# Thermal NO Predictions in Glass Furnaces: A Subgrid Scale Validation Study

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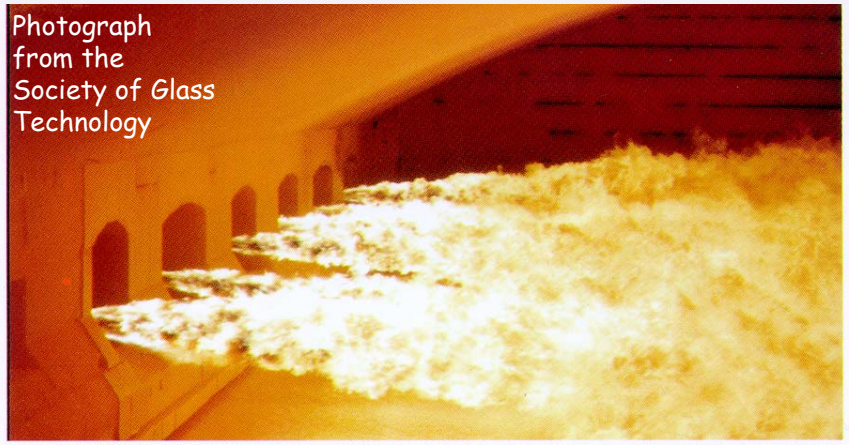
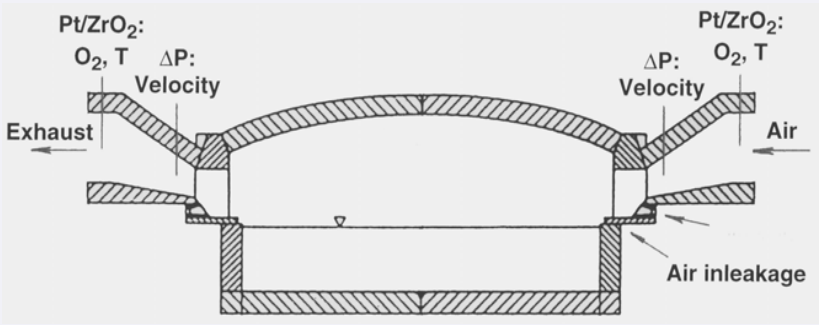
# Glass furnaces: Thermal NO

- High pre-heated air is used in the combustion for fuel efficiency, results in high peak flame temperatures (typically around 2200 K)
- Thermal NO formation is very significant above 1800 K
  - Forms in local regions, where temperature is high & radicals such as O, OH present
- To meet the environmental regulations, glass manufacturers are in need of cost-effective tools to minimize the emissions

