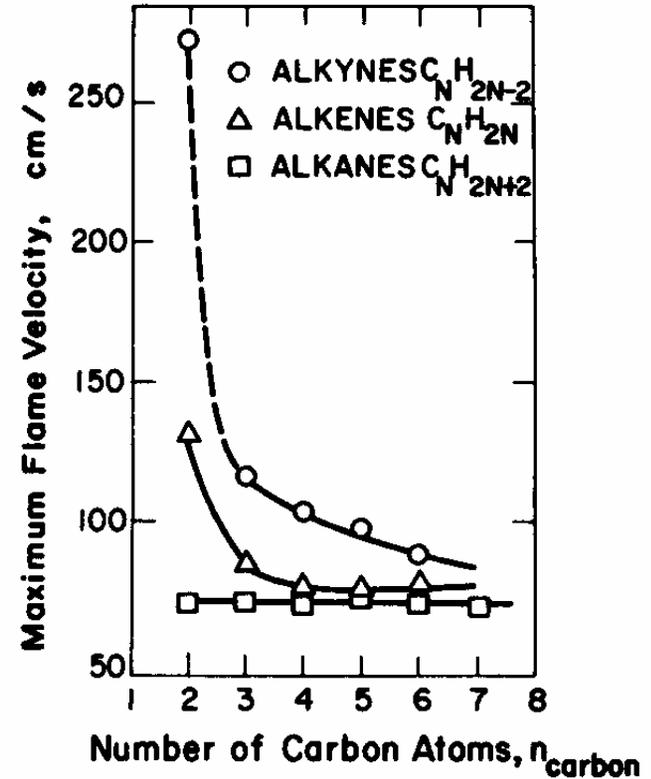
Premixed Flames

- **Effect of Chemical Properties**

- **Mixture Ratio**



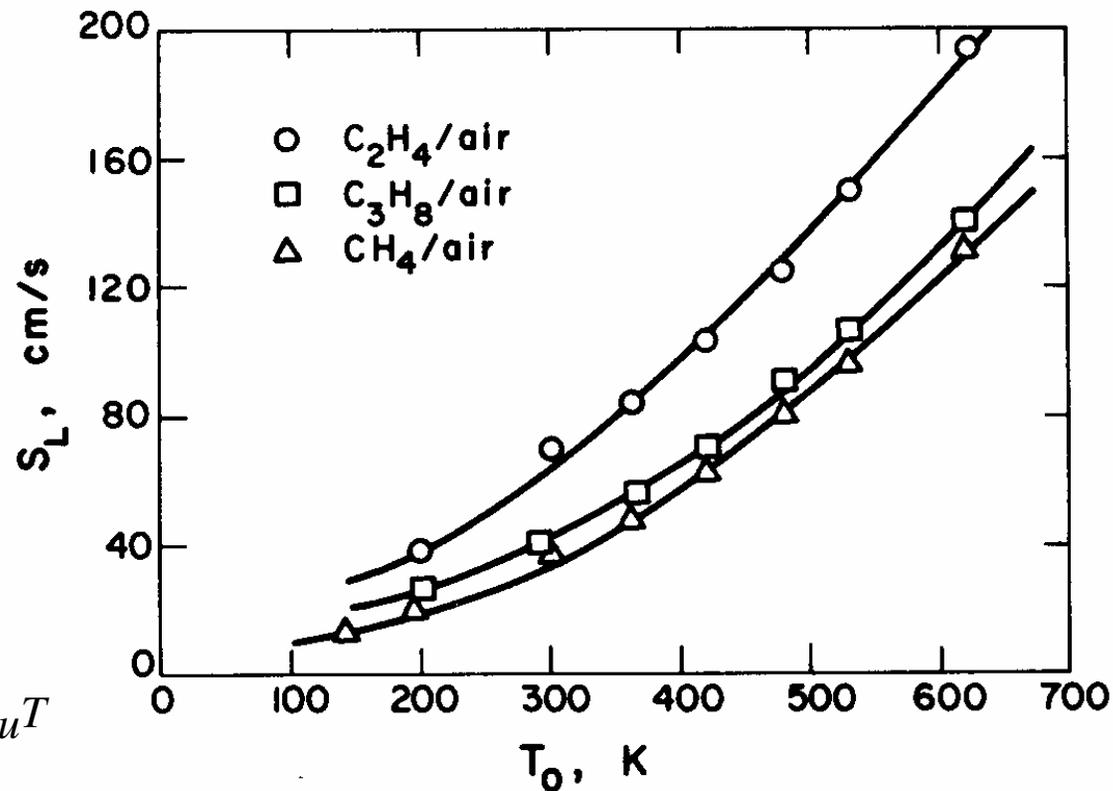
- **Fuel Molecular Structure**



Premixed Flames

- **Effect of Physical Properties**

- **Pressure** - $S_L = C_2 \cdot p^{n-2}$
- **Initial Temperature**



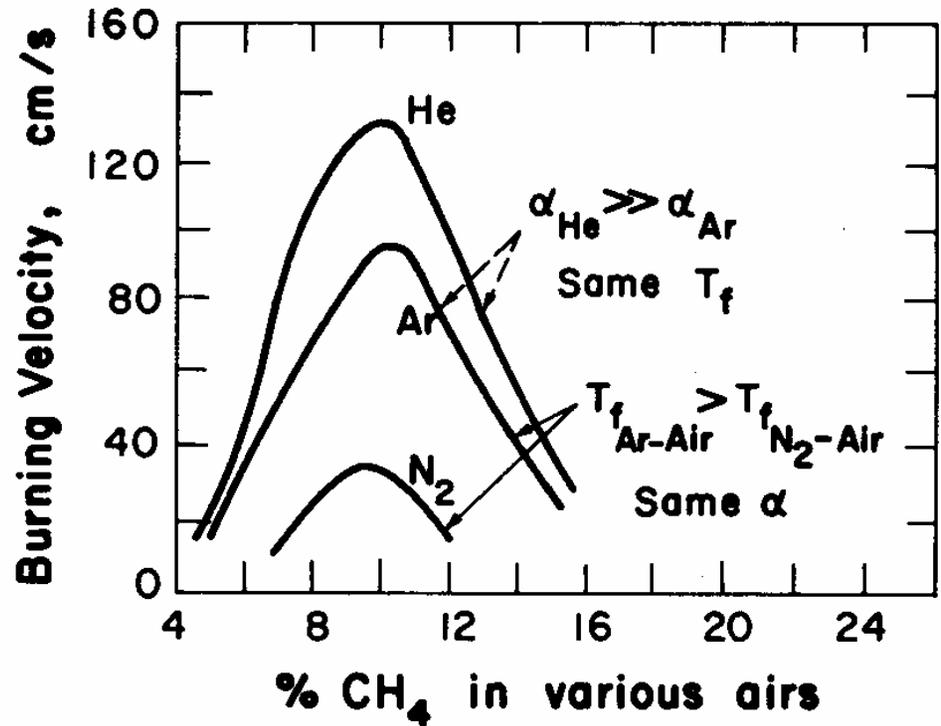
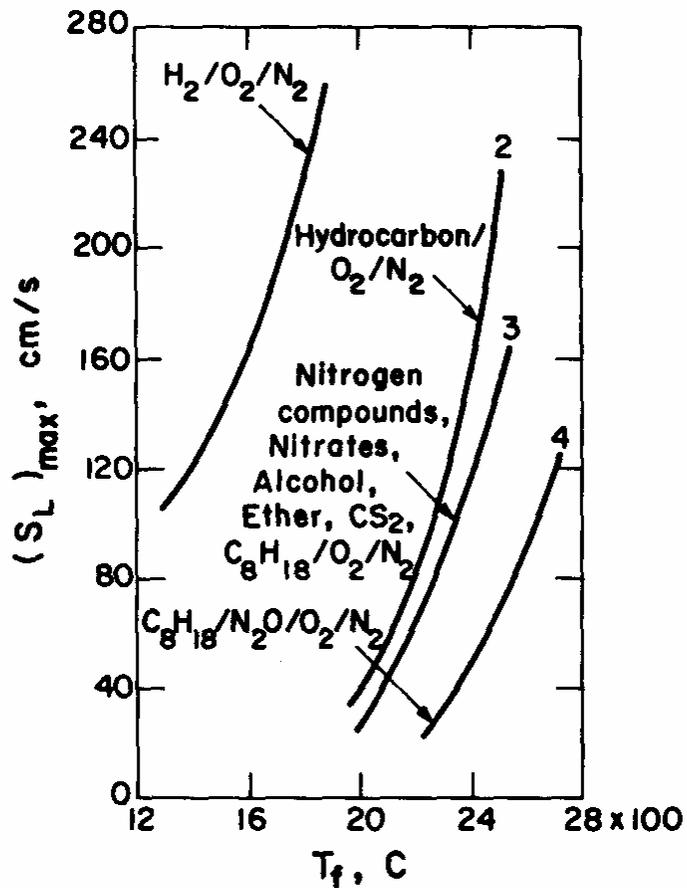
$$S_L = C_3 \cdot e^{-E/2R_u T}$$

Premixed Flames

- Effect of Physical Properties

- Flame Temperature

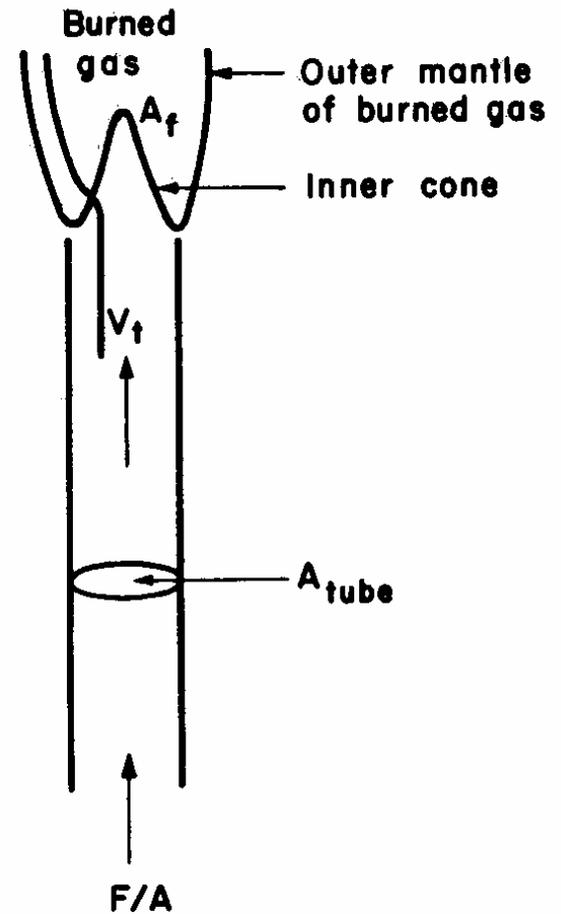
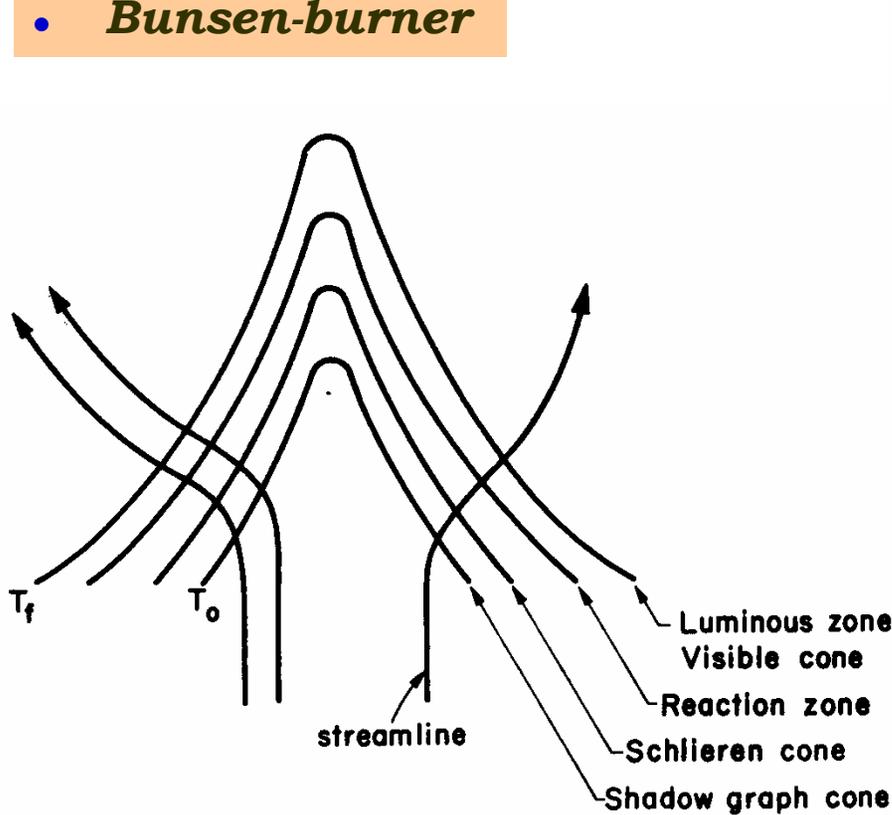
- α and C_p



Premixed Flames

- **S_L - Experimental Methods**

- **Bunsen-burner**

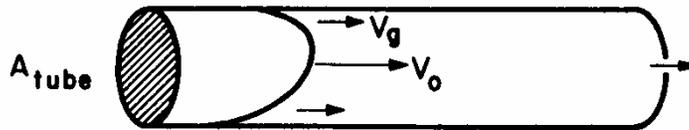


$$S_L = V_t \cdot A_t / A_f$$

Premixed Flames

- **S_L - Experimental Methods (cont.)**

- **Transparent Tube**



$$S_L = (V_o - V_g) A_{tube} / A_f$$

- **Constant-Volume Bomb**

- **Constant-Volume**
- **Temperature and pressure rise**
- **Flame accelerates**

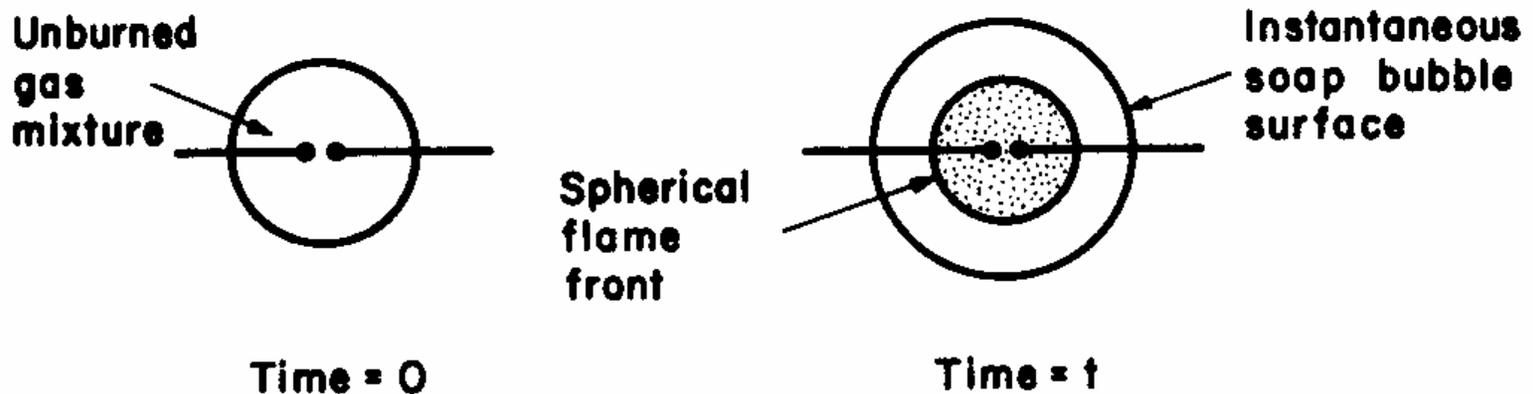
$$S_L = \frac{dr}{dt} - \frac{R^3 - r^3}{3p\gamma_u r^2}$$

Premixed Flames

- **S_L - Experimental Methods (cont.)**

- **Soap-Bubble**

- Constant Pressure

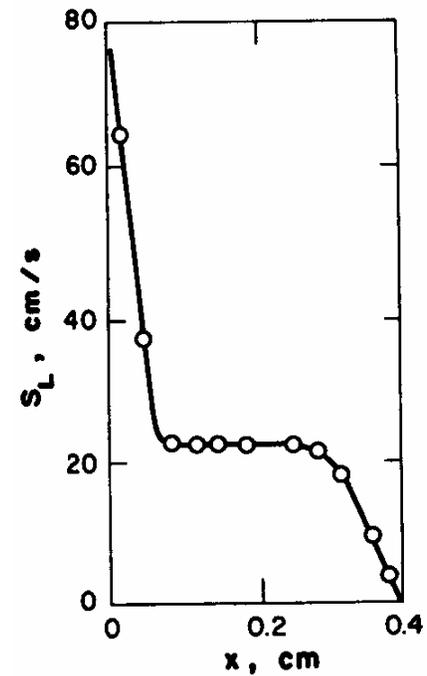
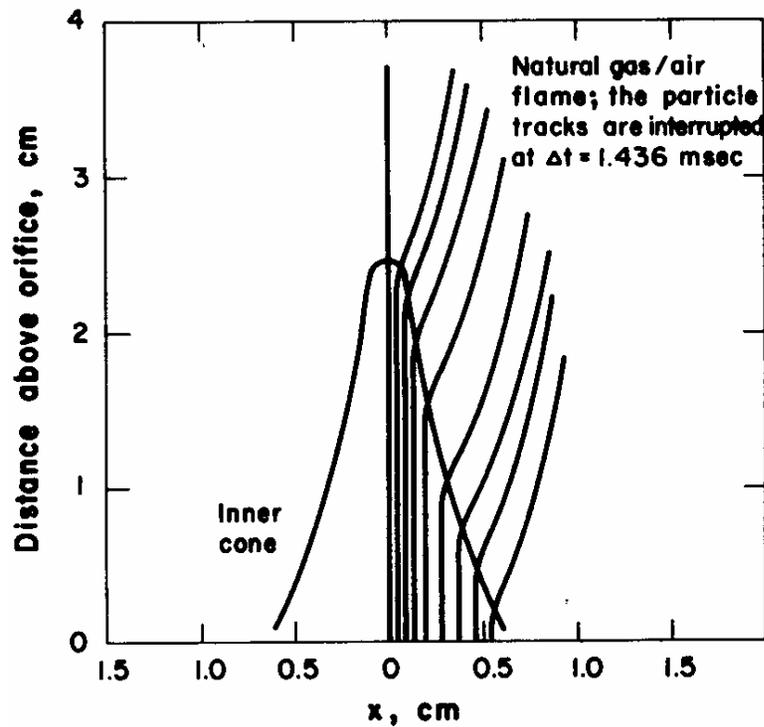


$$S_L = u_r \frac{\rho_b}{\rho_u} = u_r \frac{T_b}{T_u}$$

Premixed Flames

- S_L - Experimental Methods (cont.)

