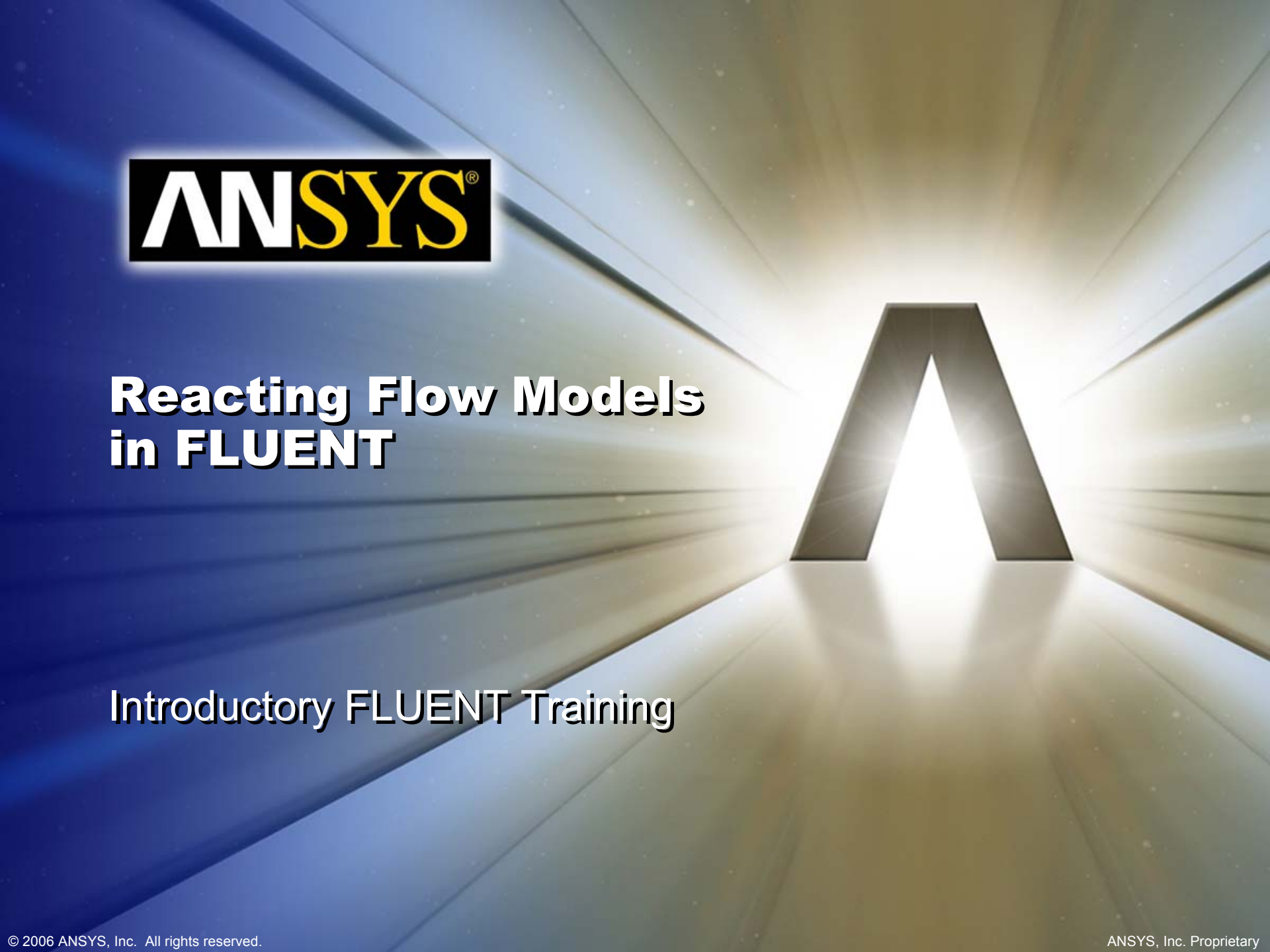


Reacting Flow Models in FLUENT

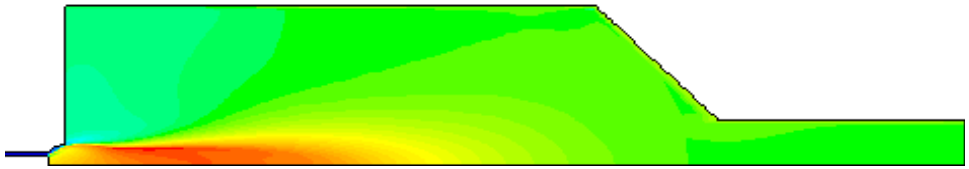
Introductory FLUENT Training

Outline

- Fundamental Concepts
- Overview of Reacting Flow Models in FLUENT
- Fast Chemistry Models
  - Eddy Dissipation Model (EDM)
  - Premixed
  - Non-Premixed
  - Partially Premixed
- Finite-rate Chemistry Models
  - Laminar Finite-Rate Model
  - Eddy Dissipation Concept (EDC)
  - Composition PDF Transport Model
  - Laminar Flamelet for Non-Premixed Flames
- Discrete Phase Model (DPM)
- Pollutant Formation Models
- Surface Reactions
- Summary
- Appendix

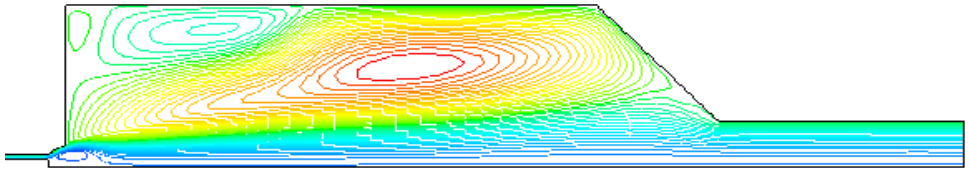
Applications of Reacting Flow Systems

- FLUENT contains models which are applicable to a wide range of homogeneous and heterogeneous reacting flows
  - Furnaces
  - Boilers
  - Process heaters
  - Gas turbines
  - Rocket engines
- Predictions of
  - Flow field and mixing characteristics
  - Temperature field
  - Species concentrations
  - Particulates and pollutants