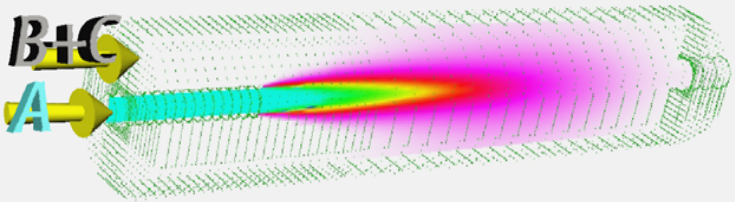



**Combustion in a glass furnace**



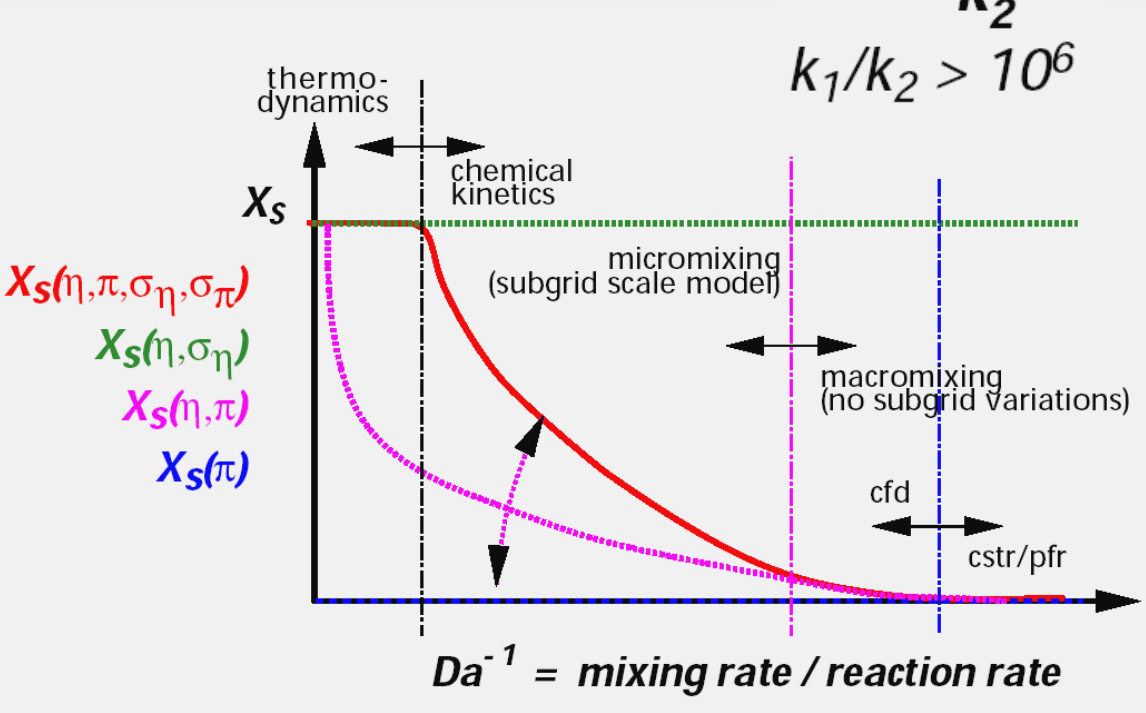

**Cross-sectional view of a single port**

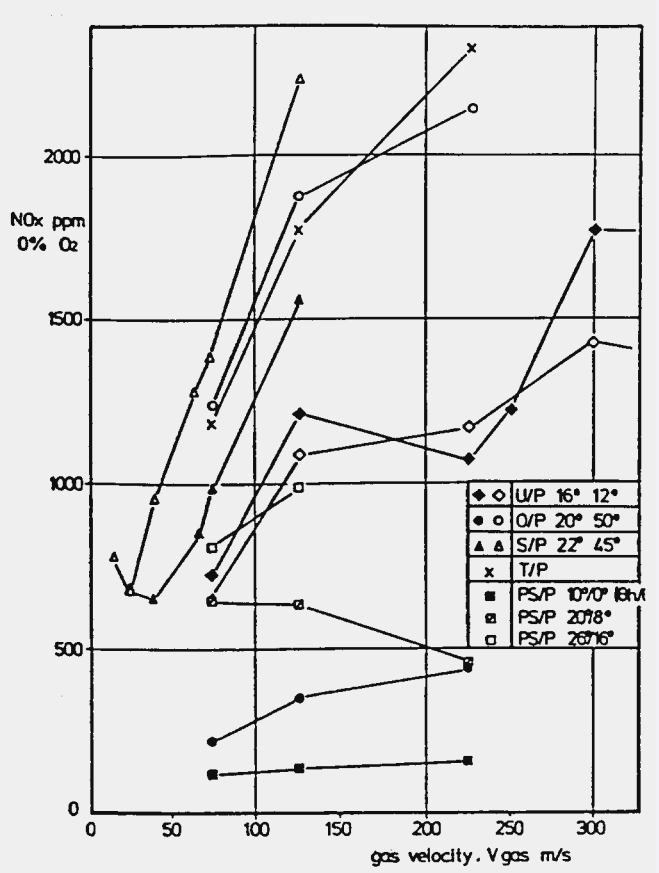
# Turbulent mixing & reaction-NOx




$$A + B \xrightarrow{k_1} P$$
$$A + C \xrightarrow{k_2} S$$

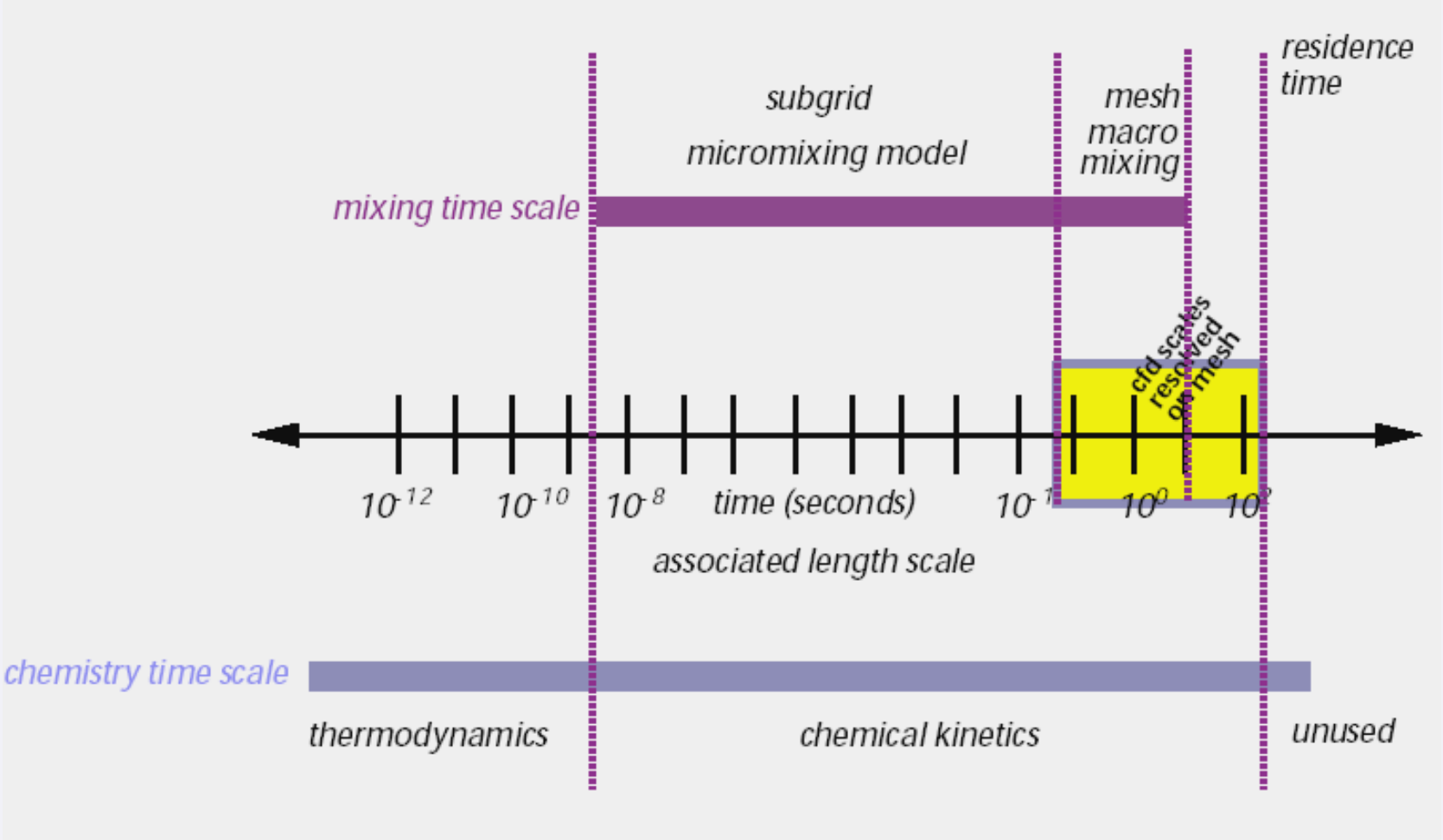
$k_1/k_2 > 10^6$




(Nakamura, Smart, and Van de Kamp, *J. Inst. Energy 69,* 1996, 39-50)

# Time & Length scales




**Mesh/subgrid**

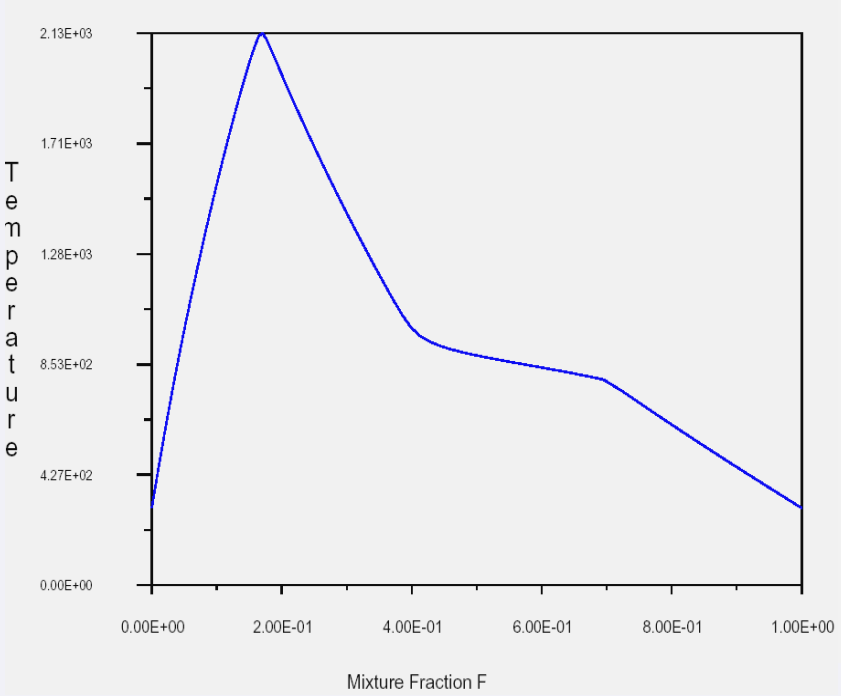
# Numerical simulation of combustion

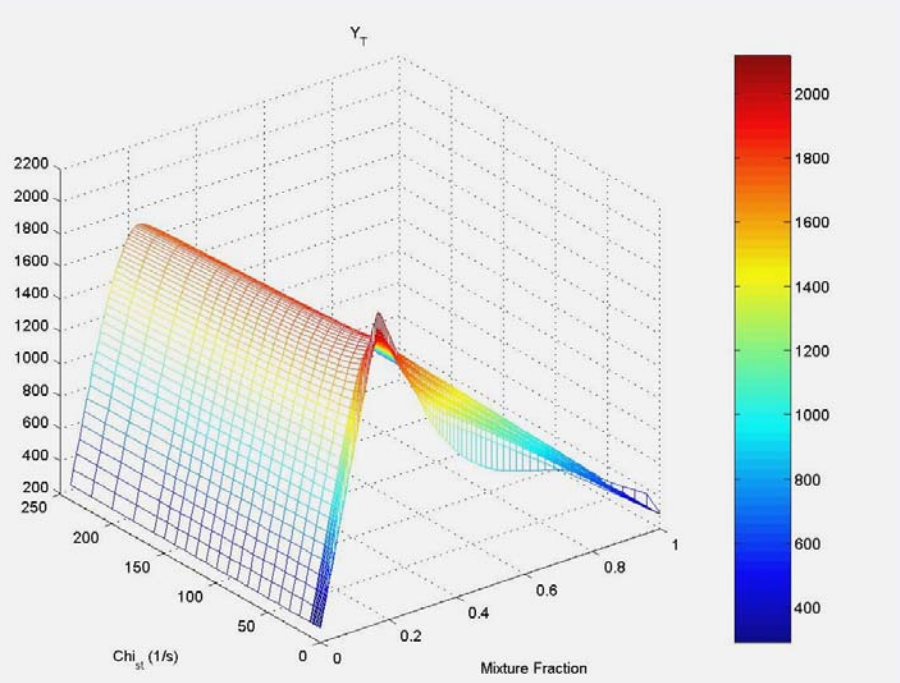
- Direct Numerical Simulations (DNS) is not possible for practical problems in the foreseeable future
  - Resolves all the scales, both spatially and temporally
- Large Eddy Simulations (LES) is difficult, but possible
  - Resolves problem-dependent large scales, models small scales
- Reynolds Average Navier Stokes (RANS) simulations is the feasible solution for industrial scale problems
  - Solves time-averaged governing equations
  - Needs subgrid scale models to account for the unresolved scales
    - Turbulence model: Accounts for the unresolved turbulent scales on the mean flow transport
    - Mixing model: Represents mixing at subgrid scales
    - Reaction model: To simplify the complex finite-rate calculations

# Reaction model (Thermo chemistry)

- Reduces the number of degrees of freedom associated with the combustion chemical reactions in CFD calculations
- If the state of the system ($ø_i$) has n+2 degrees of freedom i.e., $[\rho, T, Y_{1,}....Y_n]$ ,a reaction model parameterizes the state with one/more independent tractable variables
  - Integration of stiff PDEs can be avoided in CFD
- For non-premixed combustion, two widely used models
  - Equilibrium model: Mixture fraction (*f*)
  - Steady flamelets model : Mixture fraction (*f*) & scalar dissipation ($\chi$)
  - An important underlying assumption is that mixing is the rate limiting process compared to chemical reactions (High Damkholer number)

