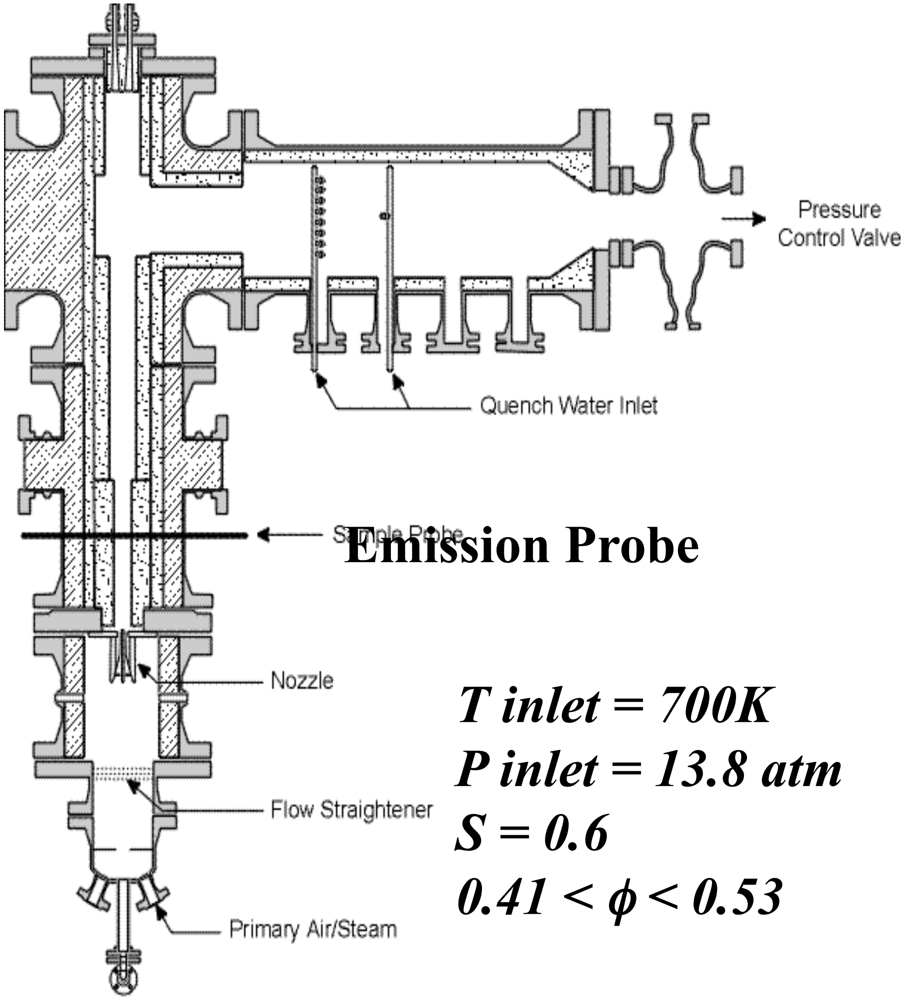
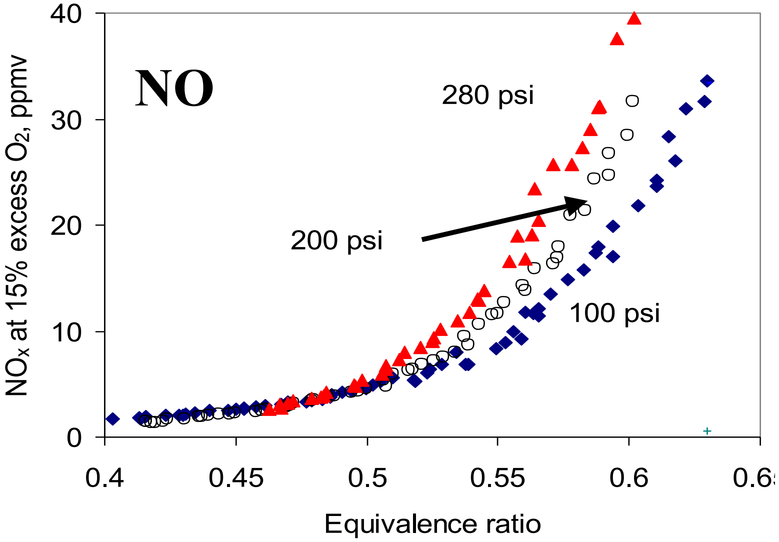
Lecture 5
Emission and Low-NOx Combustors

- Emissions: CO, Nox, UHC, Soot
- Modeling requirements vary due to difference in time and length scales, as well as processes
- In general, finite-rate kinetics is needed to predict emission
  - Flamelet approach still uses kinetics!
  - Reduced kinetics successful for heat release and global dynamic many not work for emissions
- Accuracy in PPMs is needed for reliable predictions
- Computational cost for finite-rate!
- Soot physics is relatively unknown