Temperature in a Gas Furnace

CO_2 Mass Fraction



Stream Function

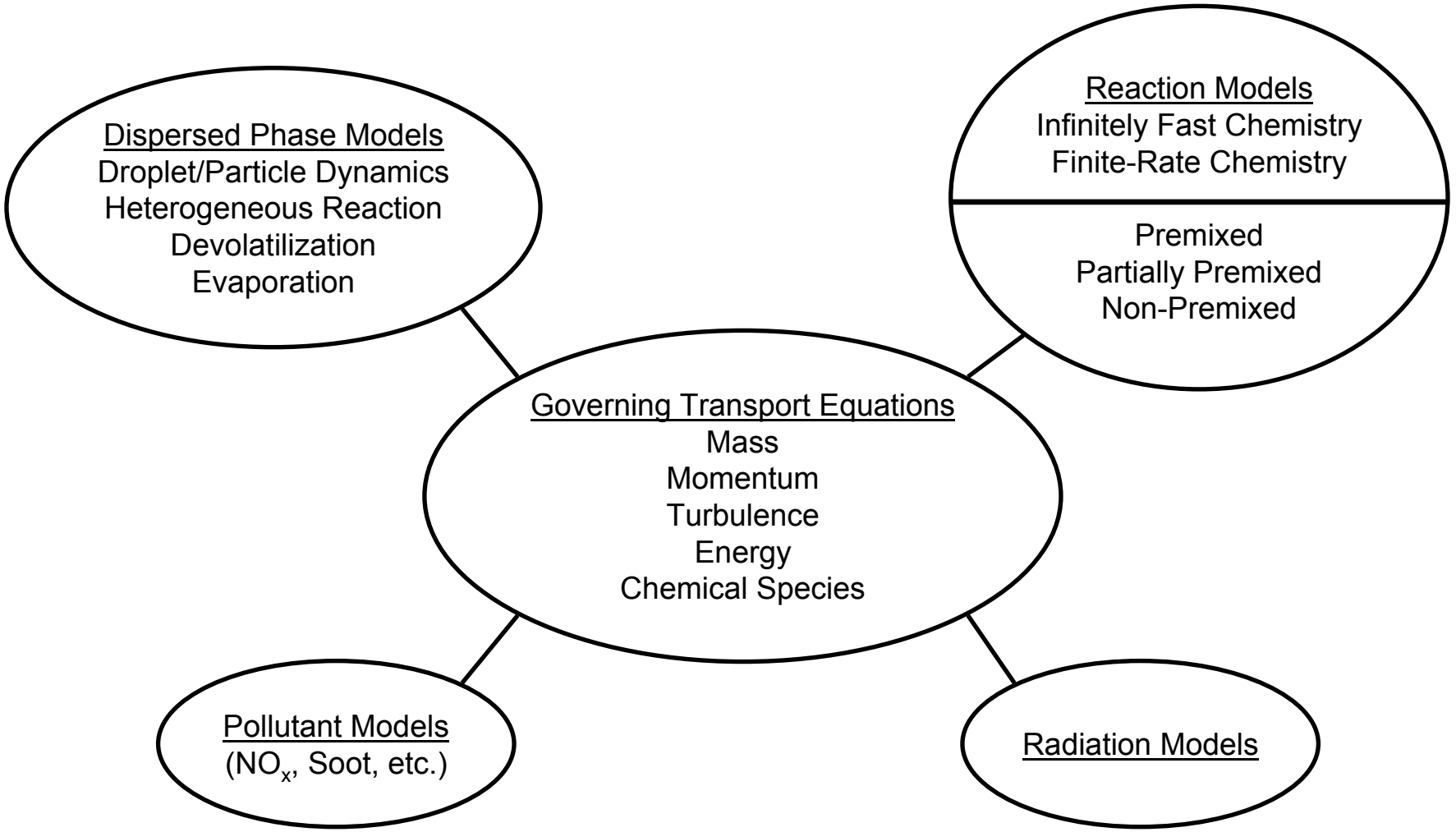
Difficulties in Modeling Reacting Flows

- Turbulence
  - Most industrial flows are turbulent.
  - DNS of non-reacting and reacting turbulent flows is not possible because of the wide range of time and length scales.
- Chemistry
  - Realistic chemical mechanisms cannot be described by a single reaction equation.
    - Tens of species, hundreds of reactions
    - Known in detail for only a limited number of fuels
  - Stiff kinetics (wide range of reacting time scales)
- Turbulence-Chemistry Interaction
  - The sensitivity of reaction rates to local changes is complicated by enhanced mixing of turbulent flows.

Modeling Chemical Kinetics in Combustion

- Simplify the Chemistry (use Finite Rate / Eddy Dissipation Approach).
  - Considers global chemical reaction mechanisms.
- Decouple chemistry from turbulent flow and mixing (use mixture fraction approach)
  - Equilibrium chemistry PDF model
  - Laminar flamelet model
  - Mixture fraction and progress variable (partially premixed model)