# Reaction model (continued)




$$\phi_i = R(f)$$

**Equilibrium**

$$\phi_i = R(f, \chi)$$

**Laminar flamelets**

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# Thermal NO chemistry

- Extended Zeldovich mechanism

$$O + N_2 \xleftrightarrow{k_{+1}} NO + N$$

$$N + O_2 \xleftrightarrow{k_{+2}} NO + O$$

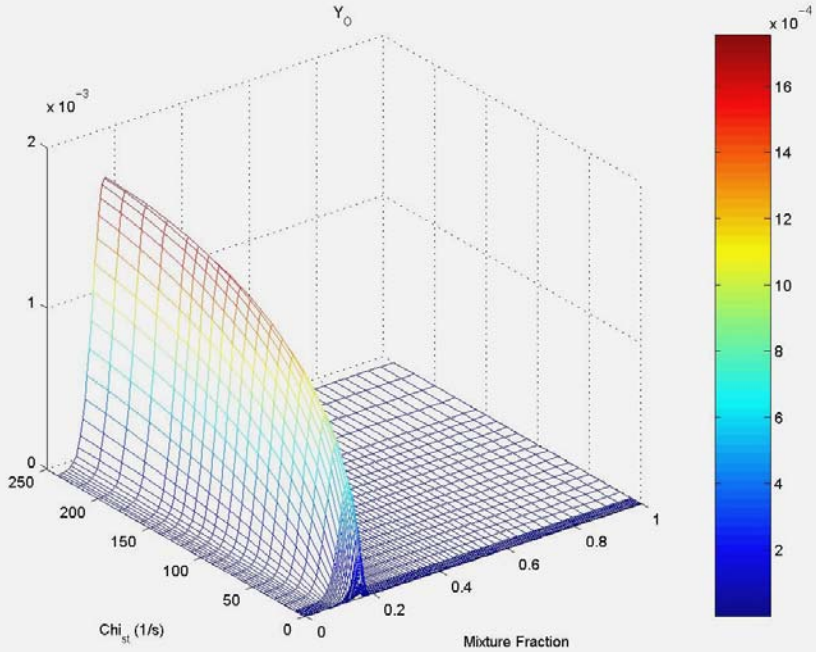
$$N + OH \xleftrightarrow{k_{+3}} NO + H$$

- With the quasi-steady state assumption for N atoms

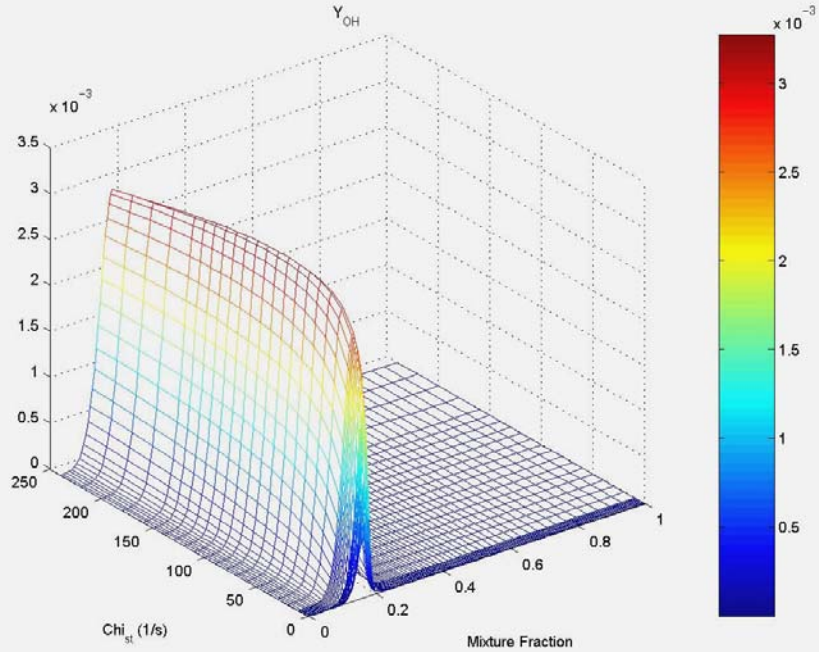
$$\frac{d[NO]}{dt} = 2k_1[O][N_2]\frac{\left(1 - \frac{k_{-1}k_{-2}[NO]^2}{k_1[N_2]k_2[O_2]}\right)}{\left(1 + \frac{k_{-1}[NO]}{k_2[O_2] + k_3[OH]}\right)} \; gmol/m^3 - s$$

- How should we choose the intermediates O & OH?
  - Equilibrium
  - Partial equilibrium
  - Instantaneous quantities from advanced subgrid reaction models (nonequilibrium effects)
- Turbulence-NO chemistry effects?
  - Needs a mixing model
  - Which NO should we select?