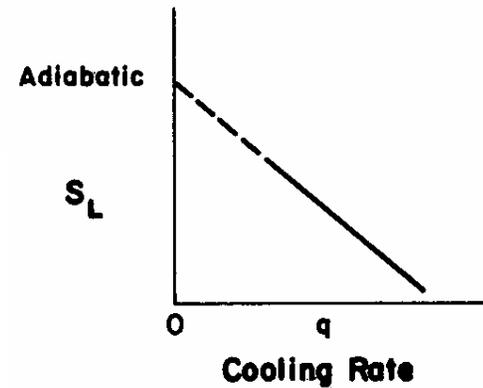
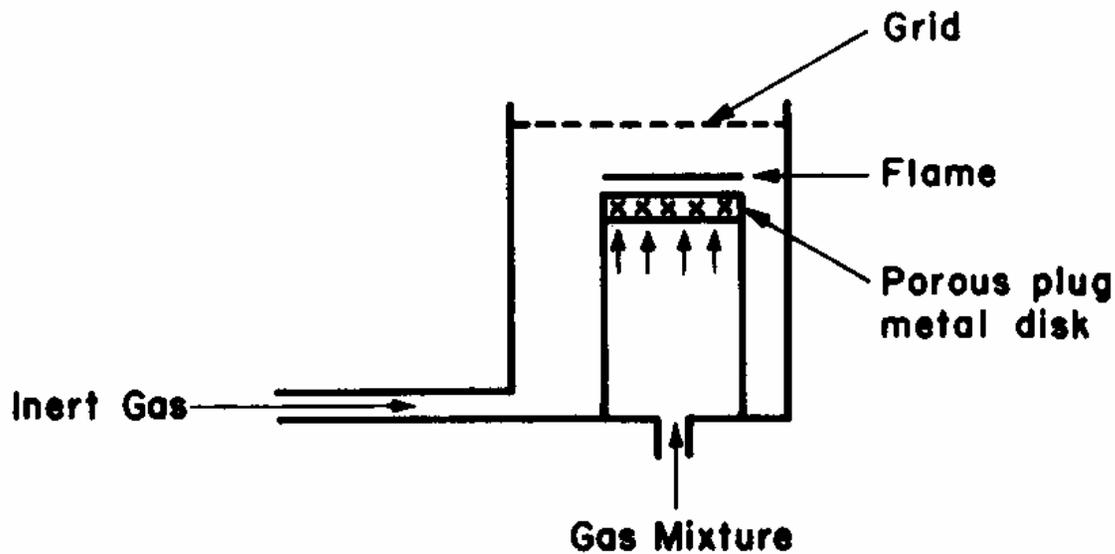
- Particle Tracking



Premixed Flames

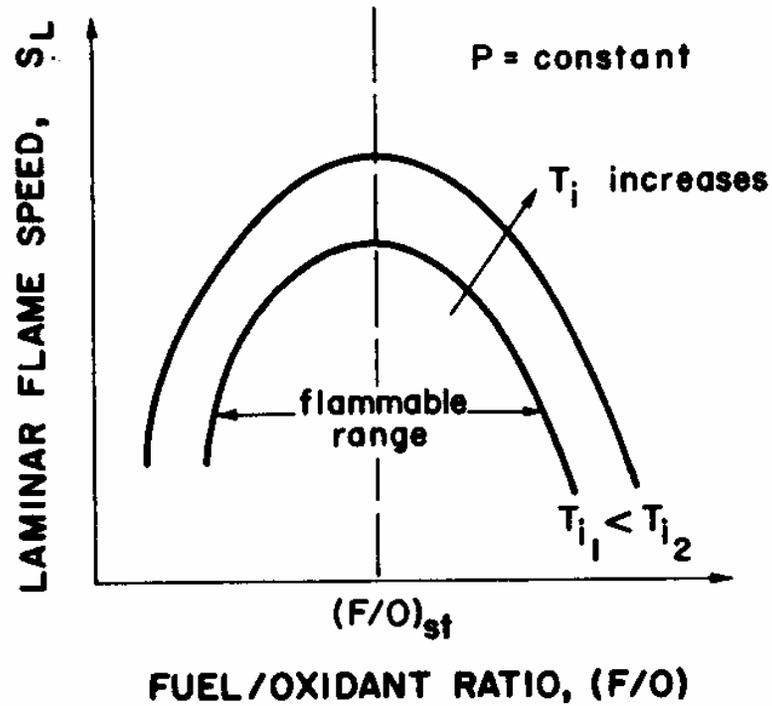
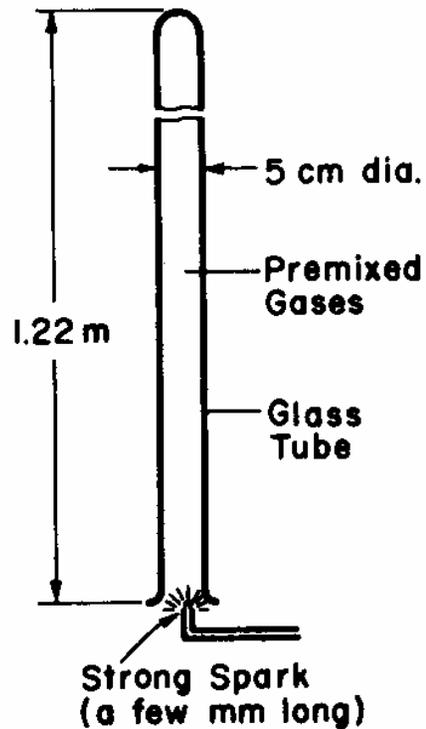
- S_L - Experimental Methods (cont.)

- Flat Burner



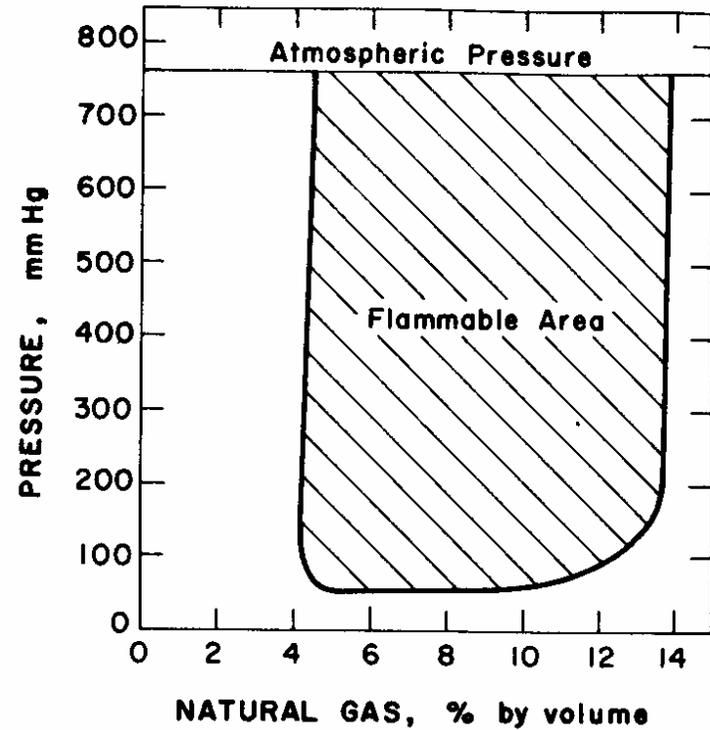
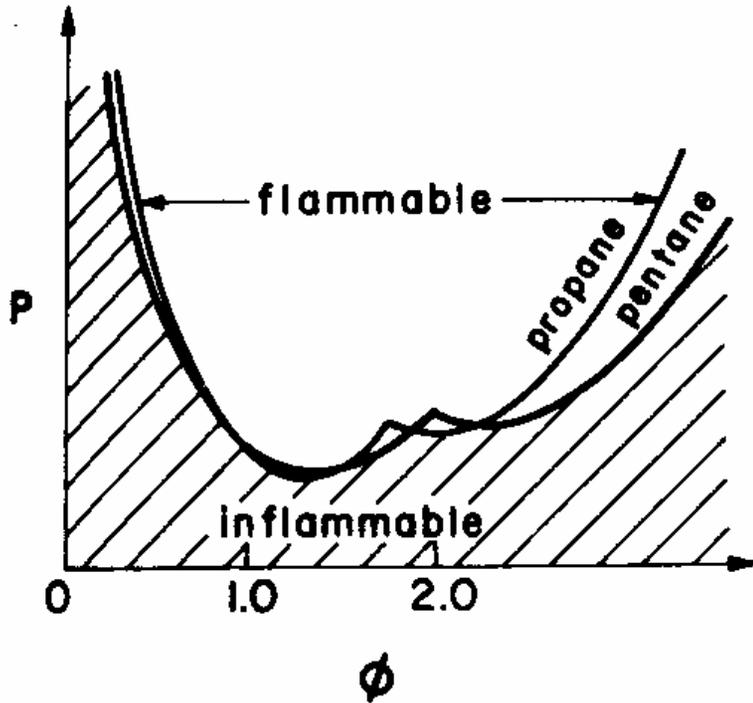
Premixed Flames

- **Flame Quenching**
- **Flammability Limits**



Premixed Flames

- **Flammability Limits**



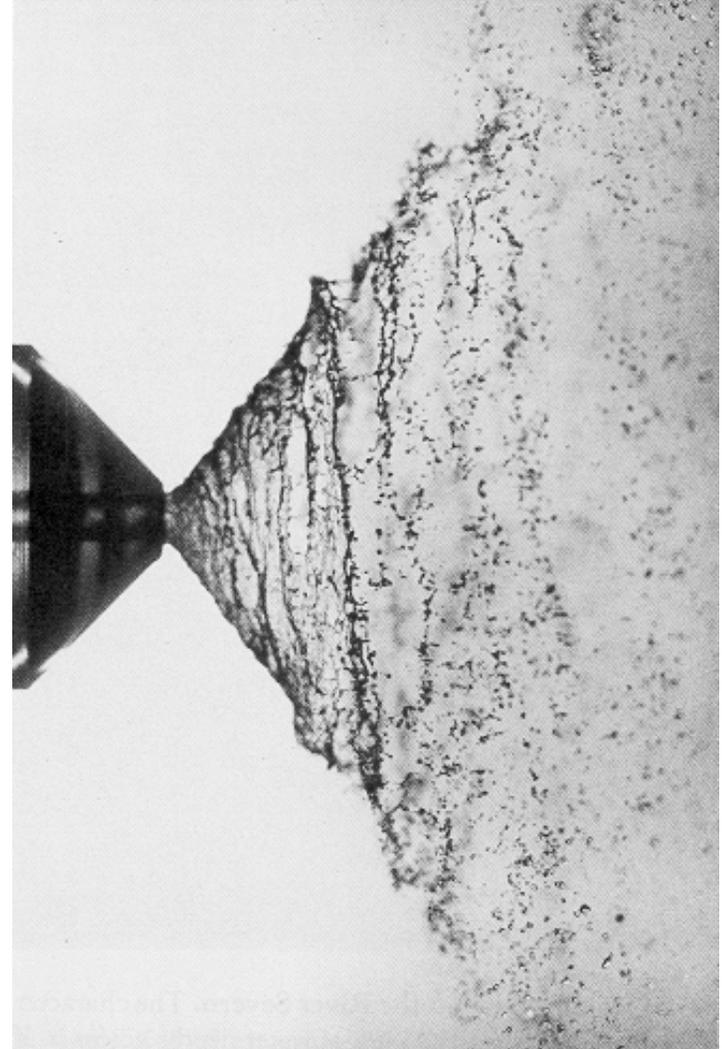
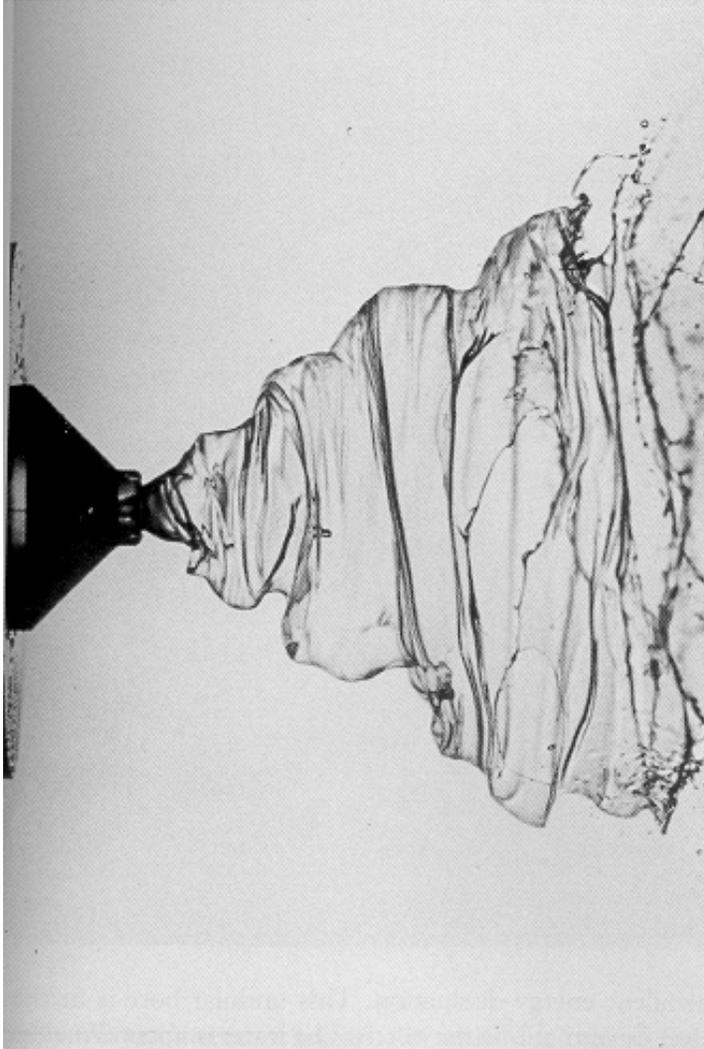
Premixed Flames

- **Flammability Limits**

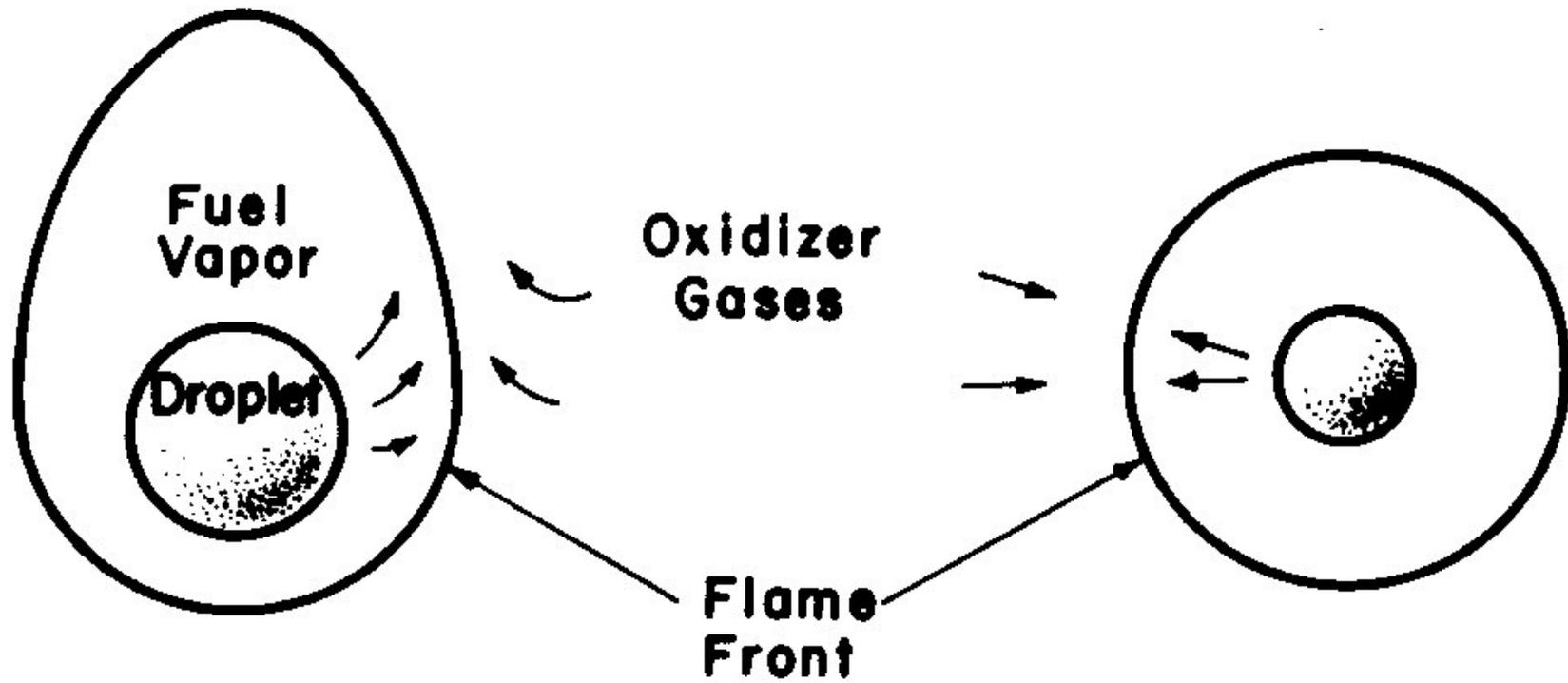
TABLE 5.5 Flammability Limits of Certain Fuel–Air Mixtures