Emission near LBO in DOE-HAT Combustor



Emission Probe

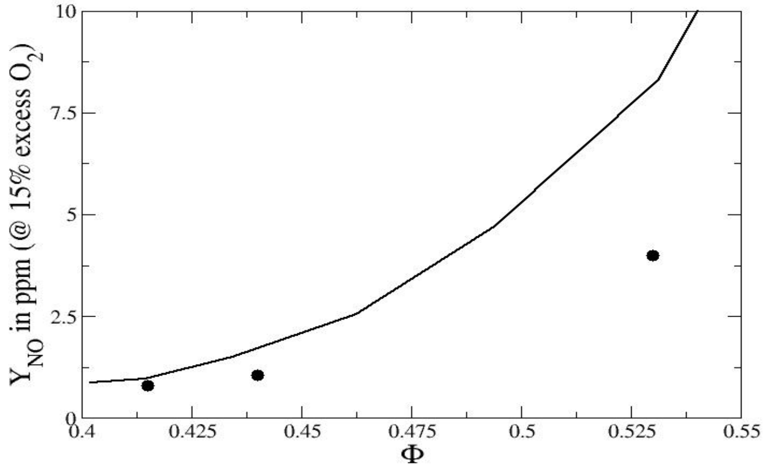


T inlet = 700K

P inlet = 13.8 atm

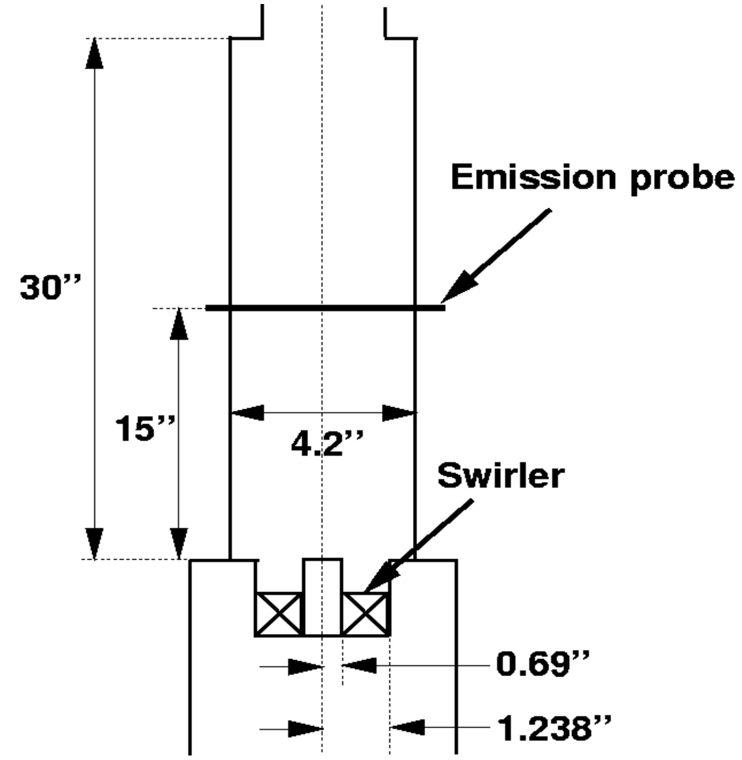
S = 0.6

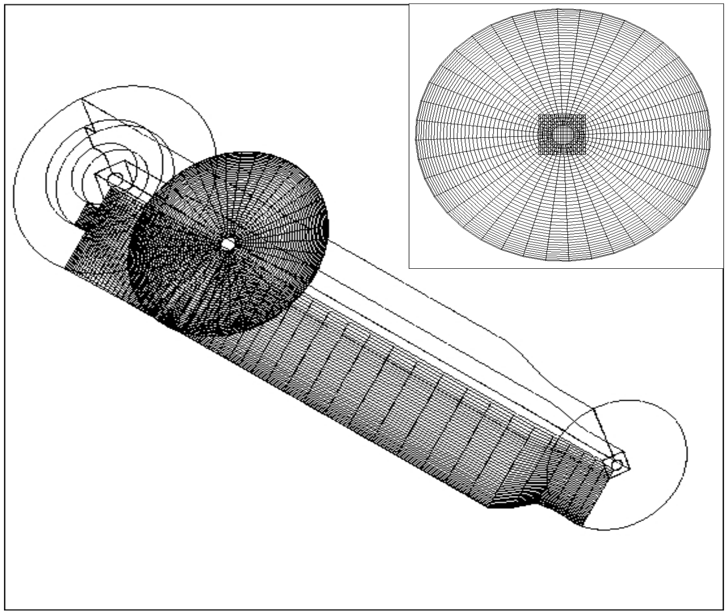
0.41 < ϕ < 0.53



DOE-HAT Setup and Conditions

Tinlet = 700K ,Pinlet = 13.8 atm
S = 0.6 , $0.41 < \phi < 0.53$





- *185 x 75 x 81 cylindrical grid*
- *185 x 24 x 24 inner Cartesian grid*
- *O(2-4) interpolation*
- *LES-LEM only in the flame zone*
    - *resolves the flame*
- *Load balancing to achieve speedup*

Simplified approach to predict emissions

- Pollutants (CO, NO, UHC) tracked at the LES level

$$\frac{\partial \bar{\rho}\widetilde{Y}_m}{\partial t} + \frac{\partial}{\partial x_j}\left[\bar{\rho}\widetilde{Y}_m\widetilde{u}_j + \bar{\rho}\left(D_m + D_T\right)\frac{\partial \widetilde{Y}_m}{\partial x_j}\right] = \bar{\rho}\widetilde{\dot{w}}$$

  - Slow chemistry, reaction rate obtained from CHEMKIN
- G-equation approach used to track flame in LES
  - Heat release in energy equation as a "thin" zone
  - Turbulent flame speed model in the LES G-equation

$$S_T = S_T(u', S_L),\ u' \text{ obtained from LDKM}$$

- LES-LEM approach
  - Global finite-rate kinetics used in the subgrid to obtain laminar flame speed and flame structure
    - Turbulent flame speed actually predicted