# Nonequilibrium effects: O & OH

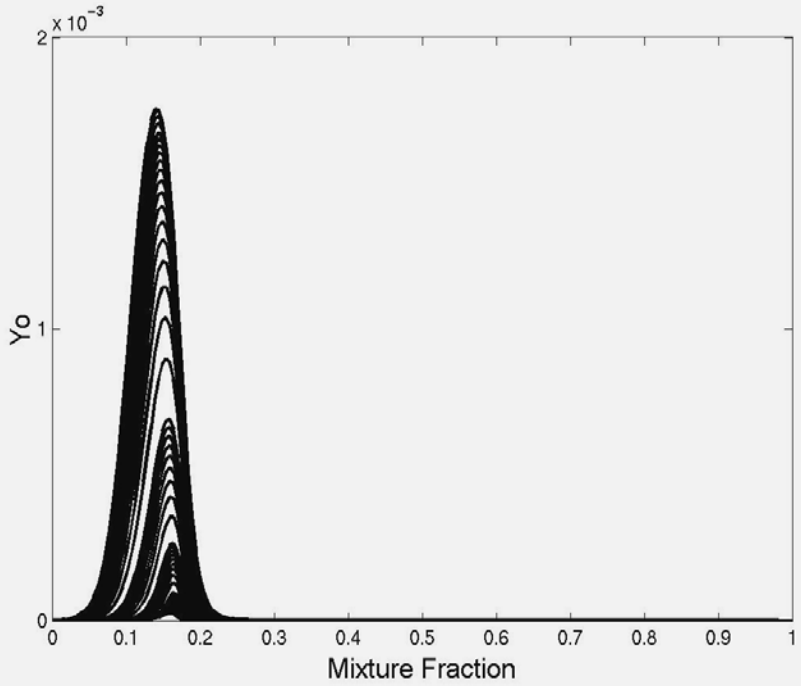



Mass fraction of O

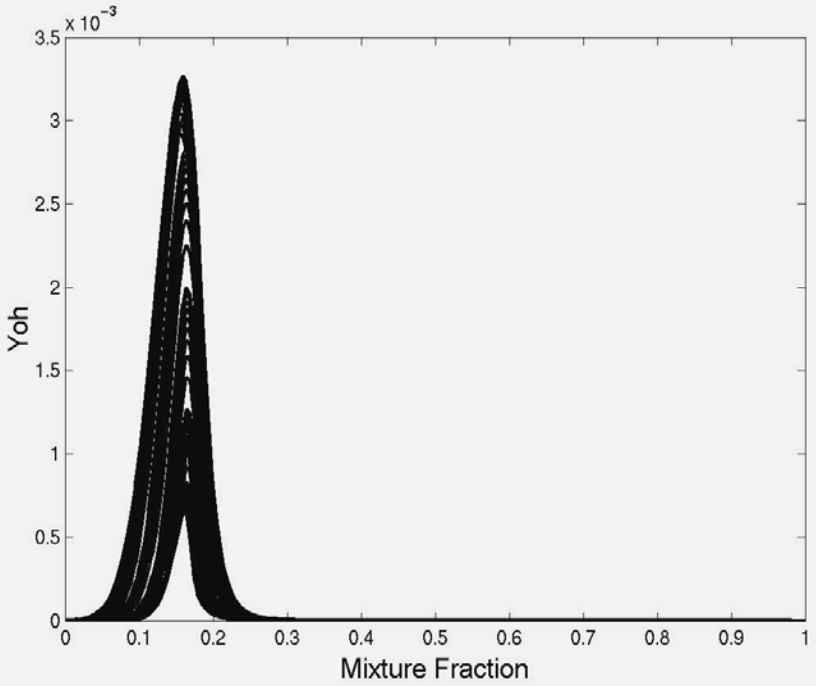



Mass fraction of OH

# Nonequilibrium effects: O & OH

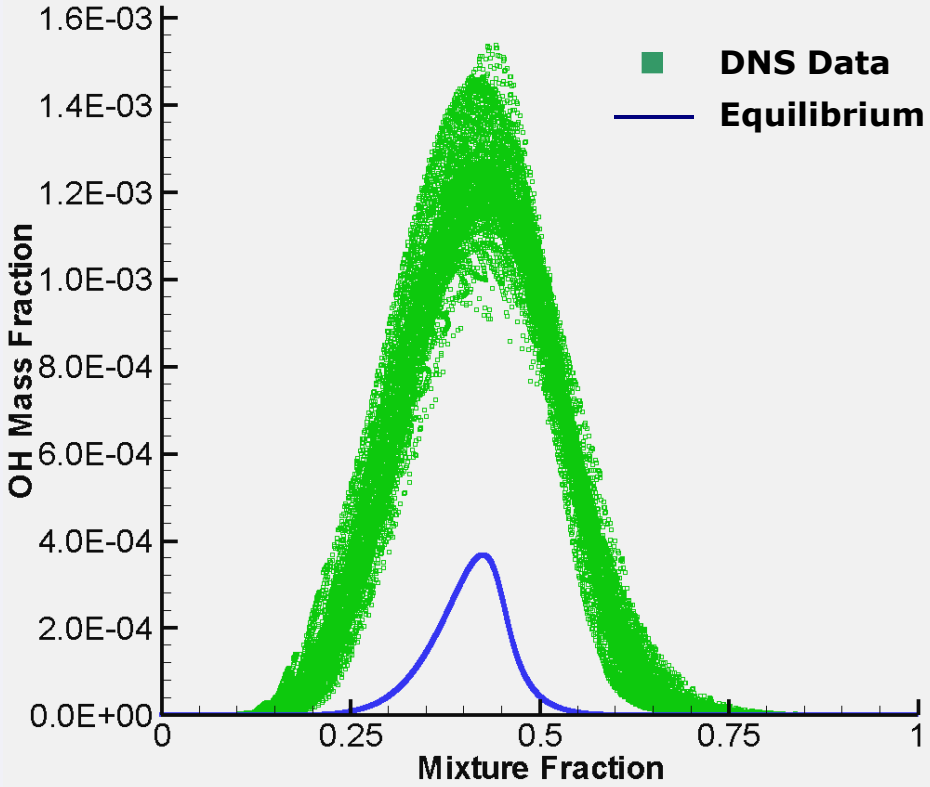


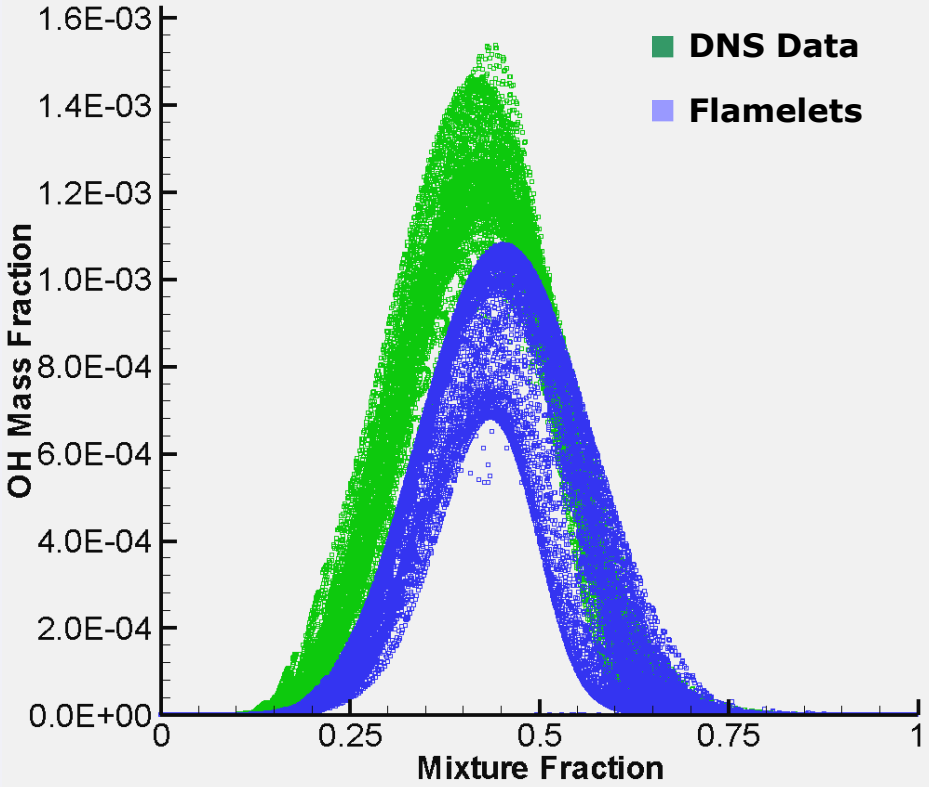

Mass fraction of O




Mass fraction of OH

# DNS validation of reaction models*




- DNS of spatially evolving non-premixed CO-$H_2$ jet
  - Compared to equilibrium chemistry models, flamelets predicted the OH concentrations reasonably

*Courtesy of James Sutherland, CRSIM

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# Mixing model

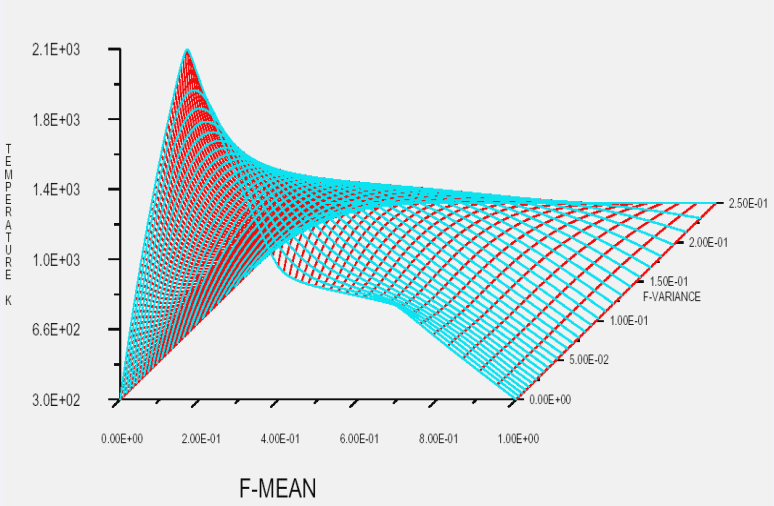
- Accounts for mixing at unresolved (subgrid) scales
- Subgrid scale statistics can be represented with a prescribed probability density function from moments of the tractable variables computed on the mesh
  - Resolving the moments at grid level is crucial to represent the subgrid scale mixing accurately

**Equilibrium**

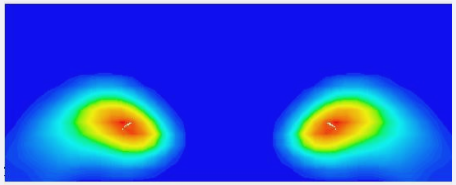
$$\overline{\phi_i} = \int \phi_i(f) P(f) df$$

**Laminar flamelets**

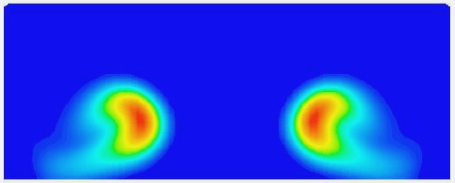
$$\overline{\phi_i} = \int \phi_i(f, \chi) P(f, \chi) df d\chi$$




**Mixing & State space**



**Low grid resolution**

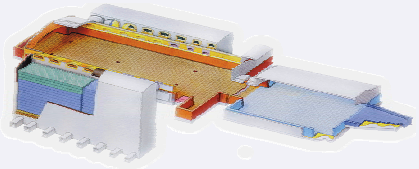


**High grid resolution**

**Resolution &mixing**

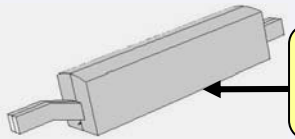
## Complete System

**Prediction/Minimization of NOx emissions from glass furnaces**



**Combustion Space**

**Glass Melt**

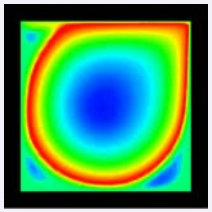
**IFRF Glass Furnace**

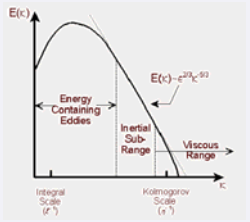
**Single Port Model**

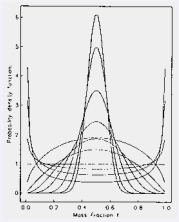
**Two Port Model**

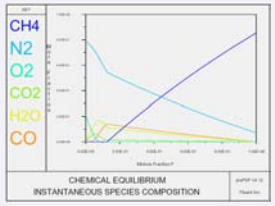
**TNF Flame**

**Laminar CFD** | **Turbulence Model** | **Mixing Model** | **Reaction Model** | **NOx Model** | **Radiation Model** | **Soot Model**





