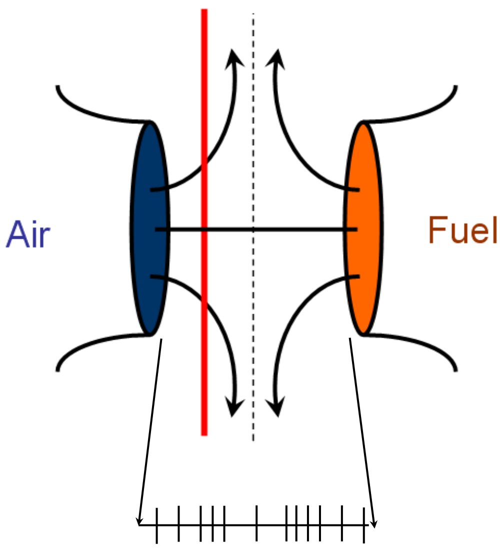
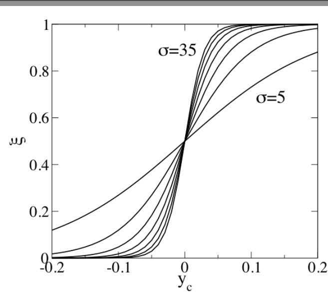
Laminar Flamelet Model

1



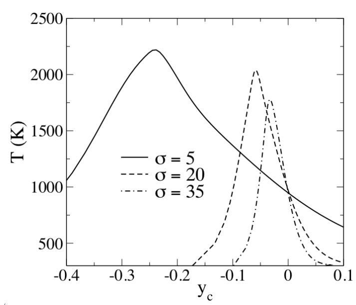
Physical Space vs. ξ Space

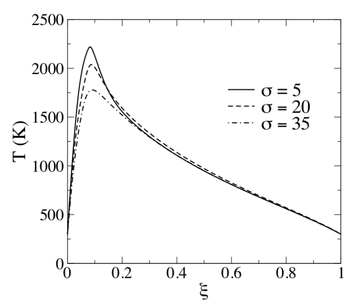
2



$$\xi(y) = \frac{1}{2}(1 + \tanh(\sigma y_c)),$$

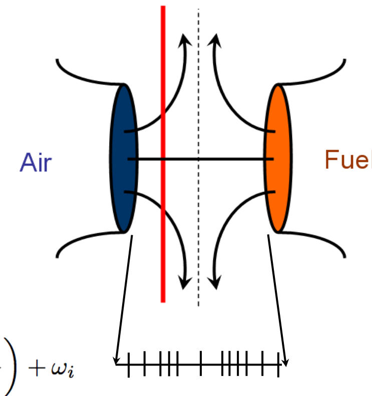
$$\chi = \frac{D_\xi}{2}\sigma^2(1 - (2\xi - 1)^2)^2$$





Laminar Flamelet Model

- Flamelets transform physical coordinate to flame coordinate.
- Assumes unity Le
- Reformulate for soot with high Le and thermophoresis



$$\rho\frac{\partial Y_i}{\partial t} = \rho v\frac{\partial Y_i}{\partial y} + \frac{\partial}{\partial y}\left(\rho D\frac{\partial Y_i}{\partial y}\right) + \omega_i$$

$$\chi = 2D\left(\frac{\partial \xi}{\partial y}\right)^2$$

$$\frac{\partial Y_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 Y_i}{\partial \xi^2} + \omega_i/\rho$$

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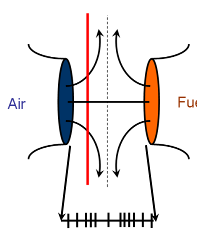

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Define mixture fraction f by transport equation

$$* \quad \rho\frac{\partial \xi}{\partial t} + \rho v\frac{\partial \xi}{\partial y} - \frac{\partial}{\partial y}\left(\rho D_\xi\frac{\partial \xi}{\partial y}\right) = 0$$

Species transport equation

$$\rho\frac{\partial Y_i}{\partial t} + \rho v\frac{\partial (Y_i)}{\partial x_i} - \frac{\partial}{\partial y}\left(\rho D\frac{\partial Y_i}{\partial y}\right)$$

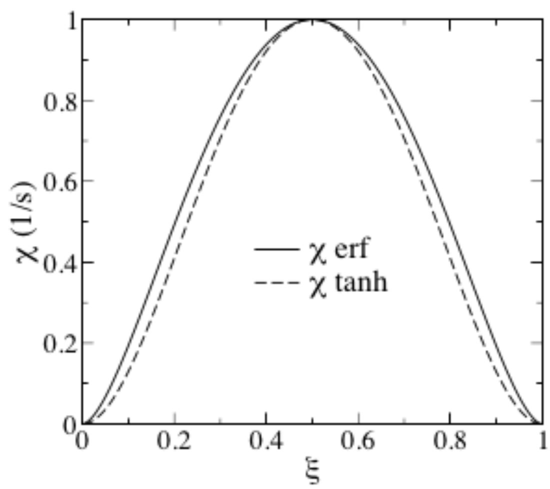
Coordinate transformation

$$\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} + \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi} \qquad \frac{\partial}{\partial y} \to \frac{\partial \xi}{\partial y}\frac{\partial}{\partial \xi}$$