CO Prediction

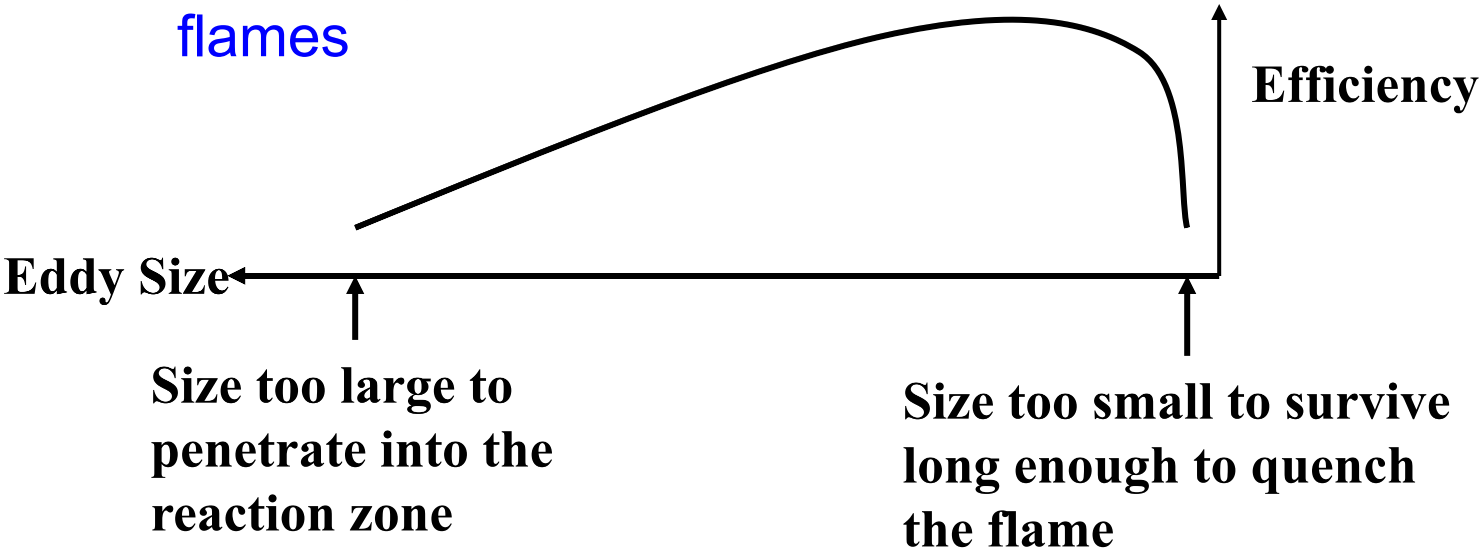
- Three mechanisms modeled
  - CO production at the flame front
    - Treated as a jump discontinuity
    - Rate obtained using CHEMKIN
  - Equilibrium between CO oxidation and CO2 dissociation

$$CO + O_2 \Leftrightarrow CO_2 + O$$

    - Forward/backward rates obtained from CHEMKIN
  - CO production via UHC oxidation
    - UHC formed due to local flame quenching
    - UHC oxidation to CO modeled as an Arrhenius rate

UHC Prediction

- Local quenching of flame due to stretch effect (Meneveau and Poinsot, 91)
  - Unburnt fuel released on the product side
  - Efficiency coefficient determines portion of quenched flames



Size too large to penetrate into the reaction zone

Size too small to survive long enough to quench the flame

NO Prediction

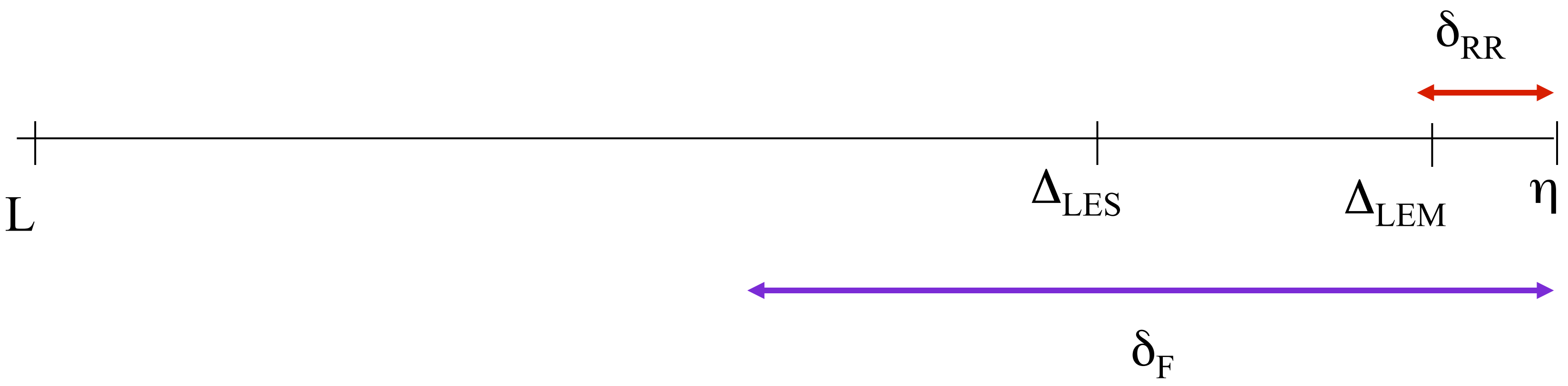
- Two mechanisms included
  - Formation at the flame front
    - Obtained from CHEMKIN
  - Formation via the Zeldovich mechanism

$$
\begin{array}{c}
N_2 + O \Leftrightarrow NO + N \\
N + O_2 \Leftrightarrow NO + O \\
\hline
N_2 + O_2 \Leftrightarrow 2NO
\end{array}
$$