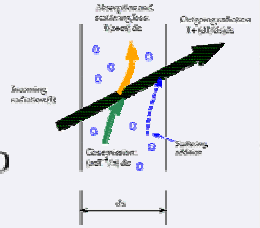



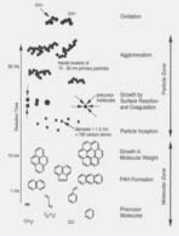



$$O + N_2 \underset{k_{-1}}{\overset{k_{+1}}{\rightleftharpoons}} N + NO$$

$$N + O_2 \underset{k_{-2}}{\overset{k_{+2}}{\rightleftharpoons}} O + NO$$

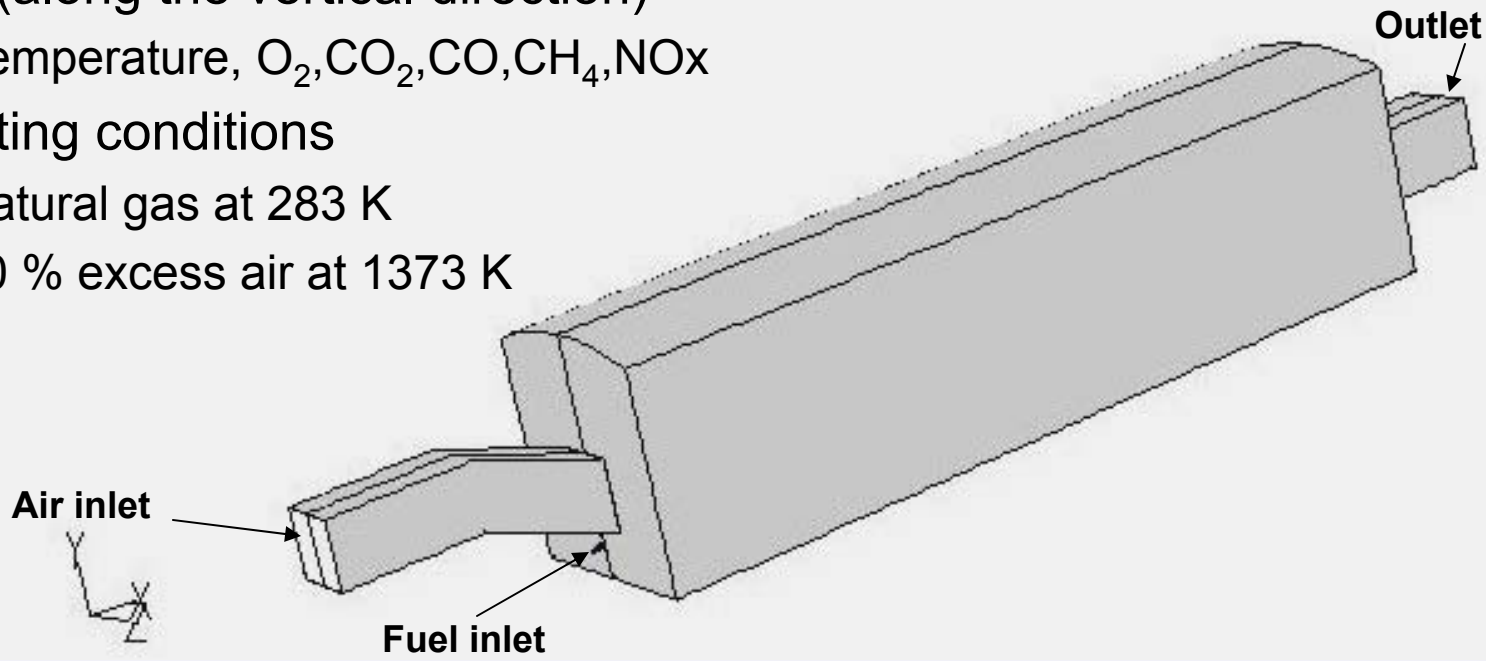
$$N + OH \underset{k_{-3}}{\overset{k_{+3}}{\rightleftharpoons}} H + NO$$





# IFRF glass furnace

- Furnace Dimensions: 3.8 m long X 0.88 m wide X 0.955 m high
- Grid: Modeled only half the domain
  - 420,000 hexahedral elements (after grid adaption)
- Validation data* on the plane of symmetry at x=0.6, 0.9, 1.2, 1.8 & 2.4 m (along the vertical direction)
  - Temperature, $O_2$,$CO_2$,CO,$CH_4$,NOx
- Operating conditions
  - Natural gas at 283 K
  - 10 % excess air at 1373 K




* *T.Nakamura, W.L. Vandecamp and J.P. Smart,"Further studies on high temperature gas combustion in glass furnaces", IFRF Doc No F 90/Y/7, August 1991*

# Simulation details

- Parallel version of FLUENT 6.0 on 4 processors
- Flow & Turbulence: Time-averaged Navier-Stokes equations with standard $\kappa$-$\varepsilon$ model & RSM for turbulence closure
- Combustion: Mixture fraction with equilibrium chemistry & flamelets
  - Flamelets: GRI Mech2.11* chemical mechanism
- Radiation: Discrete-ordinates with weighted-sum-of-gray-gases model (WSGGM) for gas absorption coefficients
- Soot: Two-step Tesner model (soot formation & combustion) with participation in radiation
- Boundary conditions:
  - Velocity is specified at the fuel and air inlets
  - Wall B.C.s & glass surface are treated by specifying heat flux

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* C.T. Bowman, R.K. Hanson, D.F. Davidson, W.C. Gardiner, Jr., V. Lissianski, G.P. Smith, D.M. Golden, M. Frenklach and M. Goldenberg, http://www.me.berkeley.edu/gri_mech/