- Model stiff chemistry (expensive)
  - Typically requires the use of very small time steps to achieve numerical stability and convergence (can be impractical).
  - Use of the stiff solver will allow larger time steps to be used.

Overview of Reacting Flow Modeling

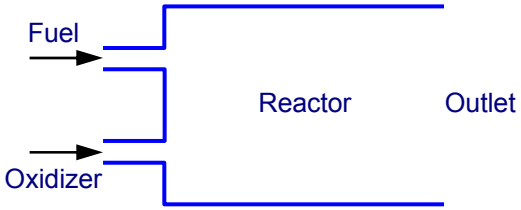


Definitions of Reacting Systems

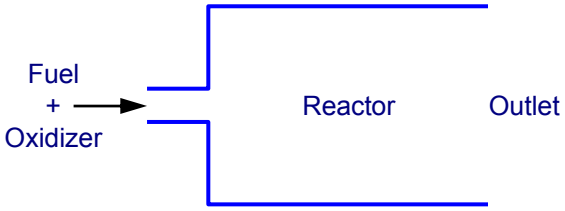
- Reacting flow systems can be divided into two distinct categories.
  - Homogeneous reactions
    - Reaction occurs among products and reactants that are in the same phase.
  - Heterogeneous reactions
    - Reactions involve reactants and products in different phases.
    - If applicable, chemical species deposited onto surfaces are treated as distinct from the same chemical species in the gas.
      - The rate of deposition is governed by both chemical kinetics and the diffusion rate from the fluid to the surface.
      - Wall surface reactions create sources (and sinks) of chemical species in the bulk phase and determine the rate of deposition of surface species
    - Surface reaction: CVD, catalytic conversion.