	Lower (Lean) Limits, Vol. (%) in Air	Upper (Rich) Limits, Vol. (%) in Air	Stoichiometric, Vol. (%) in Air
Methane, CH ₄	5	15	9.47
Heptane, C ₇ H ₁₆	1	6	1.87
Hydrogen, H ₂	4	74.2	29.2
Carbon monoxide, CO	12.5	74.2	29.5
Acetylene	2.5	80	7.7
Ethane, C ₂ H ₄	2.82	15.34	5.64
Ethylene oxide, C ₂ H ₄ O	3.0	100	7.72
Propane, C ₃ H ₈	2.05	11.38	4.02
Methanol (g), CH ₃ OH	5.88	49.94	12.24

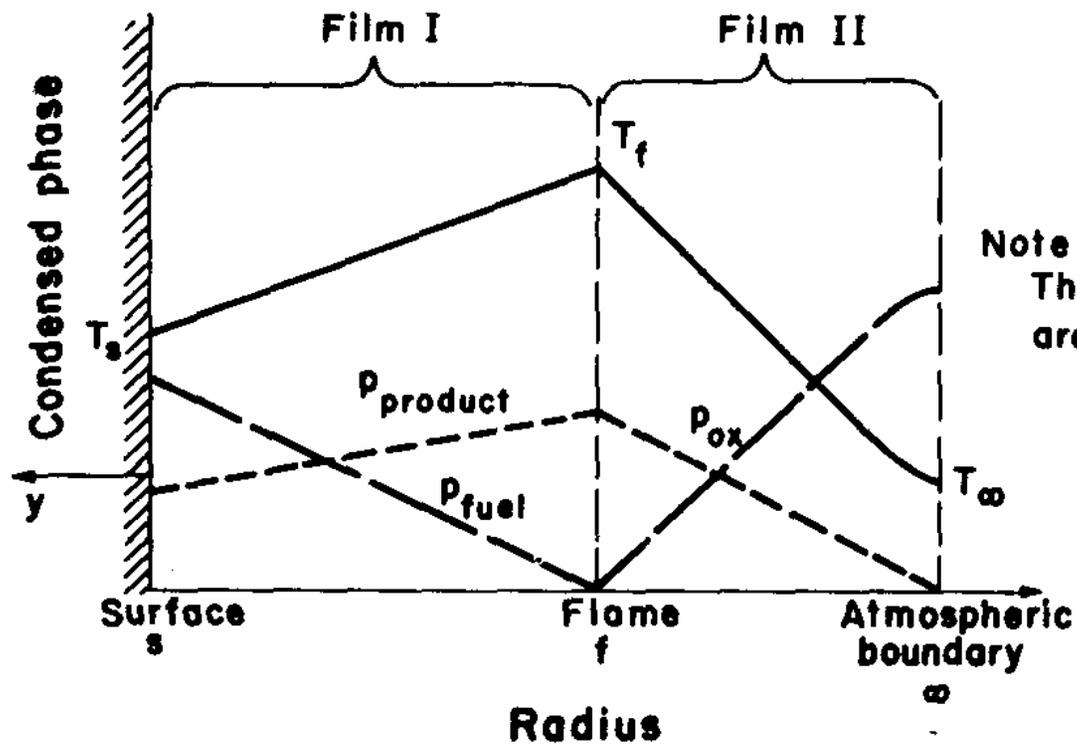
Liquid Sprays



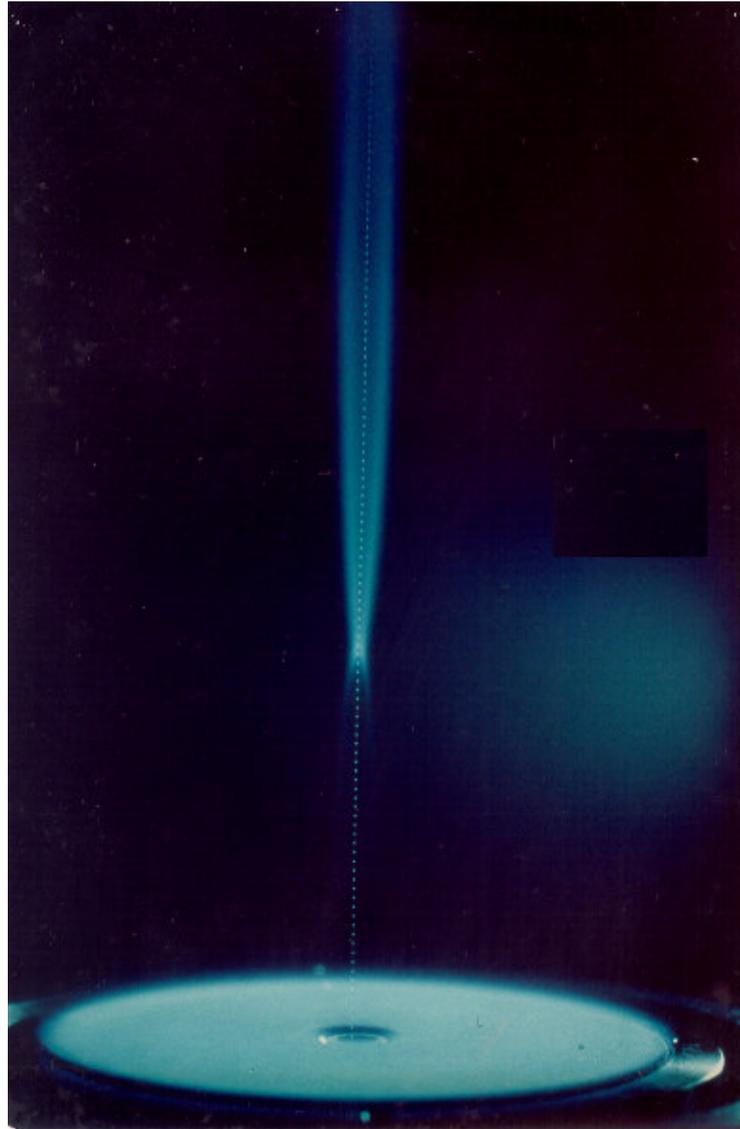
Isolated Droplets



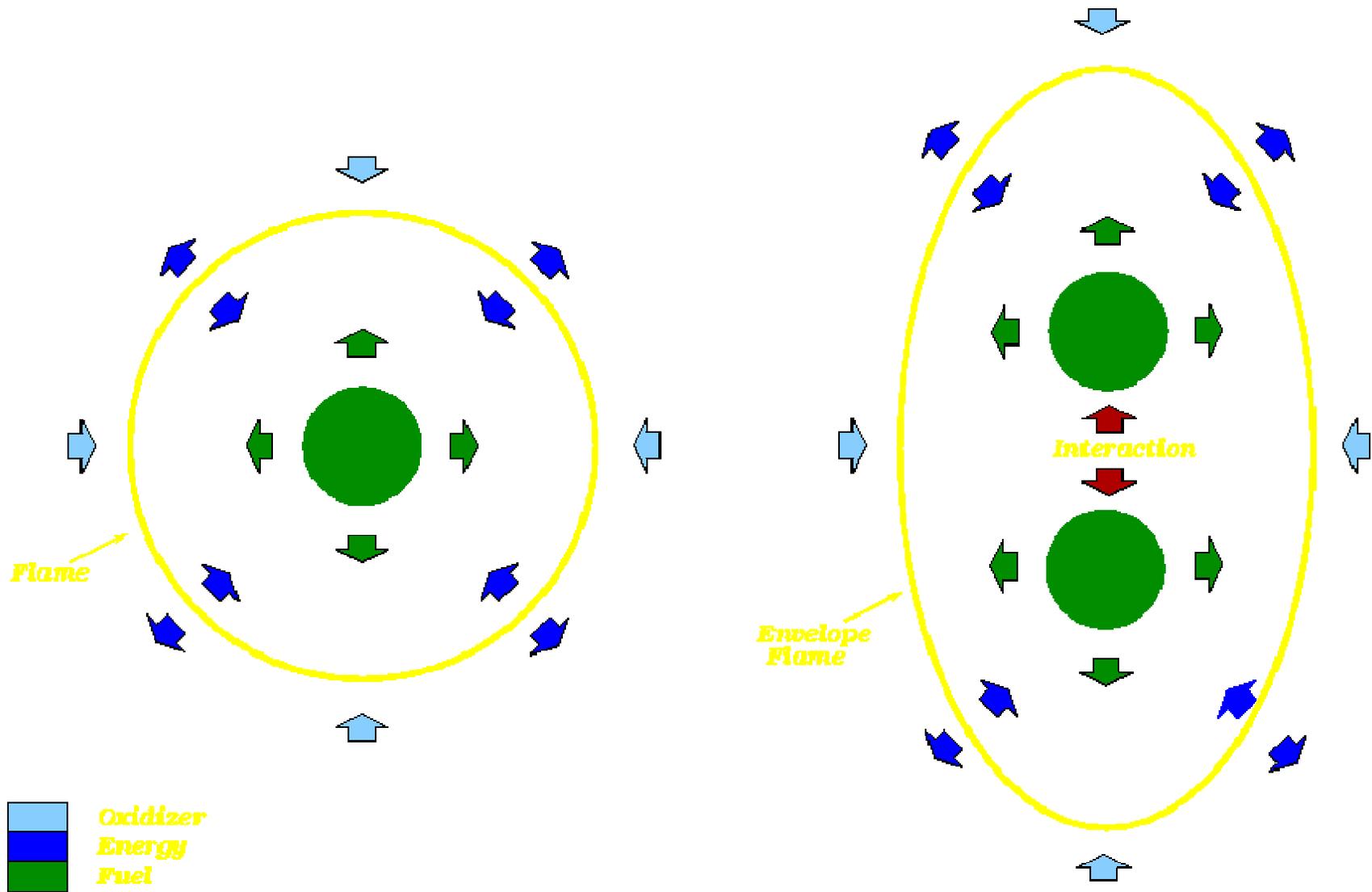
Isolated Droplets



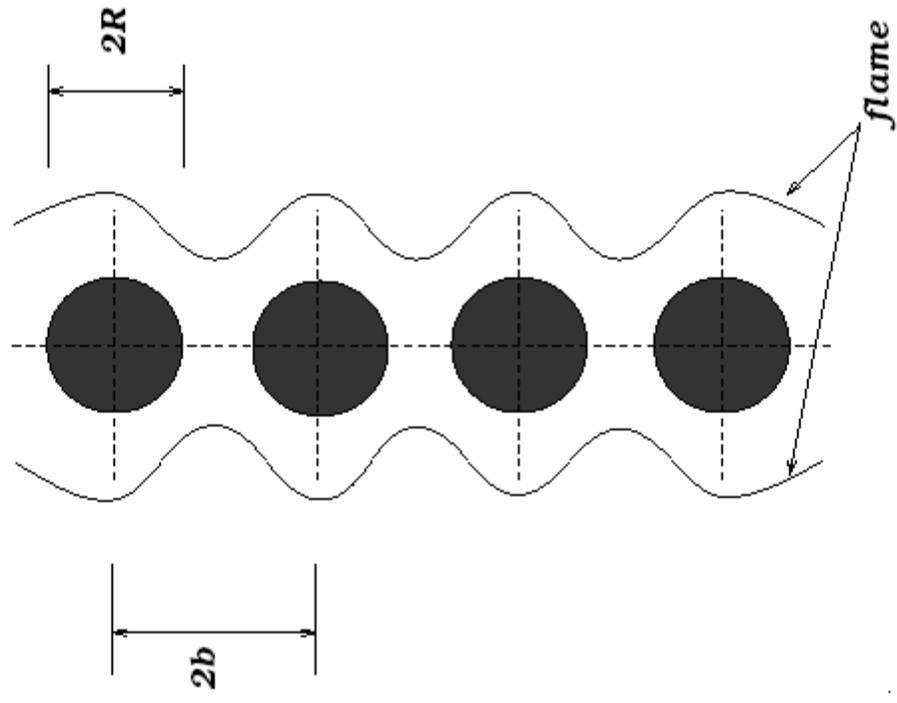
Droplet Stream



Interaction Phenomenon

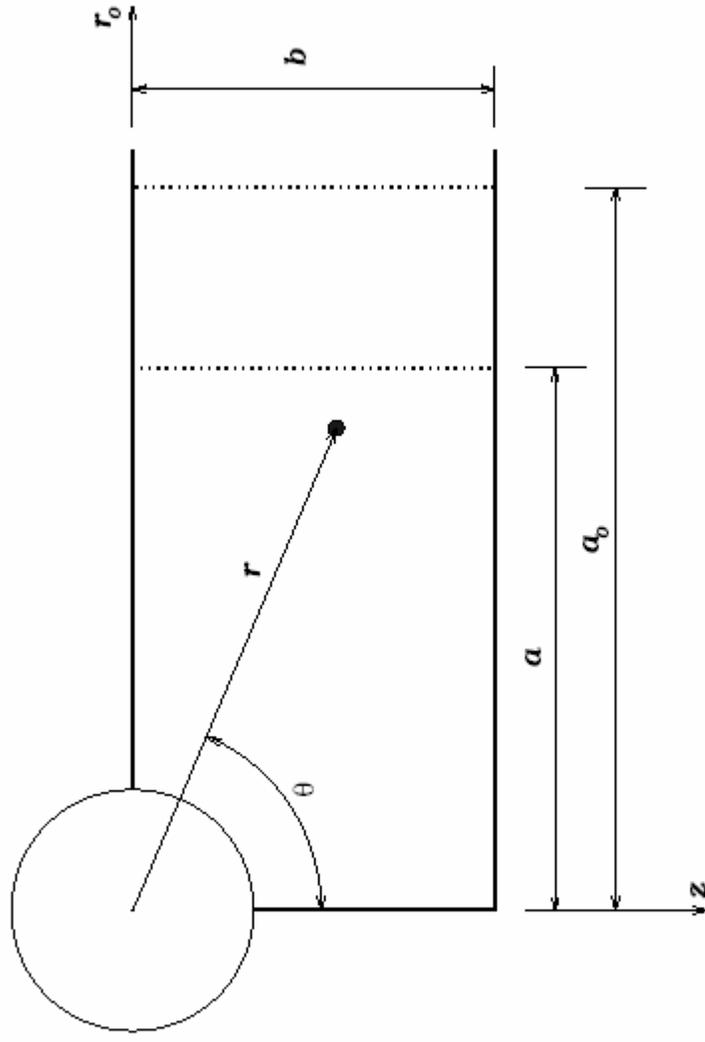


Stream of Droplets



Center portion of a stream of droplets and principal dimensions.

Physical Domain



Physical domain and principal dimensions.