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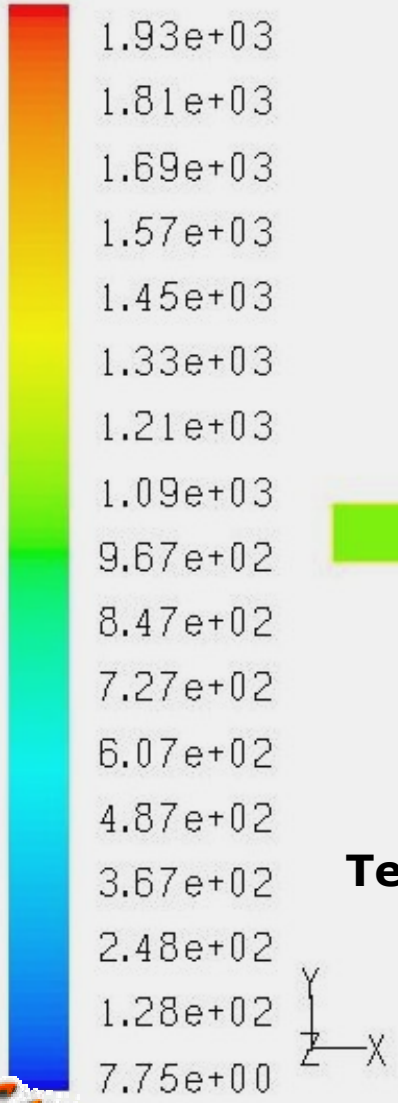
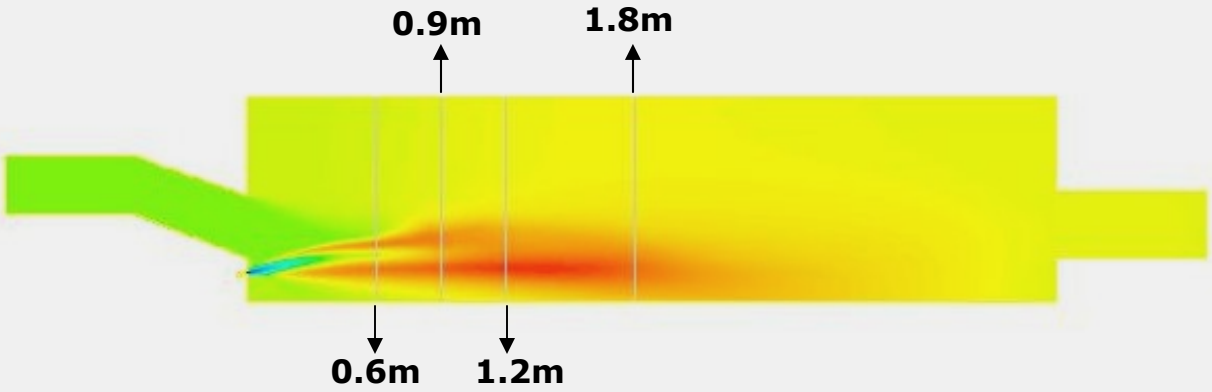
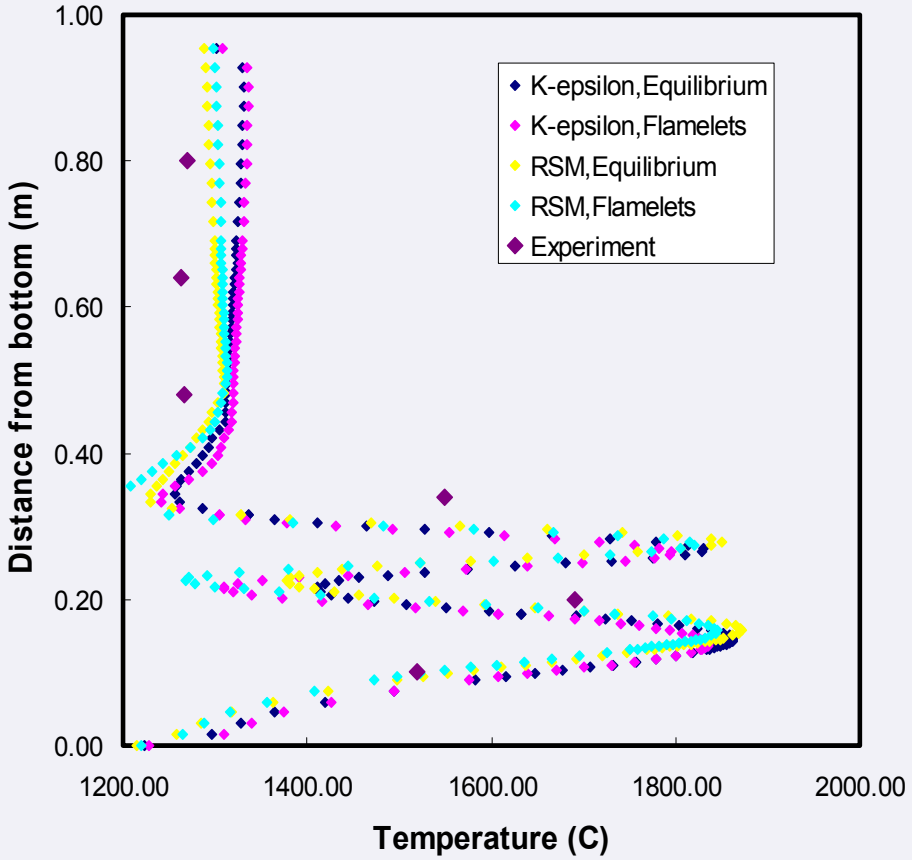
# Temperature Distribution



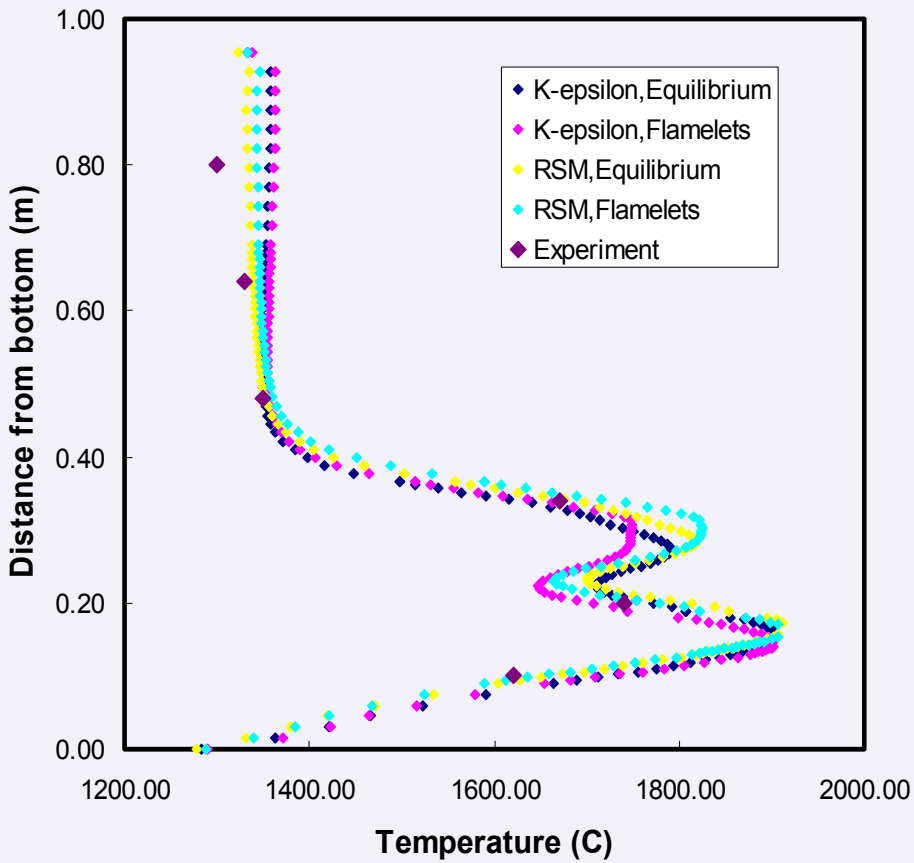




**Temperature($^0$C) contours in the plane of symmetry**

# Temperature validation




**X=0.6 m**




**X=0.9 m**

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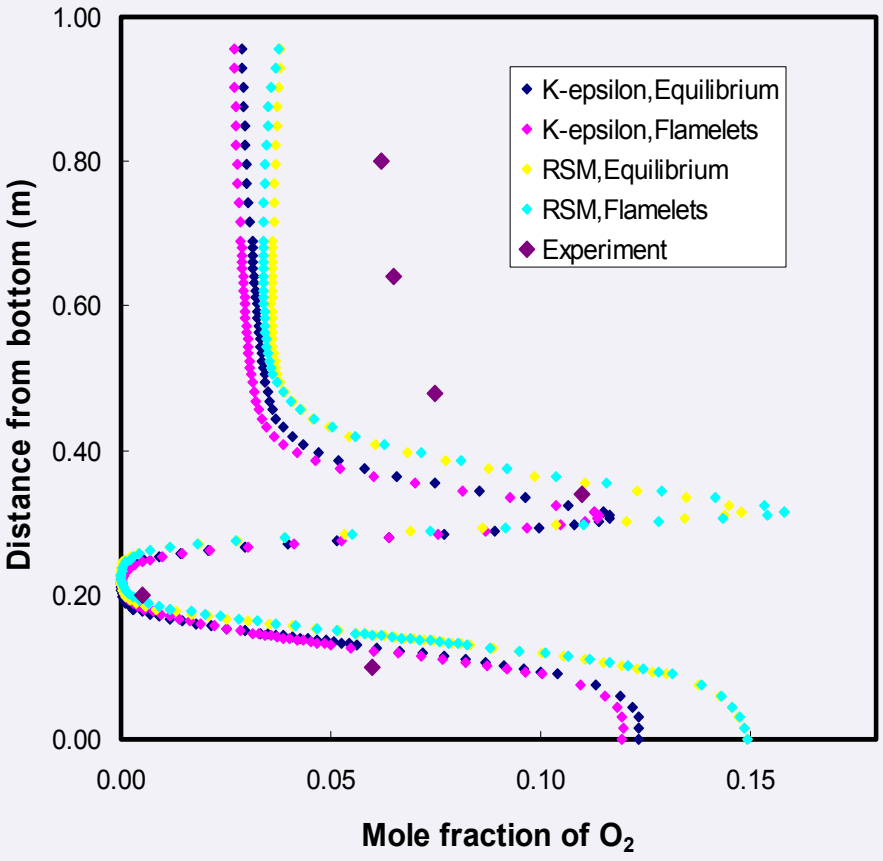
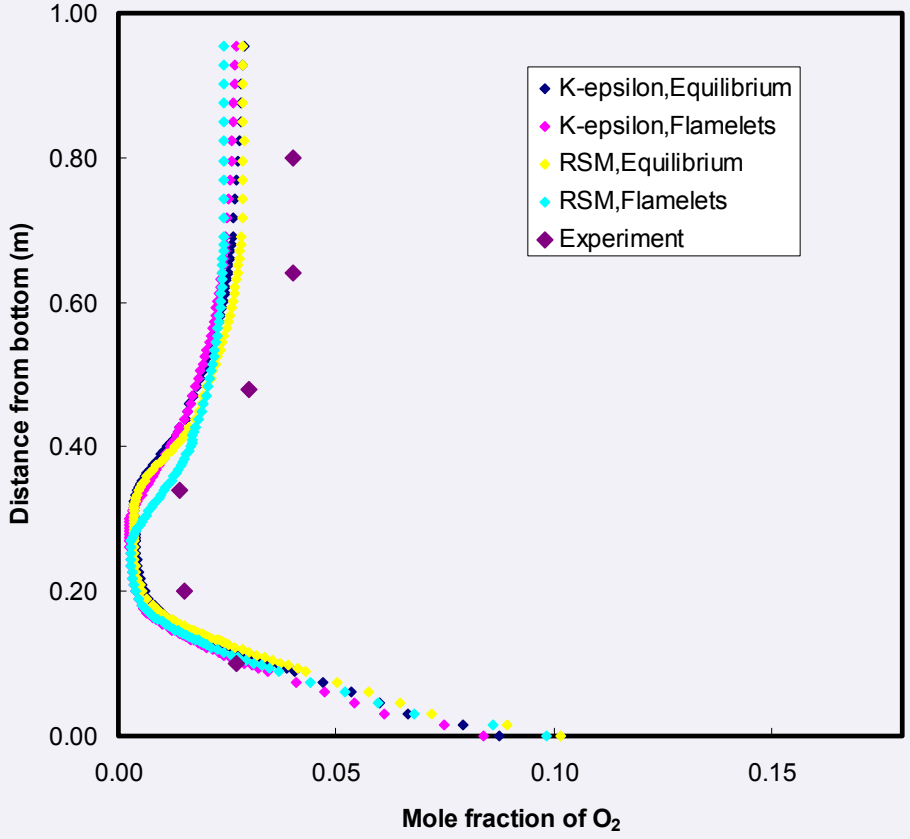
# $O_2$ validation