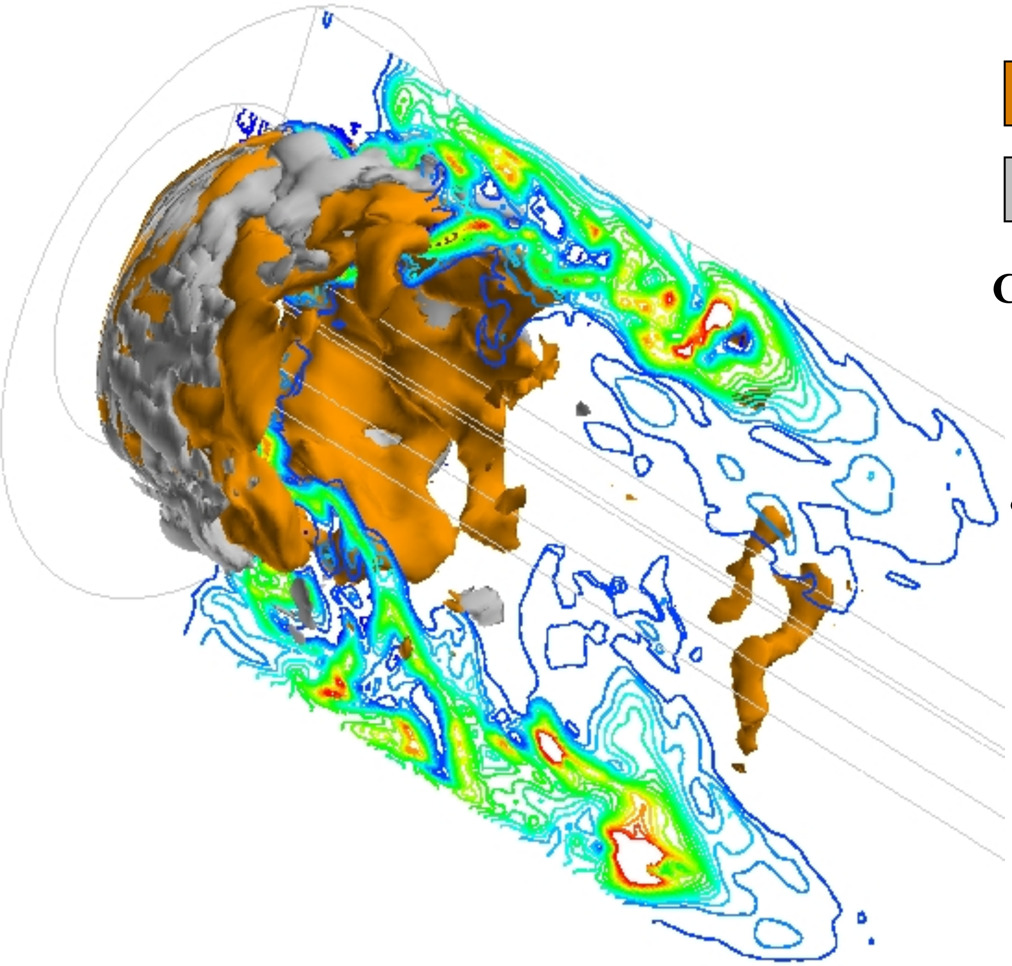
    - O and N assumed to be in equilibrium

LES-G versus LES-LEM Resolution Issues

- Eddies larger than flame thickness resolved in LES-G and LES-LEM
- LES-G barely resolves flame thickness while LES-LEM has around 12 cells within flame
  - heat release implemented in energy equation as a thin-zone
- Eddies of size of flame preheat zone are resolved in LES-LEM
  - Flame broadening effect included in LES-G via a model
- Eddies of size of flame reaction zone are partially resolved in LEM
  - Not resolved in LES-G



Emission predictions: UHC (ϕ = 0.41)