Governing Equations

Droplet-Stream Combustion

$$\frac{1}{r^{*2}} \frac{\partial}{\partial r^{*2}} \left(r^{*2} \frac{\partial \Phi^{*}}{\partial r^{*2}} \right) + \frac{1}{r^{*2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Phi^{*}}{\partial \theta} \right) = 0$$

$$u_r^{*} \frac{\partial T^{*}}{\partial r^{*2}} + \frac{u_{\theta}^{*}}{r^{*}} \frac{\partial T^{*}}{\partial \theta} = \frac{1}{Ja} \left(\frac{1}{r^{*2}} \frac{\partial}{\partial r^{*2}} \left(r^{*2} \frac{\partial T^{*}}{\partial r^{*2}} \right) + \frac{1}{r^{*2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial T^{*}}{\partial \theta} \right) \right) + \dot{q}^{*}$$

$$u_r^{*} \frac{\partial Y_f^{*}}{\partial r^{*2}} + \frac{u_{\theta}^{*}}{r^{*}} \frac{\partial Y_f^{*}}{\partial \theta} = \frac{1}{Ja Le} \left(\frac{1}{r^{*2}} \frac{\partial}{\partial r^{*2}} \left(r^{*2} \frac{\partial Y_f^{*}}{\partial r^{*2}} \right) + \frac{1}{r^{*2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y_f^{*}}{\partial \theta} \right) \right) + \dot{w}_f^{*}$$

$$u_r^{*} \frac{\partial Y_o^{*}}{\partial r^{*2}} + \frac{u_{\theta}^{*}}{r^{*}} \frac{\partial Y_o^{*}}{\partial \theta} = \frac{1}{Ja Le} \left(\frac{1}{r^{*2}} \frac{\partial}{\partial r^{*2}} \left(r^{*2} \frac{\partial Y_o^{*}}{\partial r^{*2}} \right) + \frac{1}{r^{*2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y_o^{*}}{\partial \theta} \right) \right) + \dot{w}_o^{*}$$

Boundary Conditions

Droplet-Stream Combustion

$$\frac{\partial \Phi^*}{\partial r^*} = V_s^*(\theta) \quad T^* = T_s^* \quad Y_f^* = Y_{f,s}^* \quad Y_o^* = Y_{o,s}^* \quad ; r^* = 1 \quad 0 < \theta < \frac{\pi}{2}$$

$$\Phi^* \rightarrow 0 \quad T^* \rightarrow 1 \quad Y_f^* \rightarrow Y_{f,\infty}^* \quad Y_o^* \rightarrow Y_{o,\infty}^* \quad ; r^* \rightarrow \infty$$

$$\frac{\partial \Phi^*}{\partial \theta} = 0 \quad \frac{\partial T^*}{\partial \theta} = 0 \quad \frac{\partial Y_f^*}{\partial \theta} = 0 \quad \frac{\partial Y_o^*}{\partial \theta} = 0 \quad ; \begin{cases} \theta = 0 & 1 < r^* < b^* \\ \theta = \frac{\pi}{2} & 1 < r^* < \infty \end{cases}$$

$$-\frac{\partial \Phi^*}{\partial \theta} \sin \theta + \frac{\partial \Phi^*}{\partial r^*} b^* = 0 \quad -\frac{\partial T^*}{\partial \theta} \sin \theta + \frac{\partial T^*}{\partial r^*} b^* = 0$$

$$-\frac{\partial Y_f^*}{\partial \theta} \sin \theta + \frac{\partial Y_f^*}{\partial r^*} b^* = 0 \quad -\frac{\partial Y_o^*}{\partial \theta} \sin \theta + \frac{\partial Y_o^*}{\partial r^*} b^* = 0 \quad ; \begin{cases} r^* \cos \theta = b^* \\ 0 < \theta < \theta_c \end{cases}$$

Boundary Conditions

Droplet-Stream Combustion

Coupling condition

$$\left. \frac{\partial T^*}{\partial r^{**}} \right|_{r^{**}=1} = V_s^* = \left. \frac{\partial \Phi^*}{\partial r^{**}} \right|_{r^{**}=1}$$

$$Y_{f,s}^* V_s^* = \frac{1}{Ja} \frac{\partial Y_f^*}{Le \partial r^{**}} \bigg|_{r^{**}=1}$$

$$Y_{o,s}^* V_s^* = \frac{1}{Ja} \frac{\partial Y_o^*}{Le \partial r^{**}} \bigg|_{r^{**}=1}$$

non-dimensional variables

$$r^{**} = \frac{r}{R}$$

$$\Phi^* = V_{ref} R \Phi$$

$$T^* = \frac{T - T_{sdt}}{T_{\infty} - T_{sdt}}$$

$$Y_f^* = 1 - Y_f \quad Y_o^* = Y_o$$

Coupling Functions

Droplet-Stream Combustion

$$\beta_{f,o} = \frac{Y_f^* + Y_o^* \nu}{Y_{f,s}^* + Y_{o,s}^* \nu}$$

$$\beta_{f,t} = \frac{Y_f^* - Ja.II^*}{Y_{f,s}^* - I}$$

$$\beta_{o,t} = \frac{Y_o^* \nu + Ja.II^*}{Y_{o,s}^* \nu + I}$$

Nondimensional Parameters

$$Ja = \frac{c_p(T_\infty - T_{sat})}{h_{fg}} = \frac{V_{ref} R}{\alpha} \quad Le = \frac{D}{\alpha}$$

$$I = \frac{h_{fg}}{h_r}$$

Coupling Function Equation

Droplet-Stream Combustion

$$u_r^* \frac{\partial \beta_i}{\partial r^*} + \frac{u_\theta^*}{r^*} \frac{\partial \beta_i}{\partial \theta} = \frac{1}{Ja} \left(\frac{1}{r^{*2}} \frac{\partial}{\partial r^*} \left(r^{*2} \frac{\partial \beta_i}{\partial r^*} \right) + \frac{1}{r^{*2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \beta_i}{\partial \theta} \right) \right)$$

Boundary conditions

$$\beta_i = \beta_{i;s} \quad ; \quad r^* = 1 \quad 0 < \theta < \frac{\pi}{2}$$

$$\beta_i \rightarrow \beta_{i;\infty} \quad ; \quad r^* \rightarrow \infty$$

$$\frac{\partial \beta_i}{\partial \theta} = 0 \quad \theta = 0 \quad 1 < r^* < b^*$$

$$\frac{\partial \beta_i}{\partial \theta} = 0 \quad ; \quad \theta = \frac{\pi}{2} \quad 1 < r^* < \infty$$

$$-\frac{\partial \beta_i}{\partial \theta} \sin \theta + \frac{\partial \beta_i}{\partial r^*} b = 0 \quad ; \quad r^* \cos \theta = b \quad 0 < \theta < \theta_c$$

$$i \equiv (f, o), (f, t) \text{ or } (o, t)$$

Coupling Function Equation

Droplet-Stream Combustion

Coupling Condition

$$\frac{1}{Ja} \left. \frac{\partial \beta_i}{\partial r^*} \right|_{r^*=1} = V_s^*$$

Linear Relation

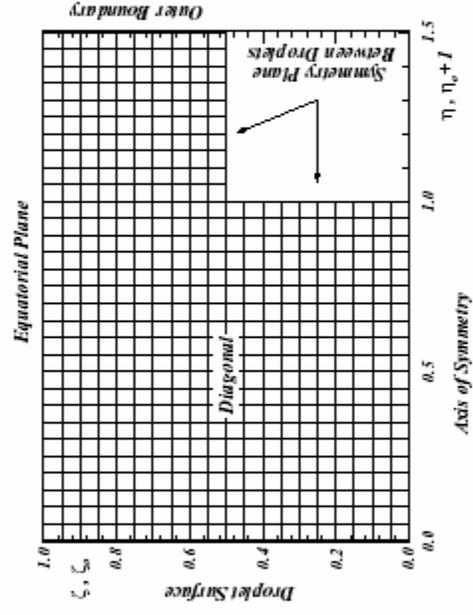
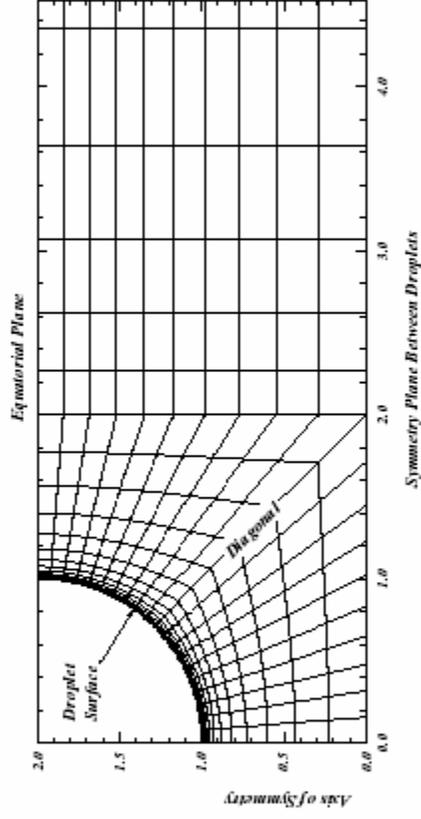
$$\beta_j = \beta_{f,o} + (\beta_{j;\infty} - \beta_{f,o;\infty})$$

$j \equiv (f, t) \text{ or } (o, t)$

Flame Position

$$\beta_{f,o} = \frac{1}{Y_{f,s}^*}$$

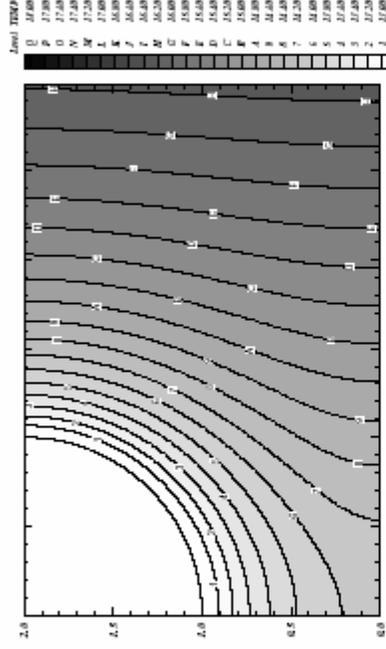
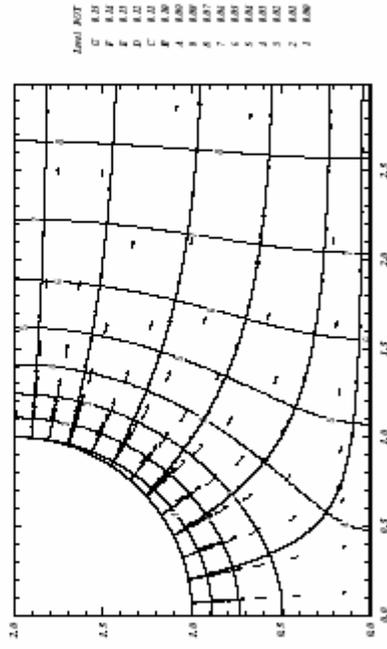
Grid



Computational 21x21 grids in the physical plane (above) and in the transformed plane (below).

Results - Stream of Porous-Spheres

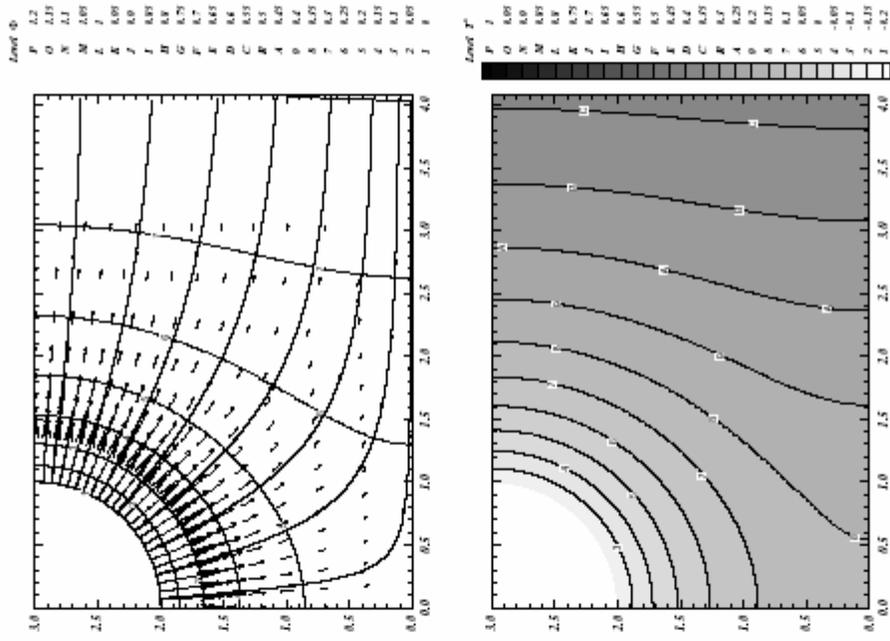
Droplet-Stream Combustion



Equip. lines, streamlines, velocity vectors (above) and temperature regions - $b^* = 2$ (16x161 points)

Results - Stream of Droplets

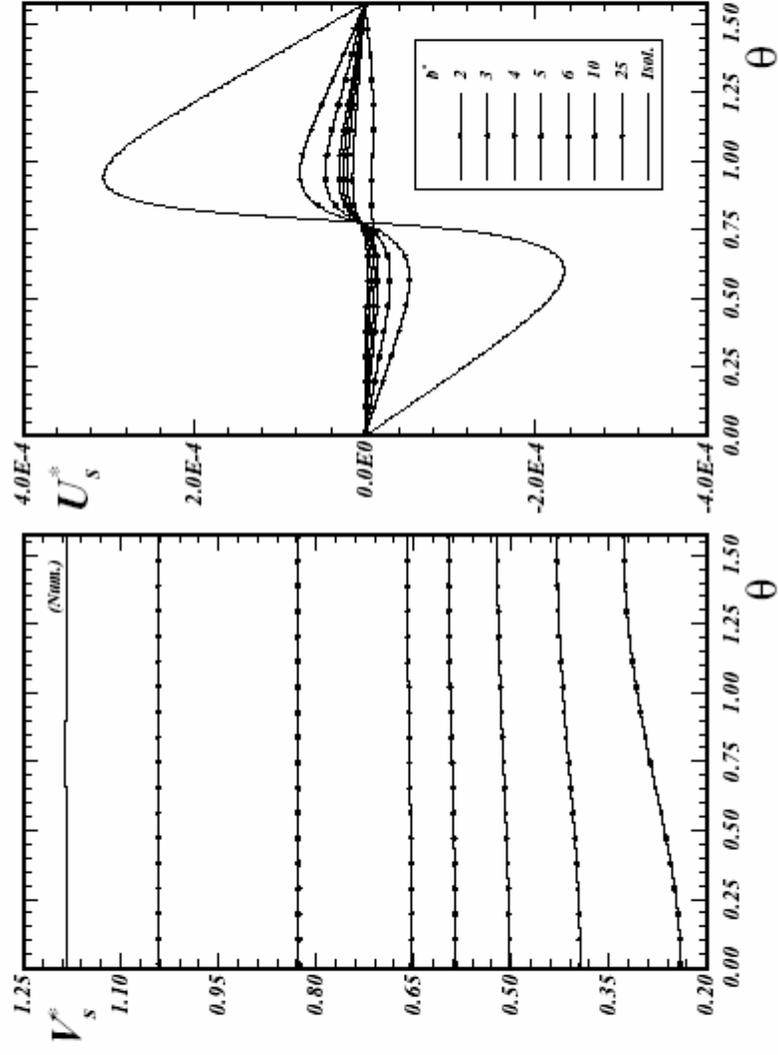
Droplet-Stream Combustion



Equip. lines, streamlines, velocity vectors (above) and temperature regions - $b^{36} = 3$

Results - Droplet Surface Velocity

Droplet-Stream Combustion



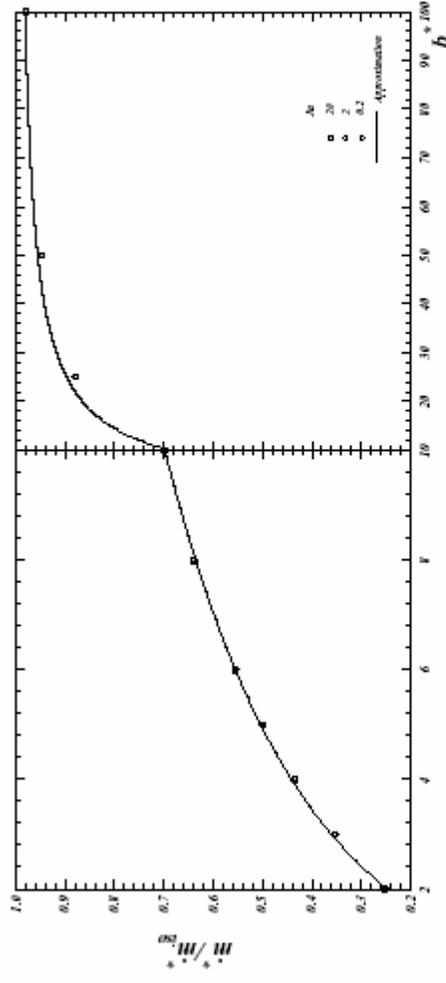
Droplet surface velocity: normal (right) and tangential (left). ($Ja = 2$)

Mass Vaporization Rate

Droplet Stream Combustion

$$\dot{m}^* = \frac{\dot{m}}{4\pi\rho R^2 V_{ref}} = \int_0^{\pi/2} V_s^*(\theta) \sin(\theta) d\theta$$

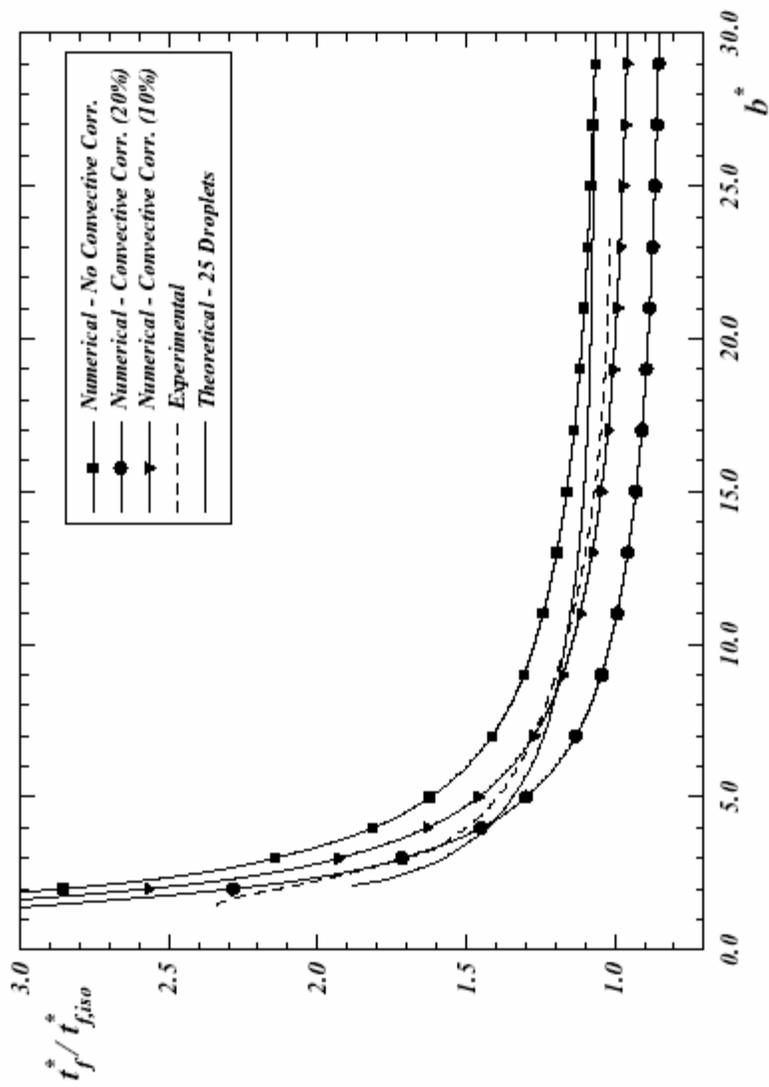
$$\frac{\dot{m}^*}{\dot{m}_{gd}^*} = 1 - g_0 (b^*)^{-g_1} \quad g_0 = 0.9972 \quad g_1 = 1.1845$$



Ratio of the Nondimensional Droplet Vaporization Rate in a Stream to an Isolated Droplet.