**X=0.6 m**




**X=1.8 m**

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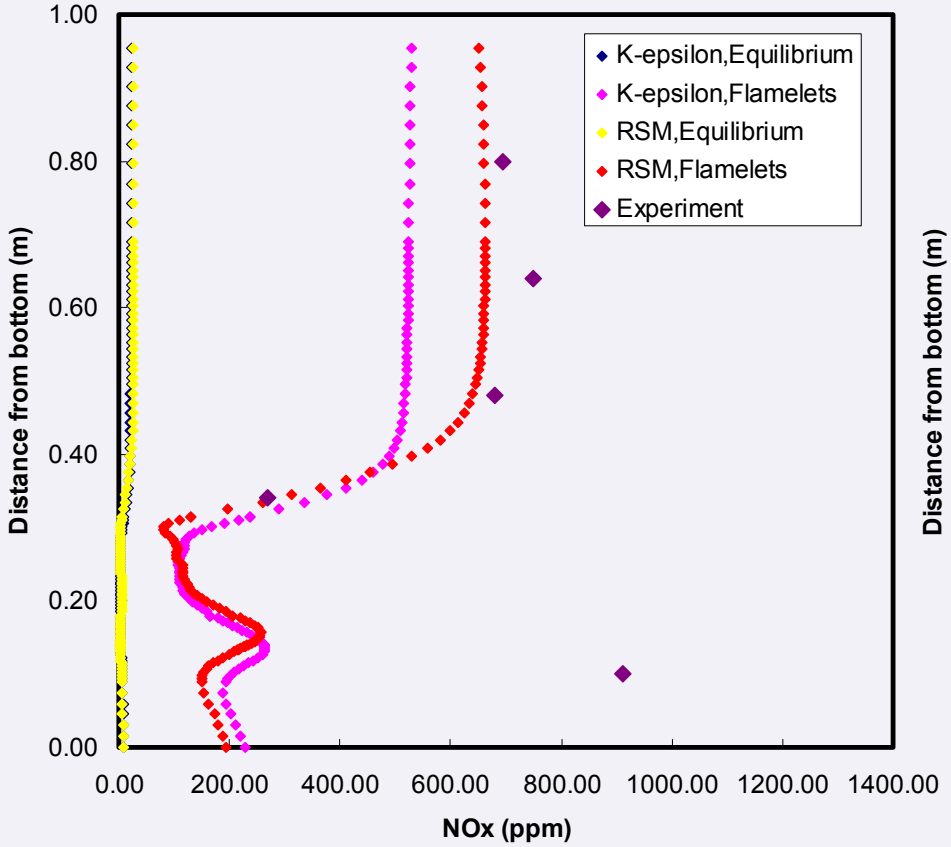
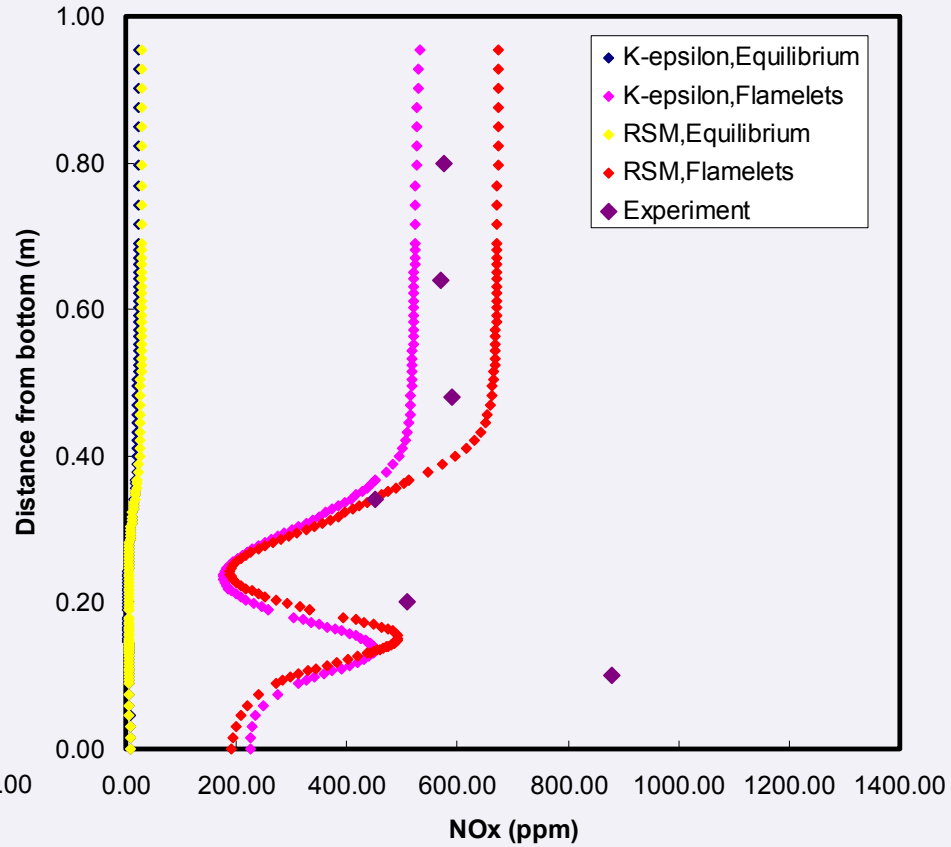
# NOx calculations

- **Turbulence**: Sensitivity of turbulence model is studied with standard κ-ε model and RSM
- **Mixing**: Turbulence effects on the NOx production rates are accounted through the mixture fraction PDF
- **Reaction model**: NOx is post-processed with the following O & OH radical concentrations
  - In the case of equilibrium combustion calculations, O & OH are taken from the partial-equilibrium approximation
  - For flamelets combustion calculations, O & OH concentrations are from flamelets PDF look-up tables