Apply Coordinate transformation, expand derivatives, use (*), and voila

$$\frac{\partial Y_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 Y_i}{\partial \xi^2} + \omega_i/\rho$$

See N. Peters, Prog. Energy Combust. Sci. 1984, Vol 10, p 319-339



Energy equation

Temperature Flamelet equation

$$\rho\frac{\partial T}{\partial \tau} = \rho\frac{\chi}{2}\frac{\partial^2 T}{\partial \xi^2} - \sum_k \frac{h_k}{c_p}\dot{m}_k''' + \left[\frac{\chi\rho}{2c_p}\frac{\partial T}{\partial \xi}\frac{\partial c_p}{\partial \xi} + \frac{\chi\rho}{2c_p}\sum_k \frac{\partial Y_k}{\partial \xi}\frac{\partial h_k}{\partial \xi}\right]$$

Or, Enthalpy Flamelet Equation (for Le=1)

$$\frac{\partial h}{\partial t} = \frac{\chi}{2}\frac{\partial^2 h}{\partial \xi^2}$$

Which, for linear initial h, remains linear

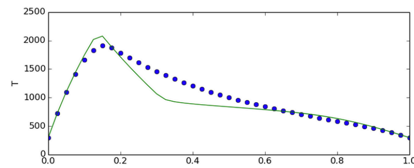
$$h(\xi) = h_{\xi=1}\xi + h_{\xi=0}(1-\xi)$$

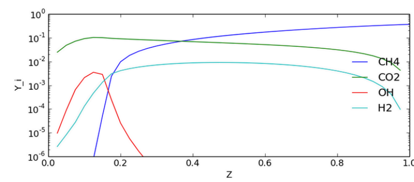
Example

Enter stream data:
Enter stream Z=0 Temperature (K) 298.15
Enter stream Z=1 Temperature (K) 298.15
Enter stream Z=0 composition as shown O2:0.21,N2:0.79
Enter stream Z=1 composition as shown CH4:1,N2:1
Mole or Mass entry: ◉ Mole ○ Mass

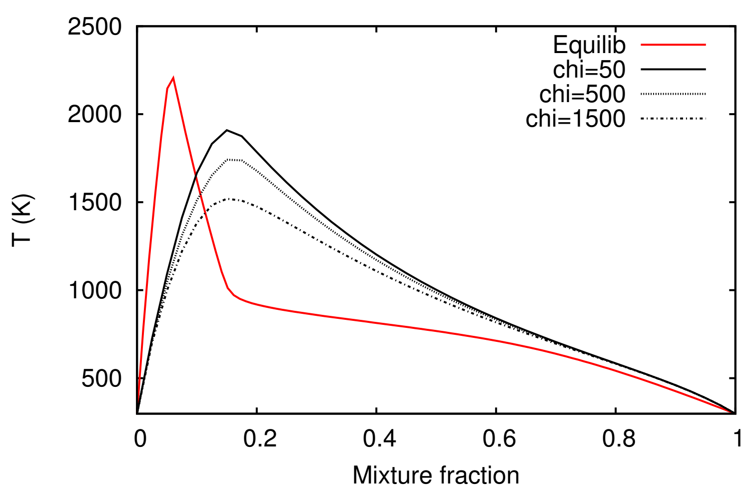
Chi max (1/s): 50.0
grid points: 41
Runtime factor * 2.0/Chi_max: 0.05
Timestep factor * 2*dZ*dZ/Chi_max: 0.5

Compute Flamelet





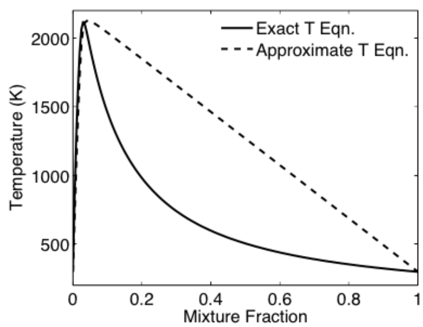
Various Chi



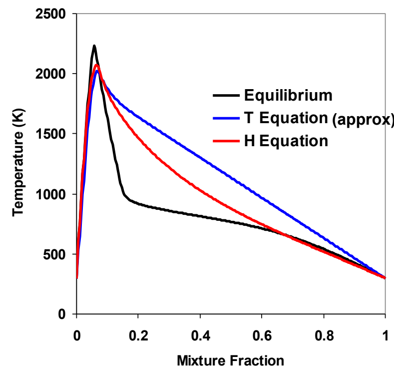
Temperature Equation

- If you ignore the term in brackets, you can get large errors

$$\rho\frac{\partial T}{\partial \tau} = \rho\frac{\chi}{2}\frac{\partial^2 T}{\partial \xi^2} - \sum_k \frac{h_k}{c_p}\dot{m}_k''' + \left[\frac{\chi\rho}{2c_p}\frac{\partial T}{\partial \xi}\frac{\partial c_p}{\partial \xi} + \frac{\chi\rho}{2c_p}\sum_k \frac{\partial Y_k}{\partial \xi}\frac{\partial h_k}{\partial \xi}\right]$$



H2-air flame



CH4-Air Flame

Soot

- Le is Not 1 for soot.