Droplet Lifetime

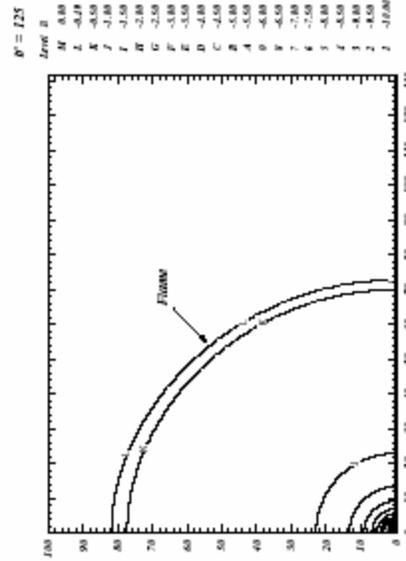
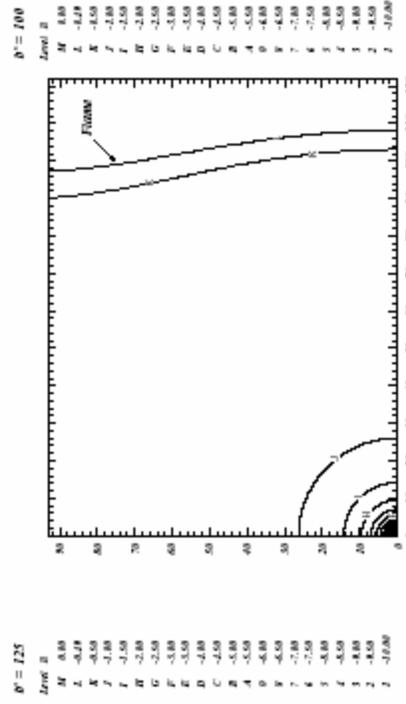
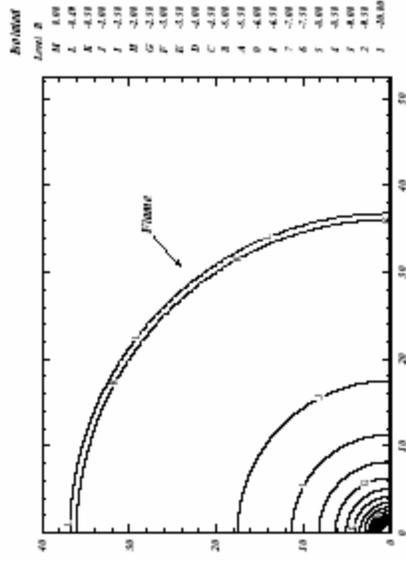
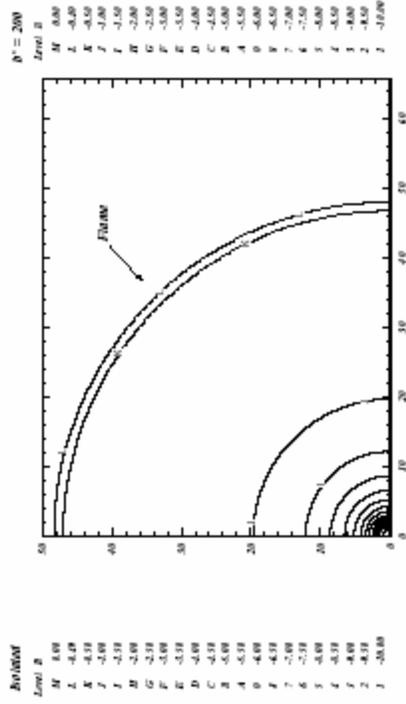
Droplet Stream Combustion



Ratio of the Nondimensional Droplet Vaporization Rate in a Stream to an Isolated Droplet.

Flame Interference

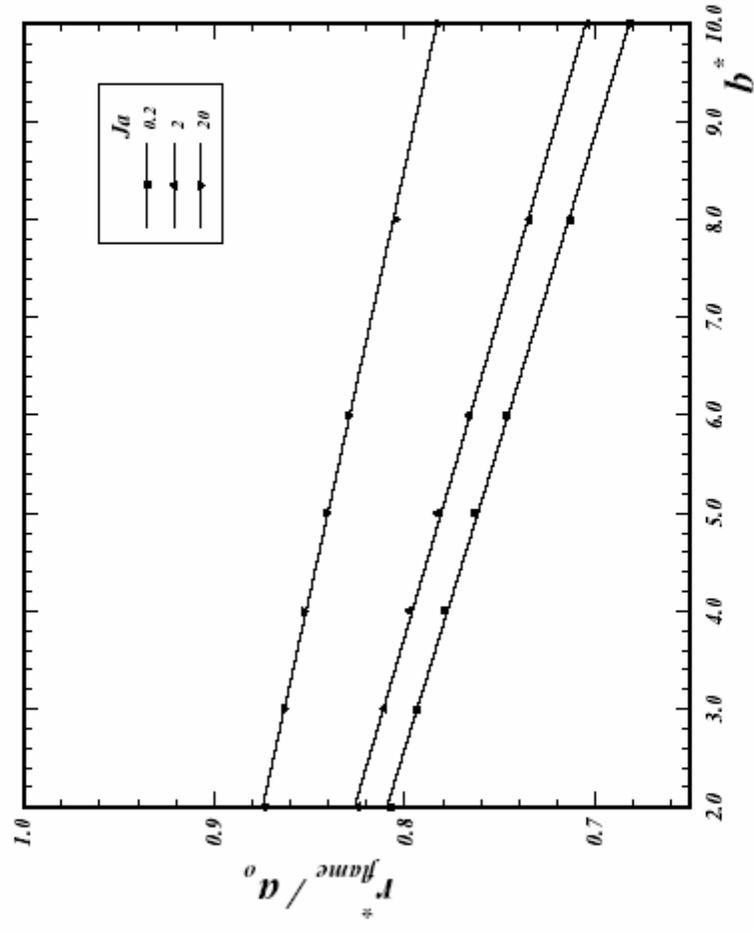
Droplet Stream Combustion



Flame distortion and position

Truncation Distance Influence

Droplet Stream Combustion



Ratio of the Cylindrical Flame-Stream distance to the truncating radius

Truncation Distance Influence

Droplet Stream Combustion

b^*	2		10		25	
	$\dot{m}_{\text{iso}}^* / \dot{m}_{\text{iso}}^*$	$r_{\text{flame}}^* / a_o^*$	$\dot{m}_{\text{iso}}^* / \dot{m}_{\text{iso}}^*$	$r_{\text{flame}}^* / a_o^*$	$\dot{m}_{\text{iso}}^* / \dot{m}_{\text{iso}}^*$	$r_{\text{flame}}^* / a_o^*$
a_o^*						
800	0.2787	0.8375	0.7344	0.7150	0.9021	0.5075
1600	0.2543	0.8244	0.6988	0.7044	0.8798	0.2211
3200	0.2327	0.7192	0.6672	0.6144	0.8592	0.4897

Mass vaporization ratio and relative flame position for different physical domain truncating distances.

Governing Equations

Velocity Field

$$\frac{1}{r^{**2}} \frac{\partial}{\partial r^{**}} \left(r^{**2} \frac{\partial \Phi^{**}}{\partial r^{**}} \right) + \frac{1}{r^{**2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Phi^{**}}{\partial \theta} \right) = 0$$

Coupling Functions

Droplet-Stream Combustion

$$\beta_{f,o} = \frac{Y_f^{**} + Y_o^{**} \nu}{Y_{f,s}^{**} + Y_{o,s}^{**} \nu} \quad \beta_{f,t} = \frac{Y_f^{**} - Ja_{IT}^{**}}{Y_{f,s}^{**} - I} \quad \beta_{o,t} = \frac{Y_o^{**} \nu + Ja_{IT}^{**}}{Y_{o,s}^{**} \nu + I}$$

Nondimensional Parameters

$$t^{**} = \frac{V_{ref} \cdot t}{a + a_o}$$

Governing Equations

Coupling Function

$$\begin{aligned} \frac{1}{a^* + a_0^*} \frac{\partial \beta_i}{\partial t^*} + u_r^* \frac{\partial \beta_i}{\partial r^*} + \frac{u_\theta^*}{r^*} \frac{\partial \beta_i}{\partial \theta} &= \\ = \frac{1}{Ja} \left(\frac{1}{r^{*2}} \frac{\partial}{\partial r^*} \left(r^{*2} \frac{\partial \beta_i}{\partial r^*} \right) + \frac{1}{r^{*2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \beta_i}{\partial \theta} \right) \right) \end{aligned}$$

Boundary conditions

$$\beta_i = \beta_{i;s} \quad ; \quad r^* = 1 \quad 0 < \theta < \frac{\pi}{2}$$

$$\beta_i \rightarrow \beta_{i;\infty} \quad ; \quad r^* \rightarrow \infty$$

$$\frac{\partial \beta_i}{\partial \theta} = 0 \quad \theta = 0 \quad 1 < r^* < b^*$$

$$\frac{\partial \beta_i}{\partial \theta} = 0 \quad ; \quad \theta = \frac{\pi}{2} \quad 1 < r^* < \infty$$

$$-\frac{\partial \beta_i}{\partial \theta} \sin \theta + \frac{\partial \beta_i}{\partial r^*} b = 0 \quad ; \quad r^* \cos \theta = b \quad 0 < \theta < \theta_c$$

$$i \equiv (f, \sigma), (f, t) \text{ or } (\sigma, t)$$

Coupling Function Equation

Droplet-Stream Combustion

Coupling Condition

$$\frac{1}{Ja} \frac{\partial \beta_i}{\partial r^*} \Big|_{r^*=1} = V_s^*$$

Linear Relation

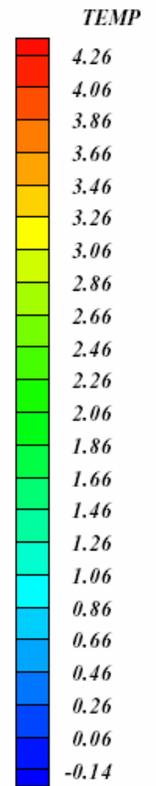
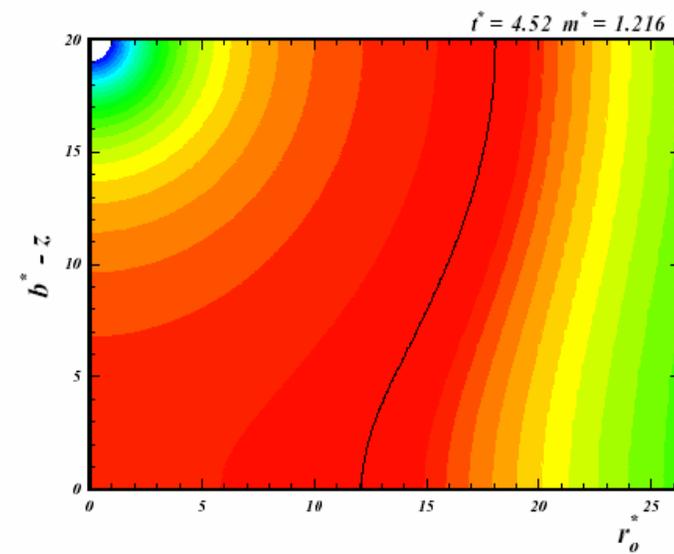
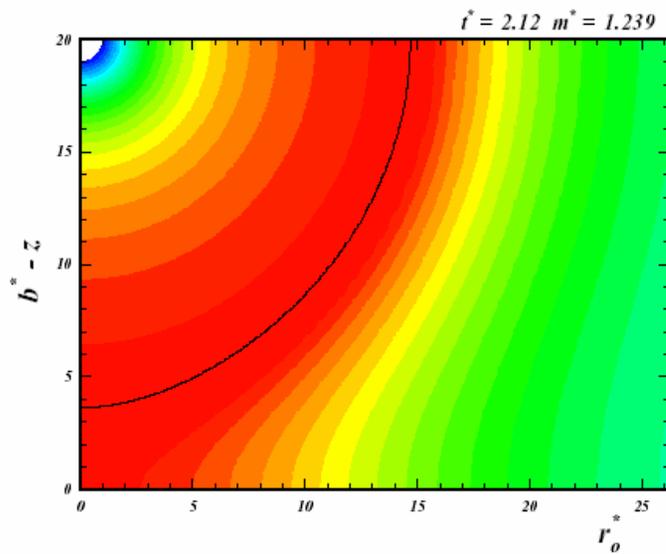
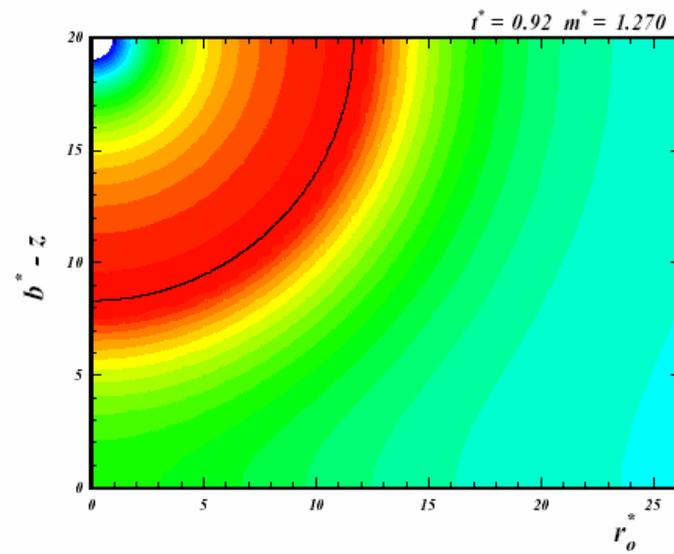
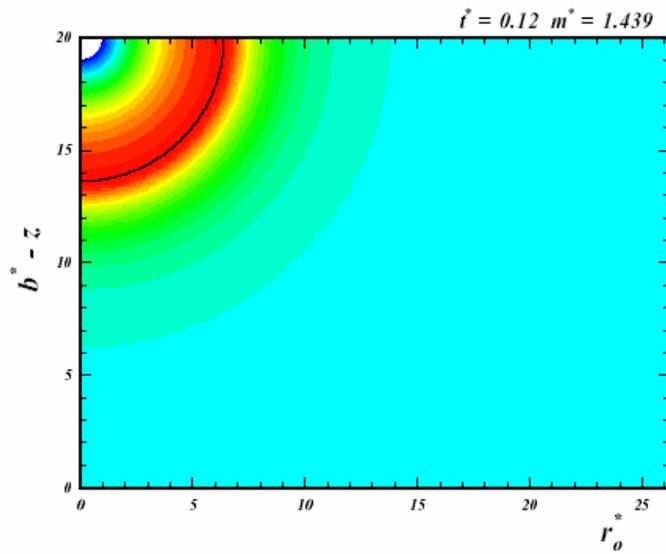
$$\beta_j = \beta_{f,o} + (\beta_{j;\infty} - \beta_{f,o;\infty})$$