# NOx validation




X=0.6 m




X=0.9 m

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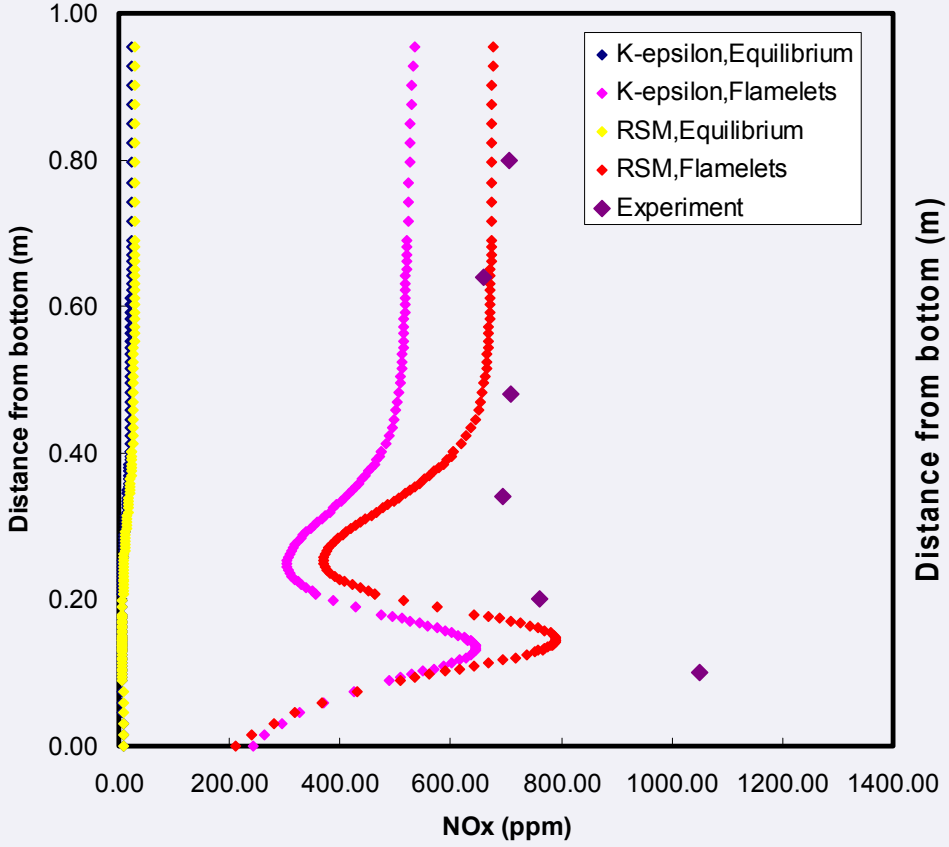
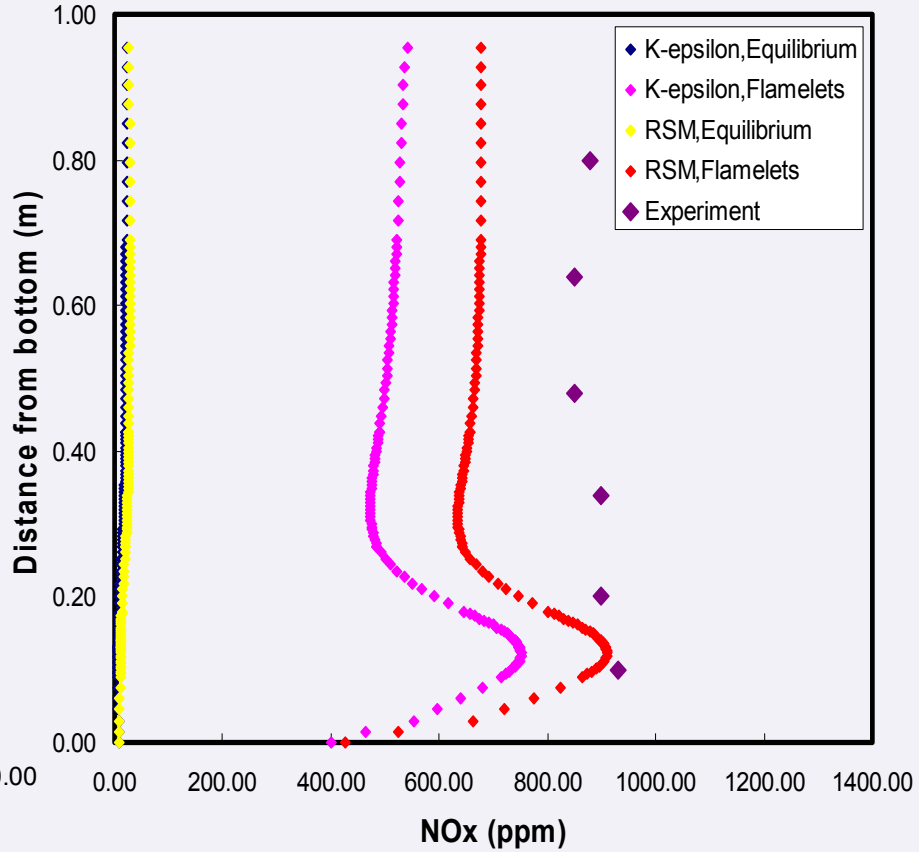
# NOx validation




X=1.2 m




X=1.8 m

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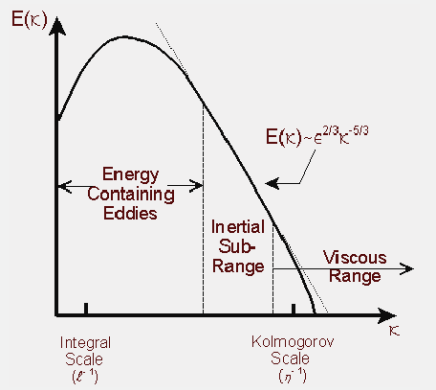
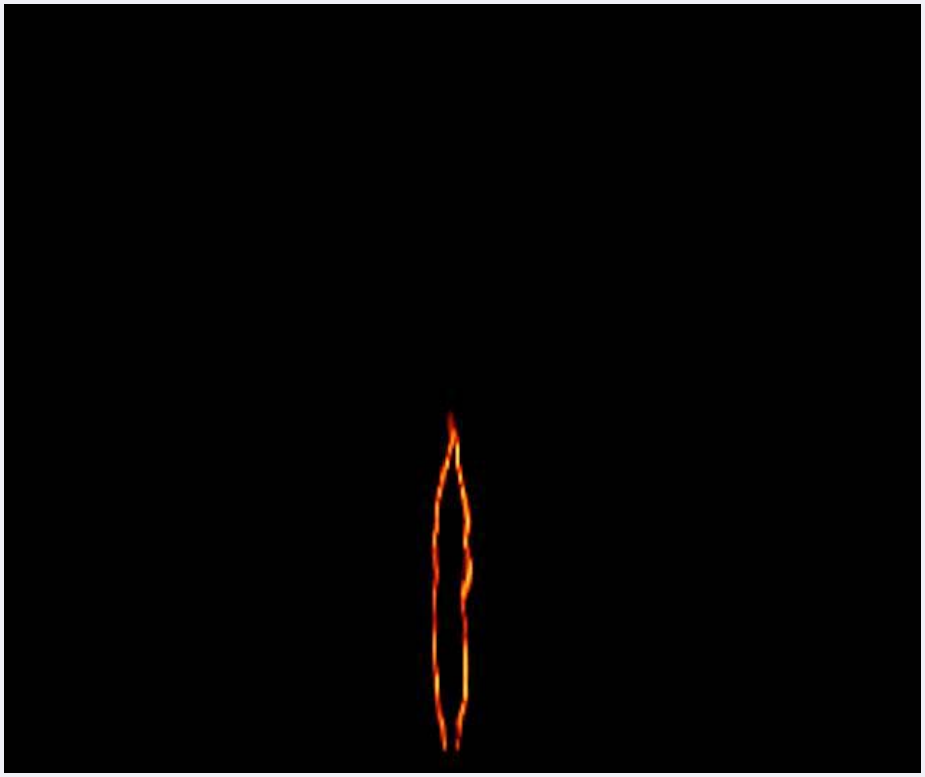
# Large Eddy Simulations (LES)

- NS equations are filtered to retain large scales of the flow
  - Large scales are more problem-dependent and contains most of the energy
  - Needs subgrid scale models for small scales, which tends to have more universal behavior
  - Resolves flow and mixing more accurately than RANS methods




**LES of a TNF workshop flame**

# LES & thermal NO



**Temperature & Thermal NO source**

# Conclusions

- **Mixing:** Resolving mixing is crucial in predicting the local thermo-chemical state of the system and pollutants
  - **Resolved scale mixing:** Predictions are very sensitive to the inlet boundary profiles
  - **Subgrid scale mixing:** LES resolves mixing more accurately than RANS, thus reduces the burden on mixing model
- **Reaction Model:** For NOx predictions, the intermediate species should be chosen from realistic reaction models, which can include the nonequilibrium effects
- **Validation:** A systematic validation strategy for NOx simulation in industrial furnaces needs to include validation at pilot and bench scales.

# Acknowledgement


- This research program is financially supported by Sandia National Laboratories & DOE Office of Industrial Technologies, under the supervision of Dr. Robert J. Gallagher