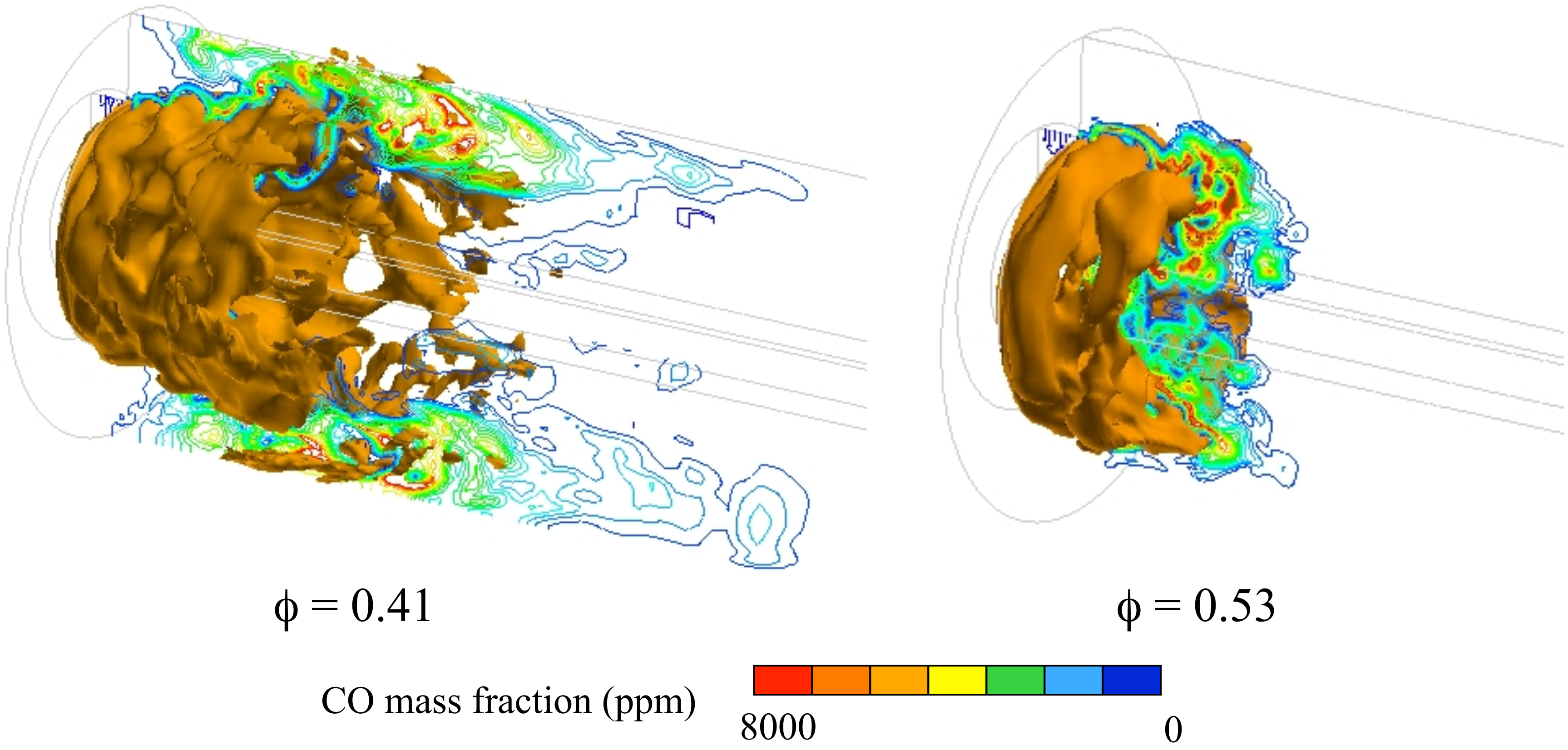
🟧 **Flame surface**

⬜ **UHC iso-surface**

Contour lines are CO mass fraction

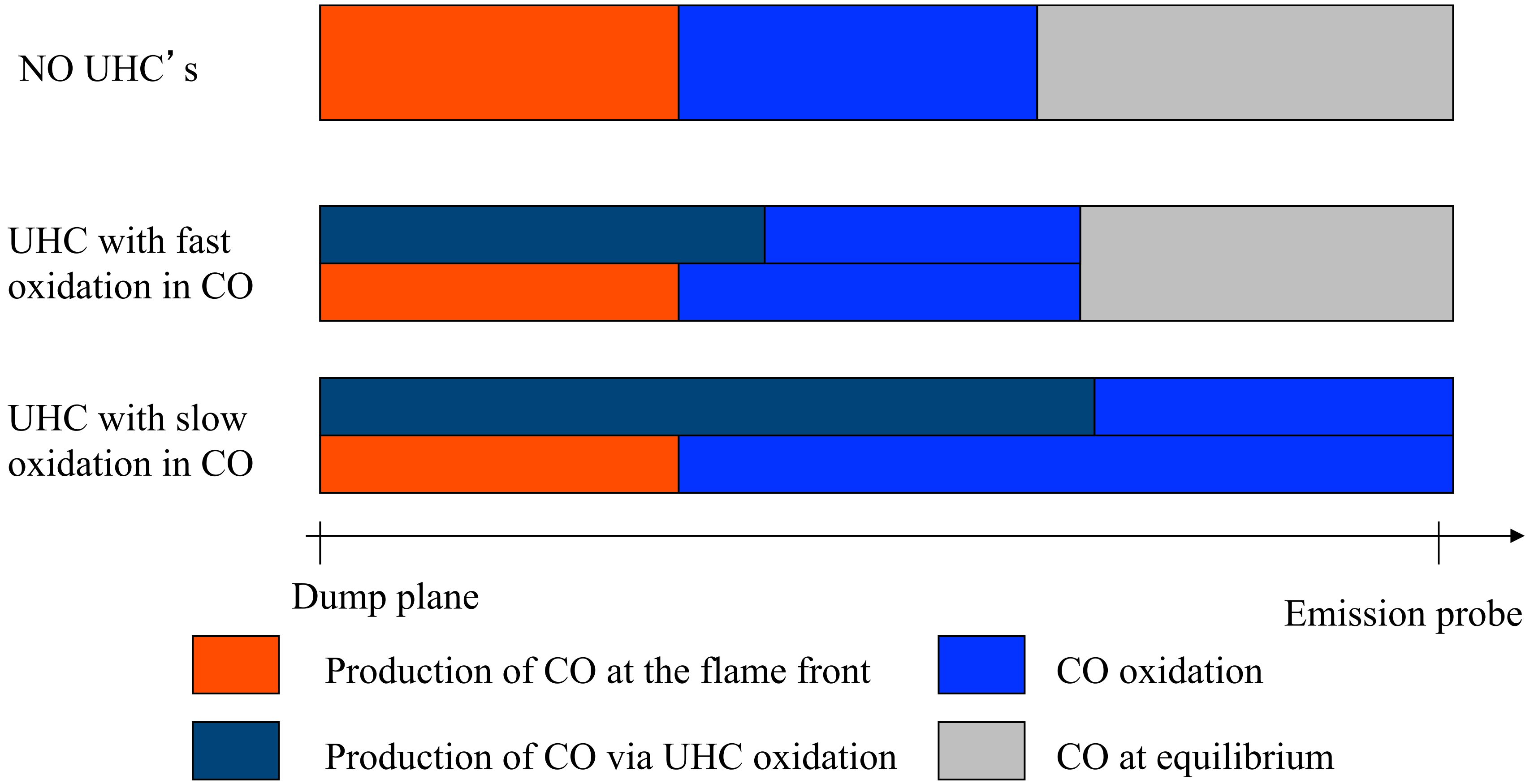
- UHC production localized in region of high shear
  - Outer boundary layer
  - Flame lift-off
  - Combustion in the distributed regime.