$j \equiv (f, t) \text{ or } (o, t)$

Flame Position

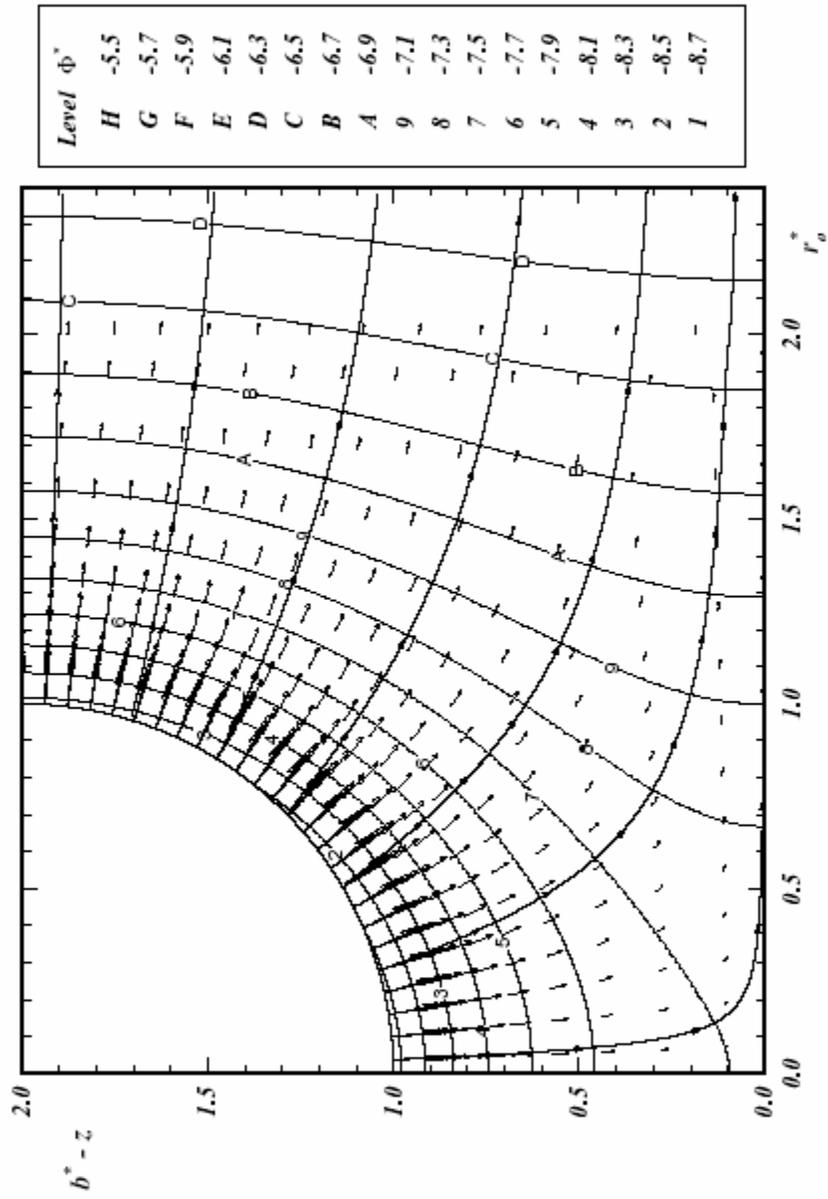
$$\beta_{f,o} = \frac{1}{Y_{f,s}^*}$$

Droplet Mass Vaporization



Velocity Field

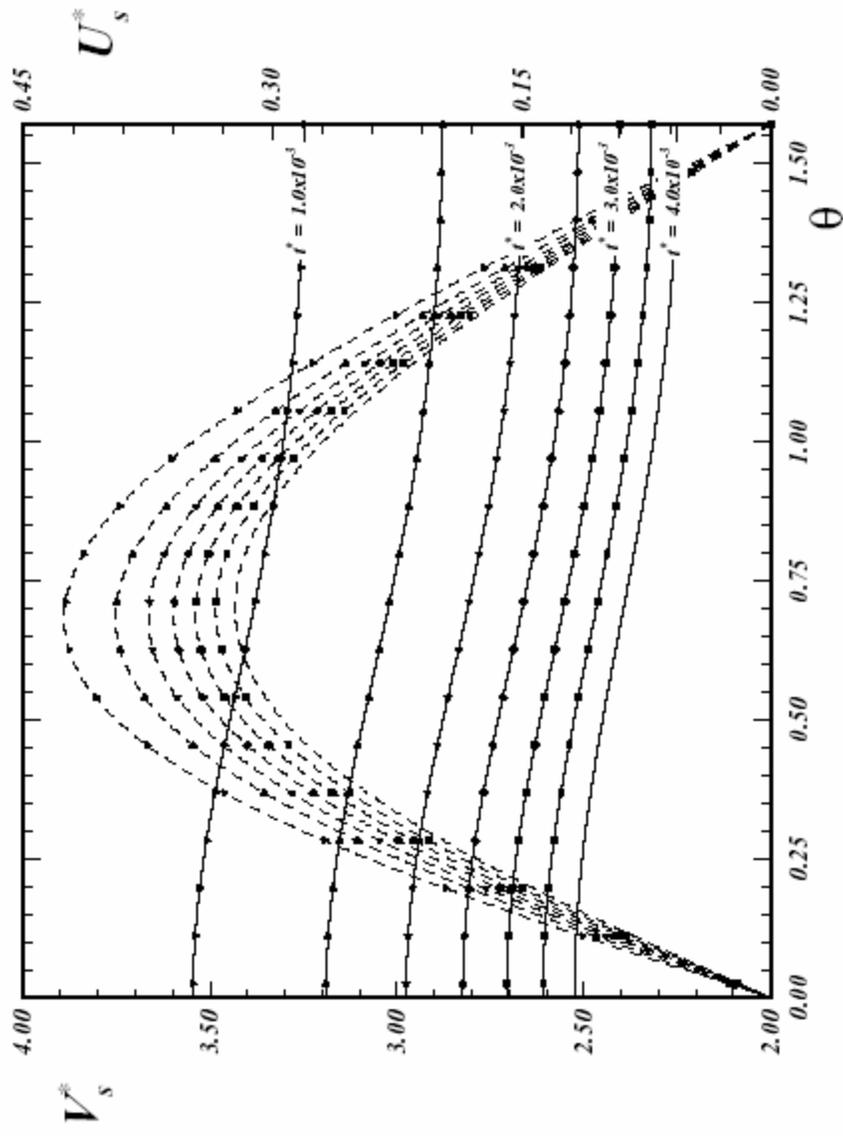
Droplet-Stream Combustion



Equip. lines, streamlines, velocity vectors for a burning droplet - $b^* = 2$ ($J_0 = 2$)

Droplet Surface Velocity

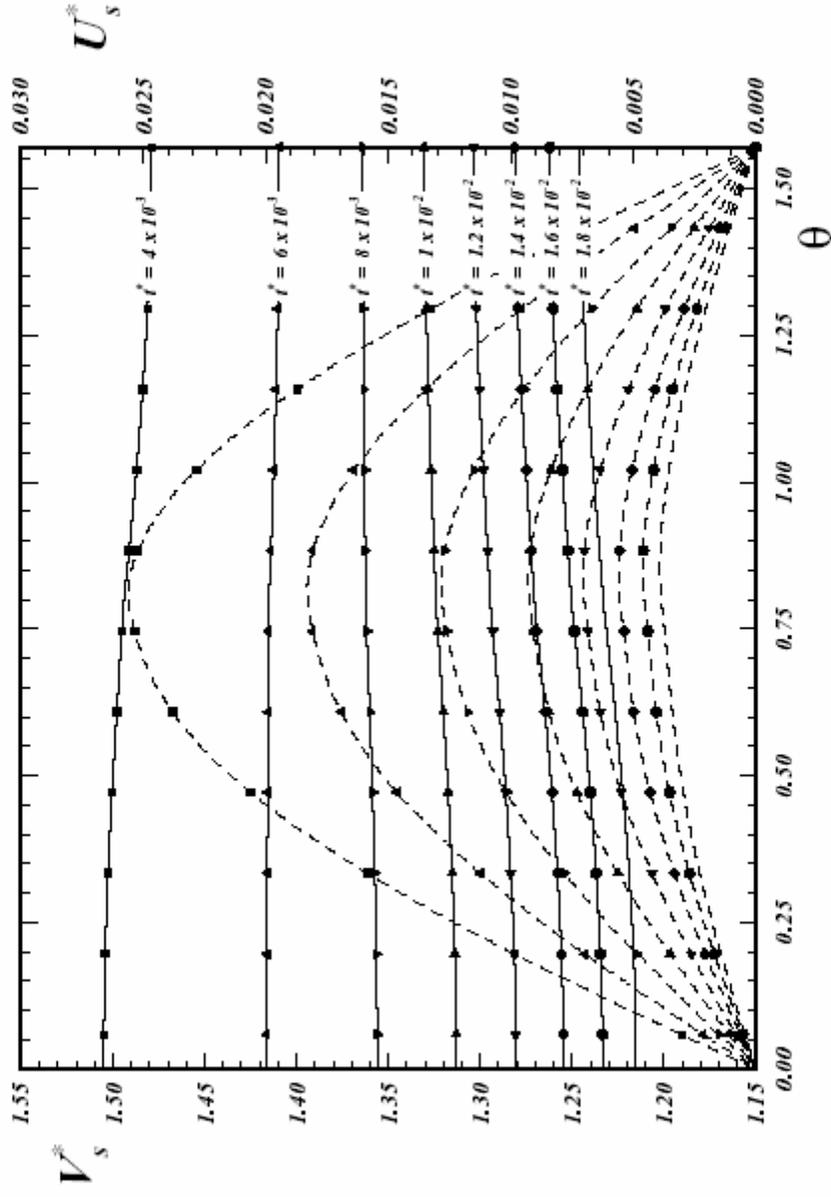
Droplet-Stream Combustion



Droplet surface velocity: normal (solid) and tangential (dashed) - $b^* = 2$.

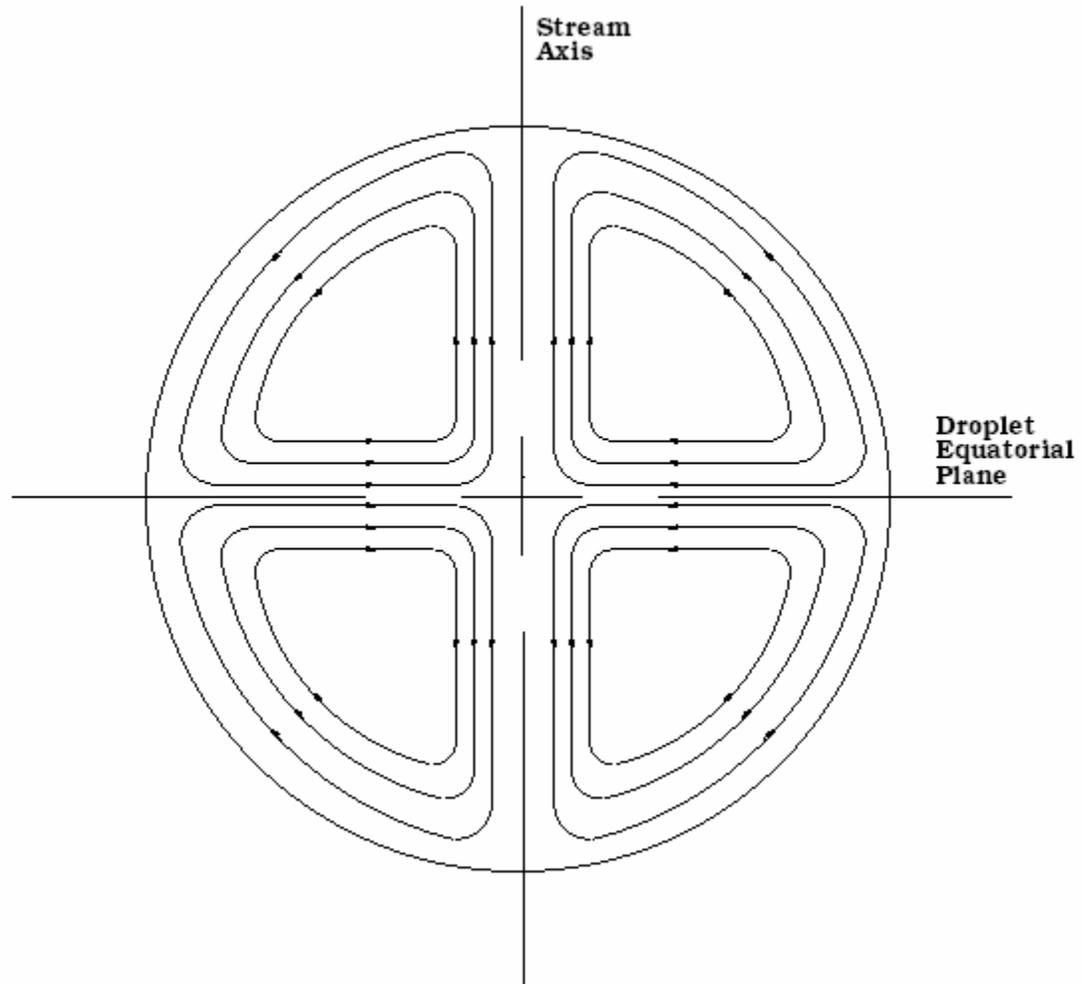
Droplet Surface Velocity

Droplet-Stream Combustion

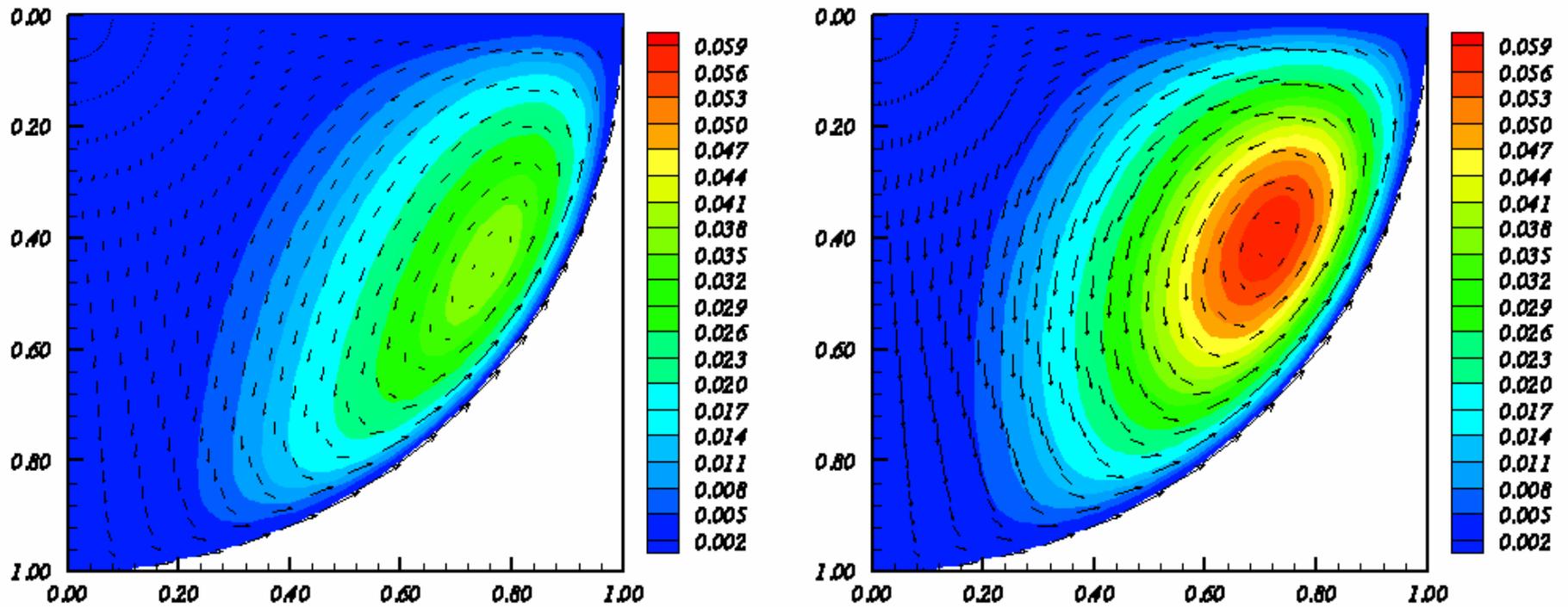


Droplet surface velocity: normal (solid) and tangential (dashed) - $d^* = 4$.

Circulation Pattern

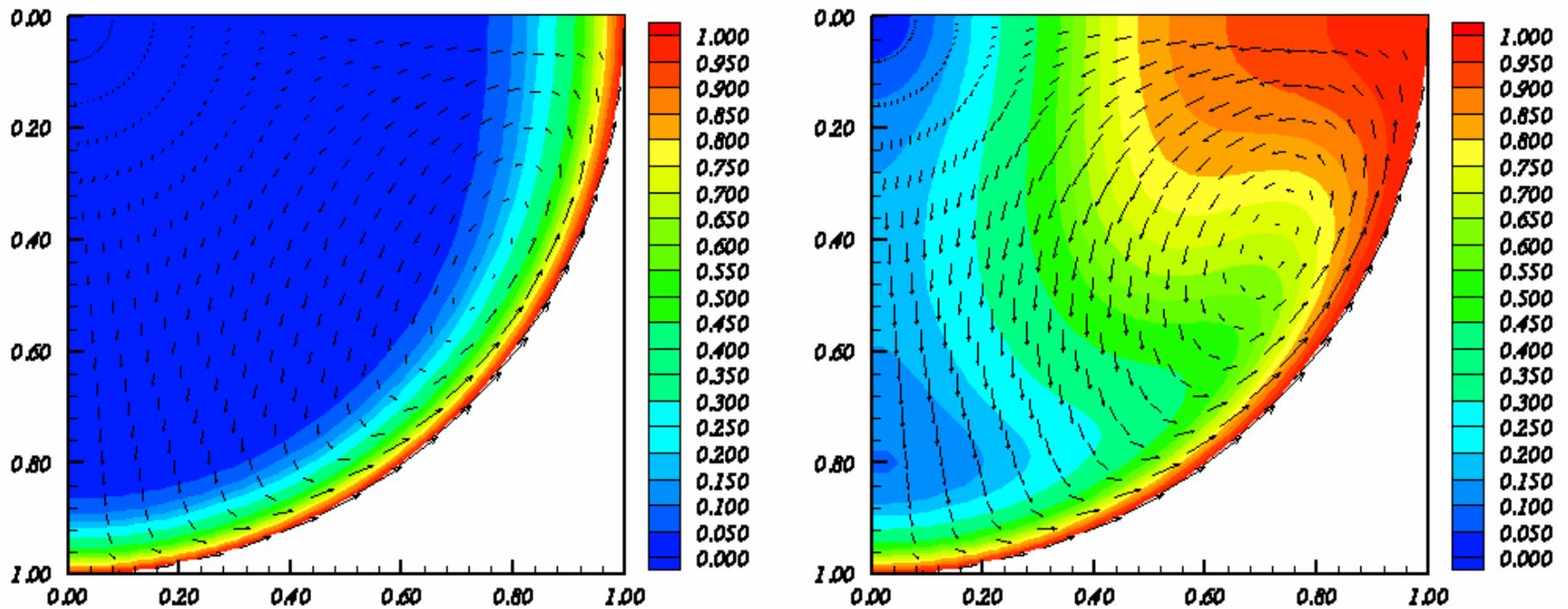


Results



Stream Function $Re=100$, $Pr=1$ for $t = 0.05$ (left) and $t = 0.95$ (right).