1-D Soot moment equation in space

$$\rho\frac{\partial m_r}{\partial t} + \rho v\frac{\partial m_r}{\partial y} - \frac{\partial}{\partial y}\left(\rho D_p\frac{\partial m_r}{\partial y}\right) - \frac{\partial}{\partial y}\left(\frac{0.554\mu}{T}m_r\frac{\partial T}{\partial y}\right) - \dot{M}_r = 0.$$

1-D Soot moment equation in mixture fraction coordinate

$$\frac{\partial m_r}{\partial t} = C\frac{\partial m_r}{\partial \xi} + S;$$

$$C = \left[\frac{0.554\mu}{\rho T}\beta^2\frac{\partial T}{\partial \xi} - \frac{\beta}{\rho}\frac{\partial(\rho D_\xi \beta)}{\partial \xi}\right],$$

$$S = \frac{m_r}{\rho}\left[\beta\frac{\partial T}{\partial \xi}\frac{\partial}{\partial \xi}\left(\frac{0.554\mu\beta}{T}\right) + \beta^2\frac{0.554\mu}{T}\frac{\partial^2 T}{\partial \xi^2}\right] + \frac{\dot{M}_r}{\rho}$$

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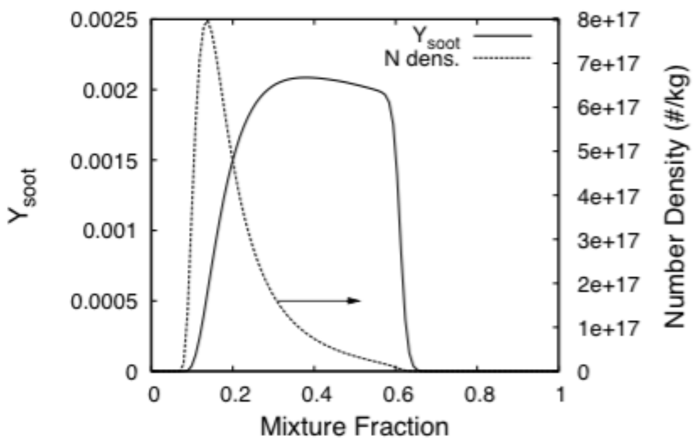
Soot



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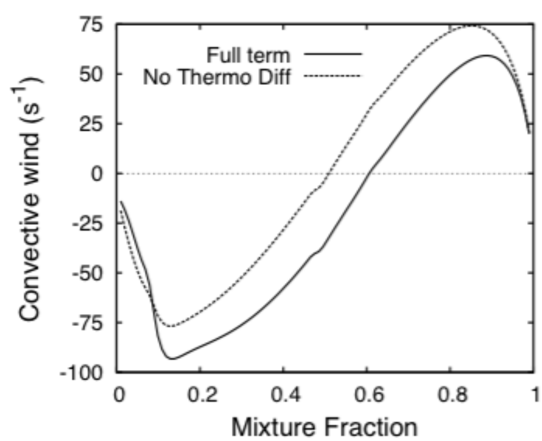
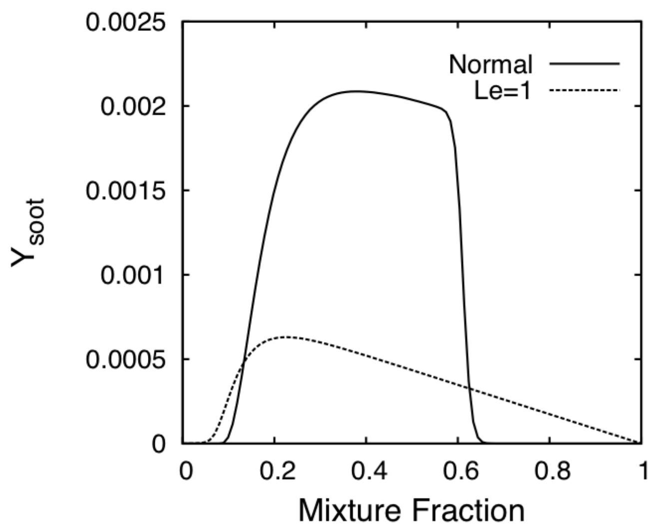
Soot "velocity"



Soot Comparison



Soot versus SDR