Emission predictions: CO



- Flame location (orange) and CO mass fraction (contour lines)
  - Low equivalence ratio: long flame and slow CO oxidation
  - High equivalence ratio: short flame and fast CO oxidation

CO Prediction for $\phi = 0.41$



NO UHC's

UHC with fast oxidation in CO

UHC with slow oxidation in CO

Dump plane

Emission probe

🟧 Production of CO at the flame front

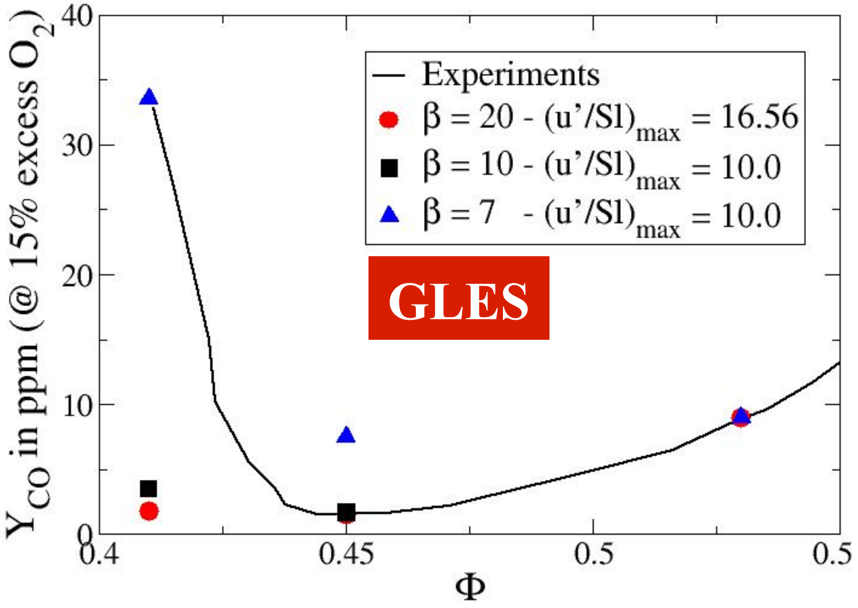
🟦 CO oxidation

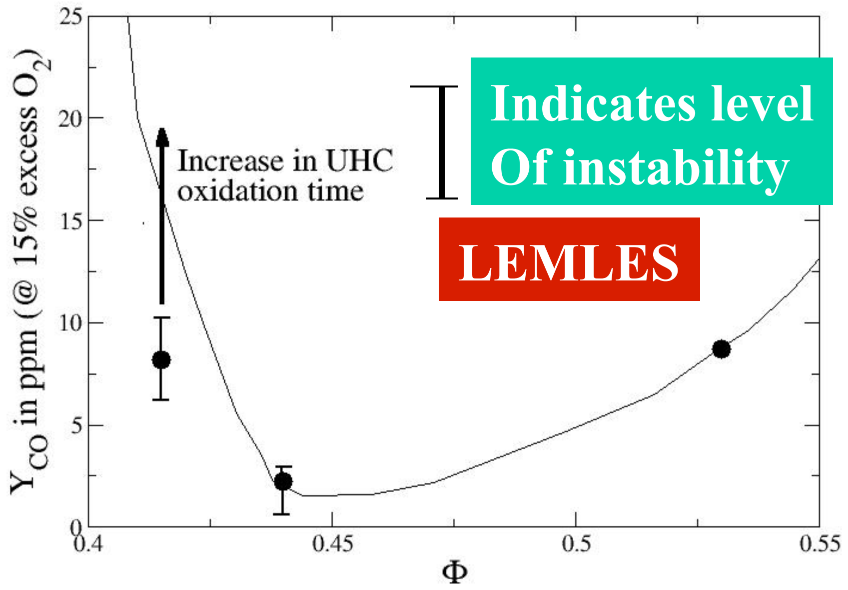
■ Production of CO via UHC oxidation

⬜ CO at equilibrium

UHC oxidation rate is essential to predict CO emission accurately

CO emission in the DOEHAT Combustor

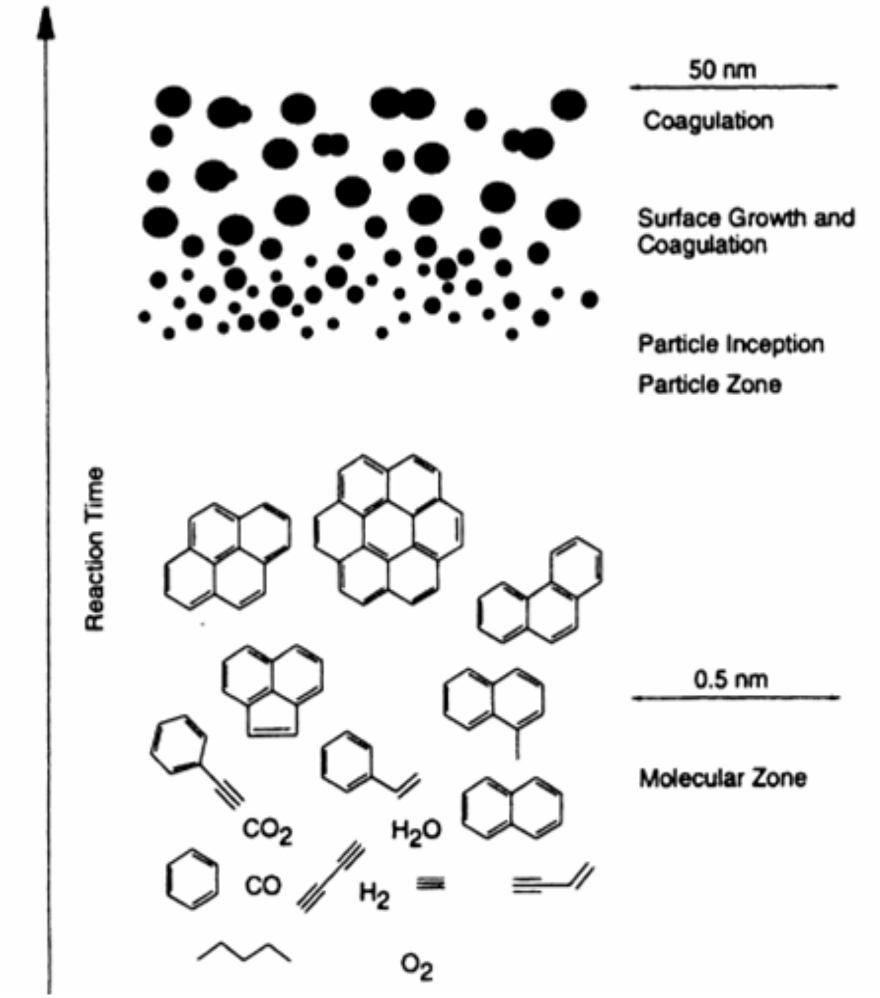




GLES: Model can be tuned to match data but with no physics
LEMLES: No parameter to adjust or control
Note: Both simulations employed the same CO emission model

How Soot is Formed?

- Steps in Soot Formation
  - Formation of precursors
  - Particle Inception
  - Surface growth
  - particle agglomeration
  - Particle oxidation
- Range of scales 0.1 – 10 nm
  - Spatially and temporally varying in the domain



Modeled Soot Related Processes

- Internal processes
  - Nucleation: Soot nuclei inception by acetylene
  - Coagulation: Particles coalesce
  - Surface growth: Mass deposition on particles
  - Agglomeration: Formation of large chain-like structures
  - Oxidation: Destruction by O2 and OH
- External processes
  - Radiation (optically thin model for absorption by soot, CO_2 H_2O gases (Kaplan 1996)
  - Thermophoresis
  - Transport by Brownian diffusion
- Other unknown processes

Radiation Model

- Current Implementation
  - Optically Thin model for absorption by soot and CO_2, H_2O gases (Kaplan 1996)
- More detailed, but relatively efficient FAST Correlated-k approach under study (Dembele and Wen, 2003)
  - Uses 43 spectral bands of variable width for H2O, CO2 and CO instead of many narrow bands
  - 5 point G-L quadrature (instead of 7 or 10 point)
  - Needs more work to check its applicability within LEMMOM

Soot Kinetics - Lindstedt (1994)