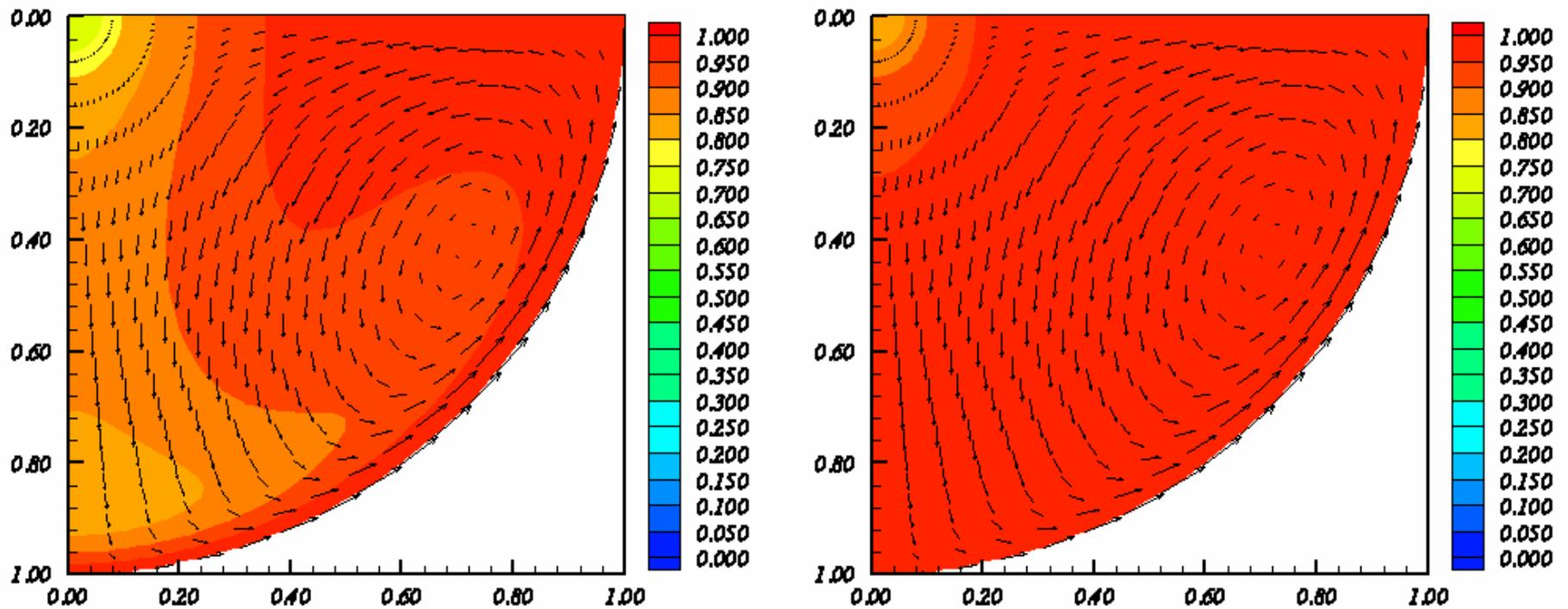
Results



Temperature field and the velocity vectors for $t = 0.05$ (left) and $t = 0.30$ (right).

$$Re = 100, Pr = 1$$

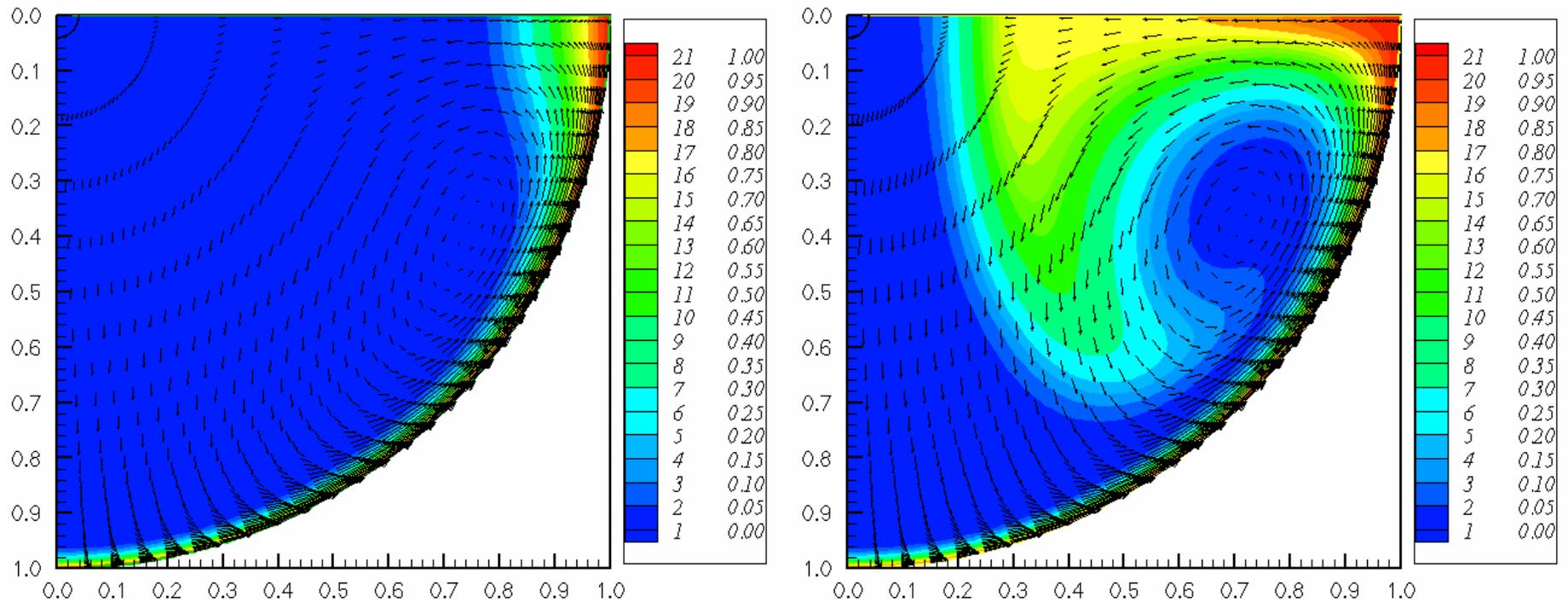
Results



Temperature field and the velocity vectors for $t = 0.6$ (left) and $t = 0.9$ (right).

$$Re = 100, Pr = 1$$

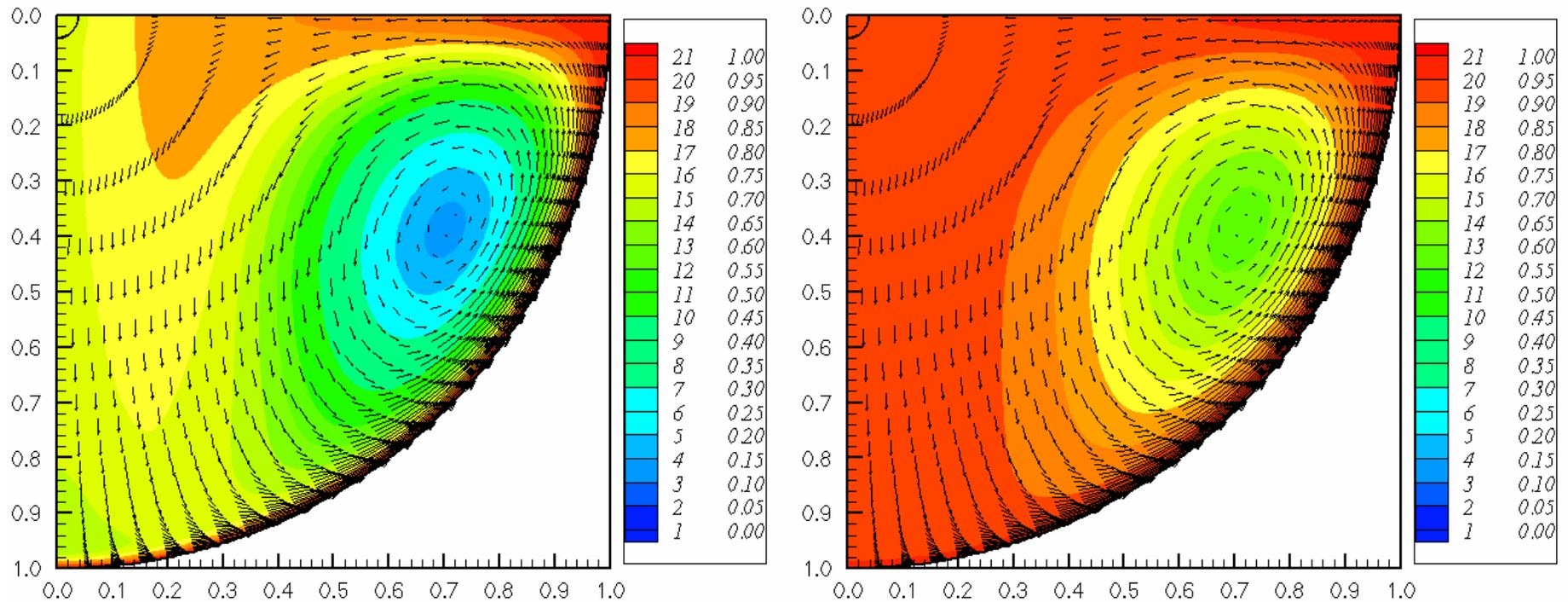
Results



Temperature field and the velocity vectors for $t = 1.0$ (left) and $t = 4.0$ (right).

$Re = 100, Pr = 10$

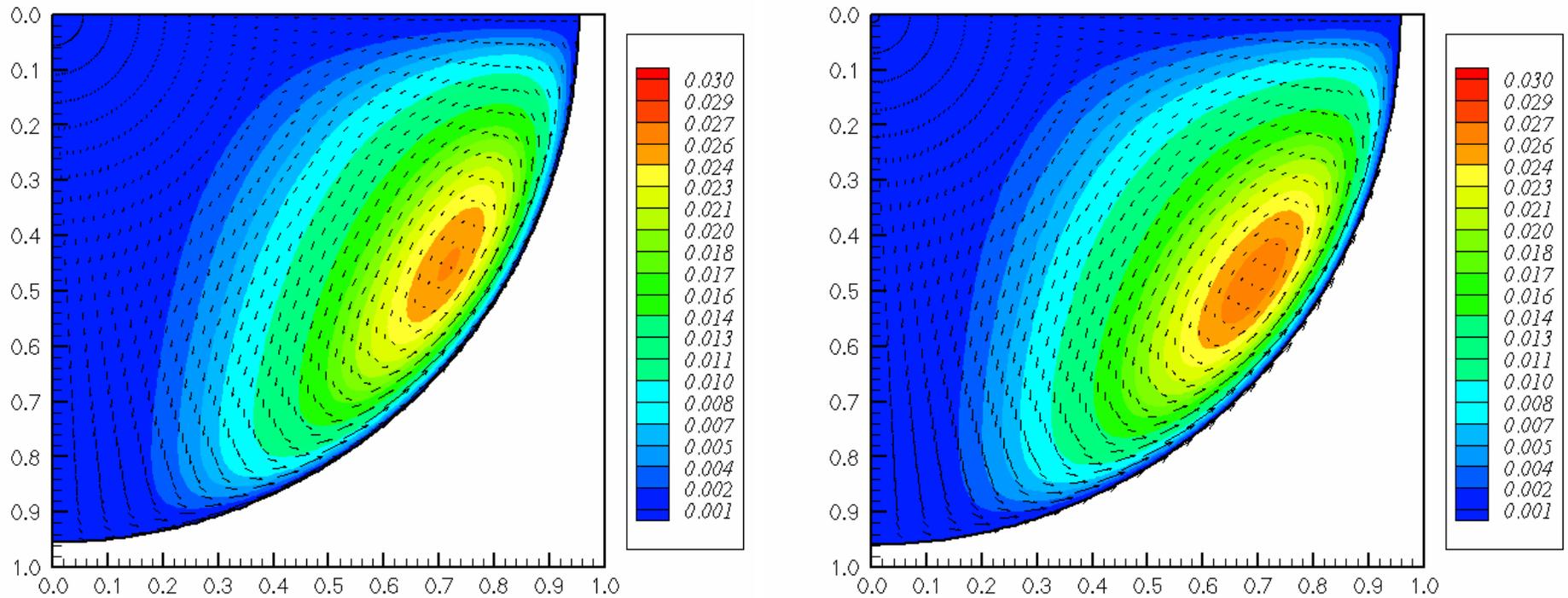
Results



Temperature field and the velocity vectors for $t = 10.0$ (left) and $t = 25.0$ (right).

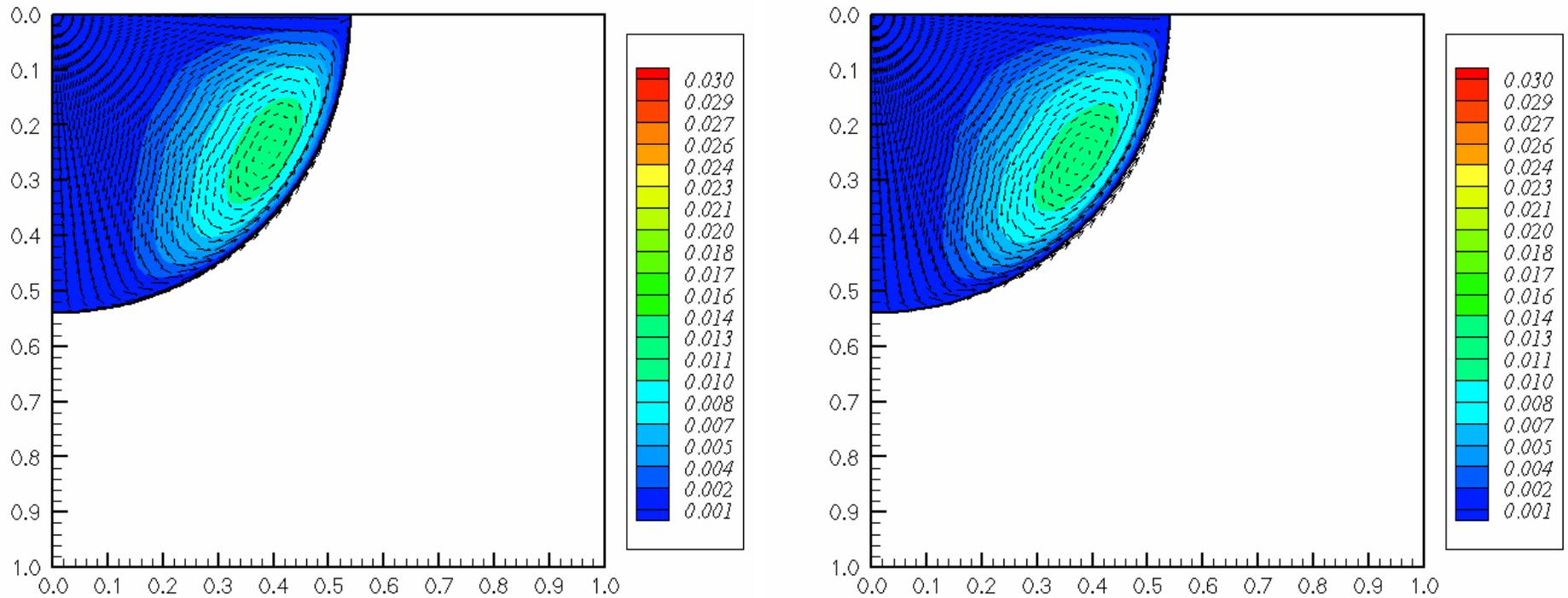
$Re = 100, Pr = 10$

Results



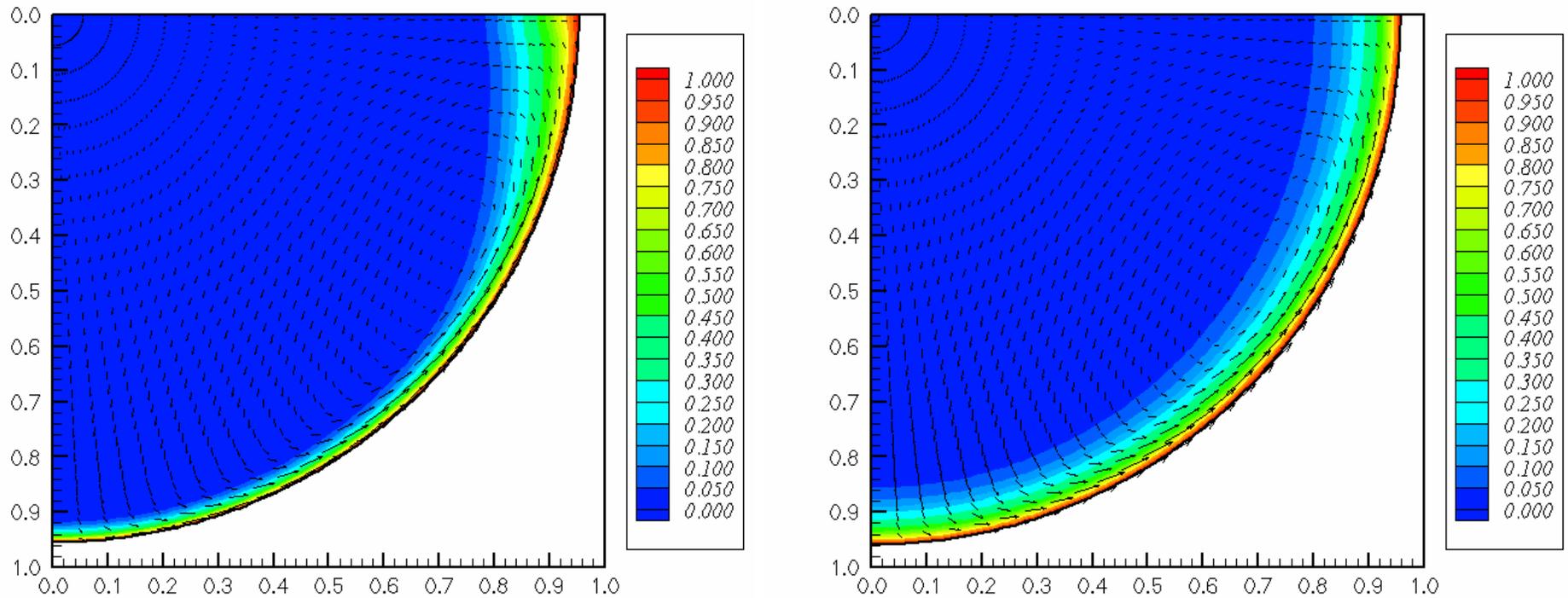
Stream Function $Re=100$ (right) and $Re=10$ (left) for $Pr=10$, $t = 1.0$.

Results



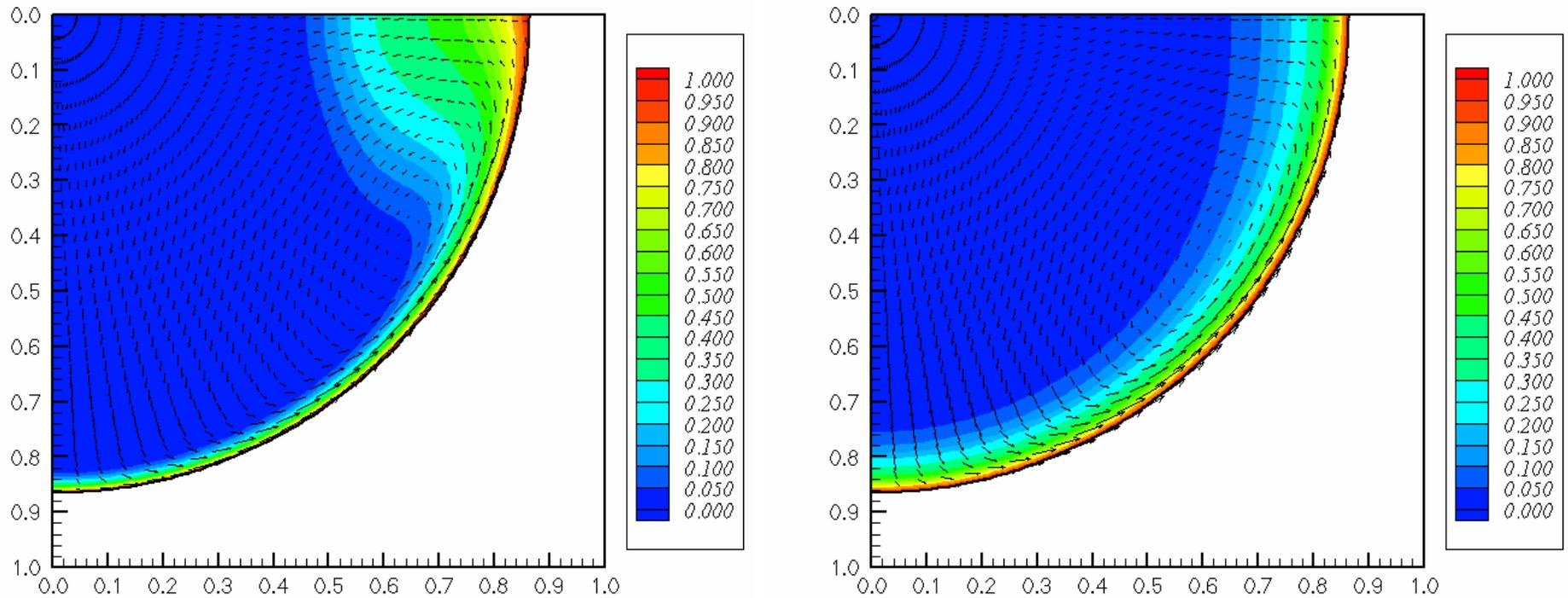
Stream Function $Re=100$ (right) and $Re=10$ (left) for $Pr=10$, $t = 7.0$.

Results



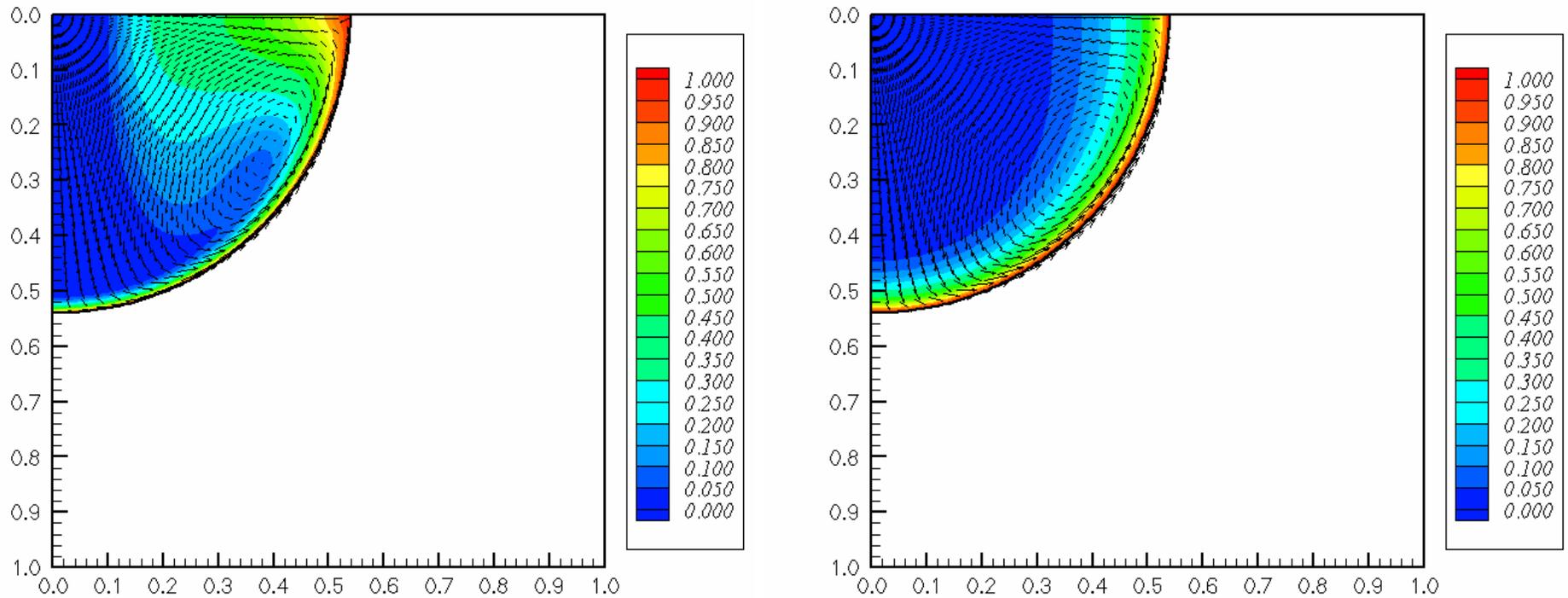
*Temperature field and the velocity vectors for $Re=100$ (right) and $Re=10$ (left)
 $Pr=10, t = 1.0$*

Results



*Temperature field and the velocity vectors for $Re=100$ (right) and $Re=10$ (left)
 $Pr=10$, $t=3.0$*

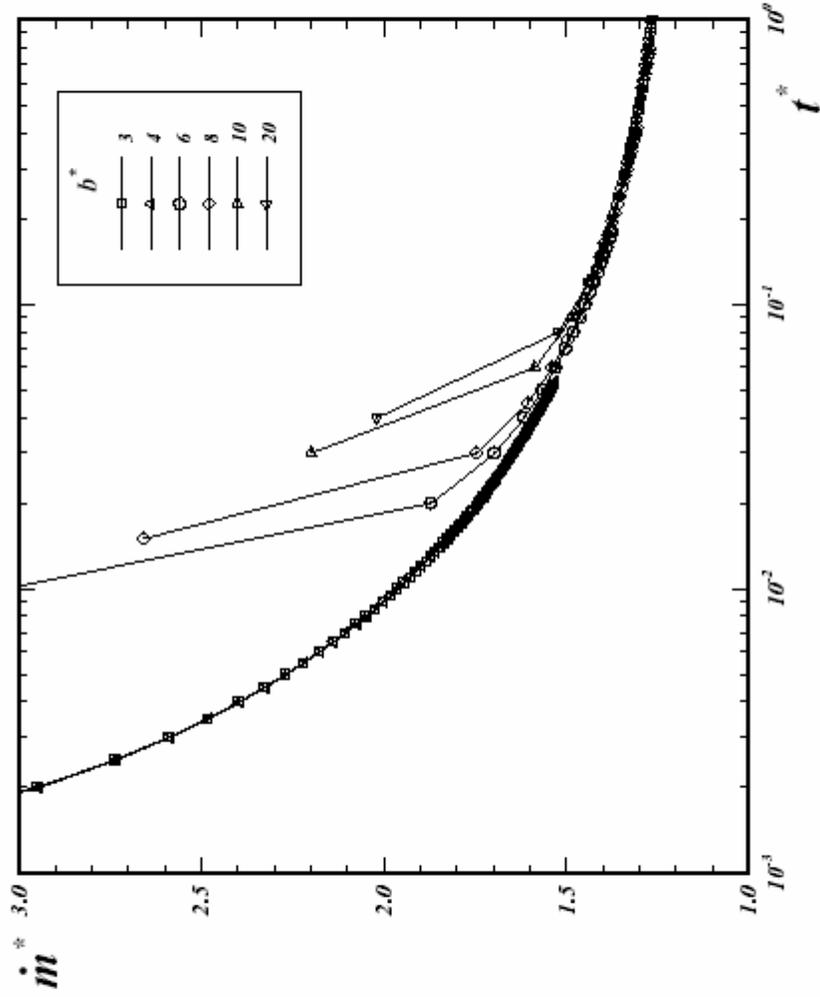
Results



*Temperature field and the velocity vectors for $Re=100$ (right) and $Re=10$ (left)
 $Pr=10$, $t = 7.0$*

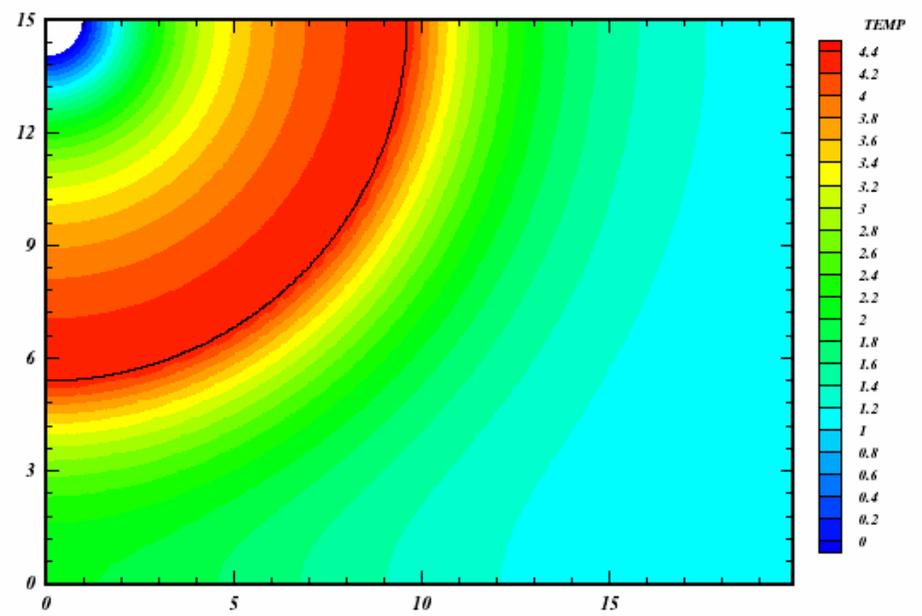
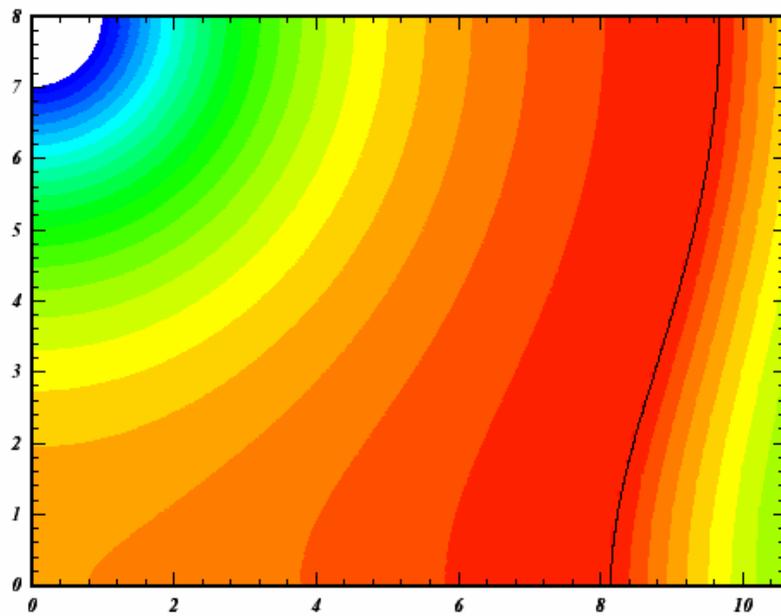
Mass Vaporization Rate

Droplet Stream Combustion



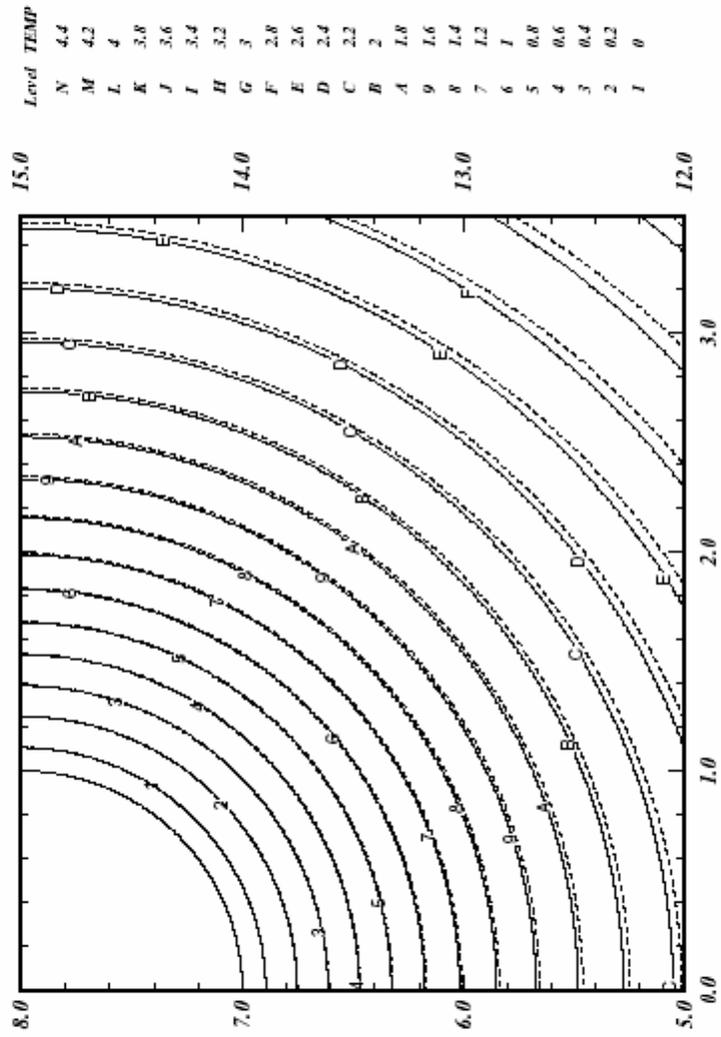
Droplet mass vaporization rate for different interdroplet spacings

Droplet Mass Vaporization



Mass Vaporization Rate

Droplet Stream Combustion



Temperature profiles and flame position for for $b^{*} = 8$ (dashed) and $b^{*} = 15$ (solid) - $t^{*} = 0.42$.

People

- *Aldélio Bueno Caldeira*
- *Andressa Araújo Abreu*
- *Antonio Roseira Junior*
- *Edson Gomes Moreira Filho*
- *Erick Galante*
- *Gulherme Bastos Machado*
- *Helcio Rangel Barreto Orlande*
- *Monique Soriano Vital*
- *Pedro Pacheco Fernandoy*
- *Roger H. Rangel*

Sponsors

CNPq, CAPES, FAPERJ, FINEP, IME, PETROBRAS, UFRJ

Contact

Albino José Kalab Leiroz
Department of Mechanical Engineering - POLI/ COPPE
Federal University of Rio de Janeiro
P.O. Box 68503 – 21945-970

leiroz @ufrj.br