Soot nucleation

$$C_2H_2 \Rightarrow^{n} 2C_s + H_2$$

Soot surface growth

$$C_2H_2 \Rightarrow 2C_s + H_2$$

Soot Oxidation

$$C_s + OH \Rightarrow CO + H$$

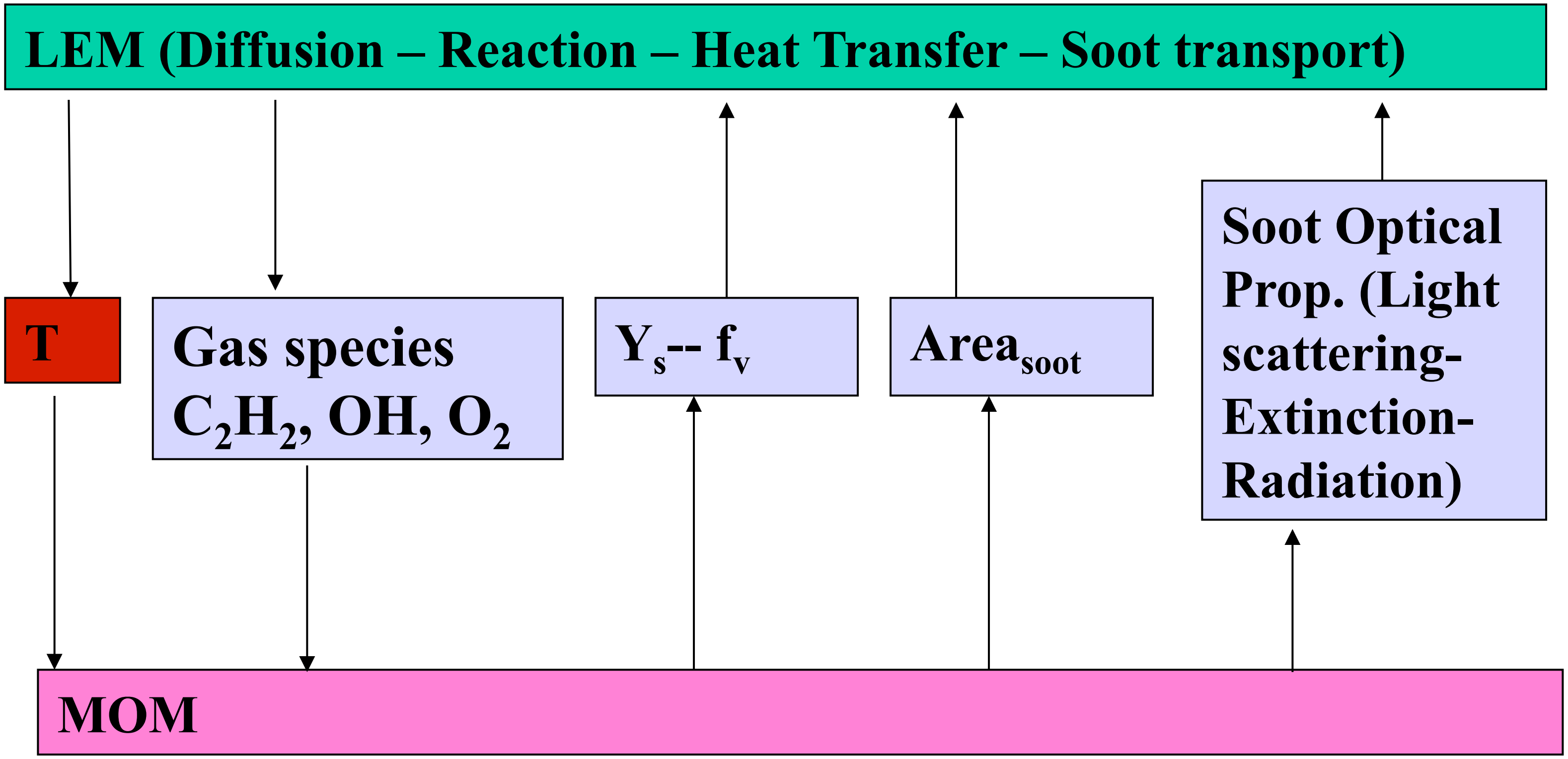
$$C_s + \frac{1}{2}O_2 \Rightarrow CO$$

- **Based on acetylene as a soot precursor**
- **Suitable for turbulent flames, with low carbon content fuels (CH_4 - C_2H_4)**

Method of Moment Approach

- The particle size distribution (PSD) is unknown in advance
- For polydisperse particles it is very hard to specify one type of PSD (Friedlander, 2000)
- However, knowing the moments is equivalent to knowing the PSD (Hudson, 1963)
- MOM with Interpolative Closure (MOMIC) developed by Frenklach and Wang used in LEMLES
  - El-Asrag et al. (Comb. Flame 2006, 2007)
- Other methods being developed (Pitsch)

LEM-MOM Subgrid Model



LEM (Diffusion – Reaction – Heat Transfer – Soot transport)

T

Gas species C_2H_2, OH, O_2

Y_s-- f_v

$Area_{soot}$

Soot Optical Prop. (Light scattering-Extinction-Radiation)

MOM

Subgrid Combustion Model for Sooting Flame

$$\frac{\partial T}{\partial t} = -\frac{1}{\overline{C}_p}\sum_{k=1}^{N_s} C_{p,k} Y_k V_k \frac{\partial T}{\partial x} + \frac{1}{\rho \overline{C}_p}\frac{\partial}{\partial x}\left(\overline{\kappa}\frac{\partial T}{\partial x}\right) - \frac{1}{\rho \overline{C}_p}\sum_{k=1}^{N_s} h_k \dot{\omega}_k W_k + \dot{q}_r + F_{Tstir}$$

$$\frac{\partial Y_k}{\partial t} = -\frac{1}{\rho}\frac{\partial \rho Y_K V_k}{\partial x} + \frac{\dot{\omega}_k W_k}{\rho} + F_{Kstir} \qquad k = 1, Ns$$

$$\frac{\partial Y_s}{\partial t} = -\frac{1}{\rho}\frac{\partial \rho Y_s \left(V_s + V_T\right)}{\partial x} + \frac{\dot{\omega}_s W_c}{\rho} + F_{Sstir}$$

$$M_r = \sum_{i=1}^{\infty} m_i^r N_i$$

$$\frac{dM_r}{dt} = R_r + G_r + S_r + M_{\text{stir}}$$

R_r = Nucleation rate

G_r = Coagulation rate

S_r = Surface Growth rate

Where M_r is the r^{th} Moment of Particle Size Distribution (PSD) Function

LEM-MOM Subgrid Model

$$\frac{\partial T}{\partial t} = -\frac{1}{\overline{C}_p}\sum_{k=1}^{N_s} C_{p,k} Y_k V_k \frac{\partial T}{\partial x} + \frac{1}{\rho \overline{C}_p}\frac{\partial}{\partial x}\left(\overline{\kappa}\frac{\partial T}{\partial x}\right) - \frac{1}{\rho \overline{C}_p}\sum_{k=1}^{N_s} h_k \dot{\omega}_k W_k + F_{Tstir} + Rad$$

$$\frac{\partial Y_k}{\partial t} = -\frac{1}{\rho}\frac{\partial \rho Y_K V_k}{\partial x} - \frac{\dot{\omega}_k W_k}{\rho} + F_{Kstir} \qquad k = 1, Ns$$

$$\frac{\partial Y_s}{\partial t} = -\frac{\dot{\omega}_s W_c}{\rho} + F_{Kstir}$$

$$M_r = \sum_{i=1}^{\infty} m_i^r N_i$$

$$\frac{\partial M_r}{\partial t} = R_r + G_r + S_r + Ox_r + F_{Mstir}$$

R_r = Nucleation rate

G_r = Coagulation rate

S_r = Surface Growth rate

Ox_r = Oxidation rate

Where M_r is the rth Moment of Particle Size Distribution Function

Soot Properties From MOM

$$N_s = M_o$$

$$Y_s = \frac{M_1}{\rho}$$

$$f_v = Y_s \frac{\rho}{\rho_s}$$

$$d_p = \left(\frac{6}{\pi} \frac{M_1}{\rho} \frac{1}{M_o} \right)^{1/3}$$

$$A_s = \pi M_o d_p^{\,2}$$

$$\omega_s = \left(\frac{M_1^{\,t} \big/ \rho^{t} - M_1^{\,t-1} \big/ \rho^{t+1}}{\Delta t} \right)$$

N_s	**Soot Number Density**
Y_s	**Soot Mass Fraction**
f_v	**Soot Volume Fraction**
d_p	**Soot Particle Diameter**
A_s	**Soot Surface Area**
ω_s	**Source Term for LEM**
M_0	**Zero Moment of PSD**
M_1	**First Moment of PSD**