Homogeneous Reactions

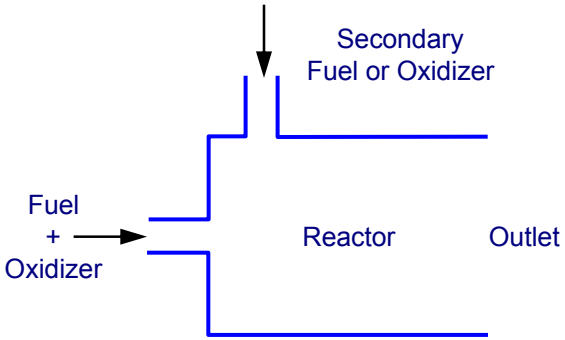
- Non-premixed reaction systems
  - Reactants convect/diffuse from either side into a flame sheet.
  - Can be simplified to a mixing problem.
  - Turbulent eddies distort the laminar flame shape and enhance mixing.



- Premixed reaction systems
  - Cold reactants propagate into hot products.
  - Rate of propagation (flame speed) depends on the internal flame structure.
    - Much more difficult to model than non-premixed combustion problems.
  - Turbulence distorts the laminar flame shape and thus accelerates flame propagation



- Partially premixed systems
  - Reacting system with both non-premixed and premixed inlet streams.



Characterization of Reacting Flow Problems

- Reacting flow problems are characterized using a number of dimensionless variables.
- The two most important dimensionless variables are the Reynolds number and the Damköhler number.
- Reynolds number

$$\mathrm{Re} = \frac{\text{Inertial Force}}{\text{Viscous Force}} = \frac{\rho U L}{\mu}$$

  - ρ, U, L, μ are characteristic density, velocity, length and dynamic viscosity, respectively.
  - Large Reynolds number indicates turbulent flow.

- Damköhler Number

$$\mathrm{Da} = \frac{\text{Mixing Time Scale}}{\text{Chemical Time Scale}} = \frac{\tau_{\text{mixing}}}{\tau_{\text{reaction}}}$$

  - Large Damköhler number (Da > 1) indicates gas phase turbulent combustion models should be used.

Characterization of Reacting Flow Problems

- Mach number

$$\mathrm{Ma} = \frac{\text{Convection velocity}}{\text{Sonic velocity}} = \frac{U}{c}$$

c ← Local speed of sound (sonic velocity)

  - High Mach number (Ma > 0.3) indicates that compressibility effects are important.
  - For low Mach number flows, the non-premixed model is valid.

- Boltzmann number

$$\mathrm{Bo} = \frac{\text{Convection Heat Flux}}{\text{Radiation Heat Flux}} = \frac{(\rho U C_p T)_{\text{inlet}}}{\sigma T_{ad}^4}$$

σ ← Stefan-Boltzmann constant 5.672×10^{-8} W/m^2·K^4

  - Large Boltzmann number indicates that convection is the primary heat transfer mechanism.
  - Radiation heat transfer should be considered when Bo < 10.

Overview of Reacting Flow Models in FLUENT

FLOW CONFIGURATION

CHEMISTRY

	Premixed	Non-Premixed	Partially Premixed
Fast Chemistry	**Eddy Dissipation Model** (Species Transport)		
	Premixed Combustion Model Reaction Progress Variable*	**Non-Premixed Equilibrium Model** Mixture Fraction	**Partially Premixed Model** Reaction Progress Variable + Mixture Fraction
Finite-Rate Chemistry	**Laminar Finite-Rate Model**		
	Eddy-Dissipation Concept (EDC) Model		
	Composition PDF Transport Model		
		Laminar Flamelet Model Steady / Unsteady	

*Rate classification not truly applicable since species mass fraction is not determined.

Homogeneous (Gas-Phase) Combustion Models

- Eddy Dissipation
  - Use one- or two-step global (heat release) reaction mechanisms.
  - The chemical reaction rate is the turbulent mixing rate.
    - Finite Rate option is a switch for the premixed flames.
- Non-Premixed
  - Uses the mixture fraction and assumed PDF instead of solving equations for species transport and reaction rate for equilibrium chemistry.
  - Laminar flamelets for moderately non-equilibrium chemistry
- Premixed
  - Treats chemistry by using a reaction progress variable, C.
  - Turbulent Flame Speed Closure – Zimont model
- Partially Premixed
  - Combines the non-premixed and premixed models.
  - Assumptions in both models apply
- Eddy-dissipation concept (EDC)
  - Turbulence / chemistry interaction model for turbulent flames
  - Includes detailed chemistry
- Composition PDF transport
  - More rigorous treatment of turbulence-chemistry interaction than EDC model.
  - Substantially more expensive!

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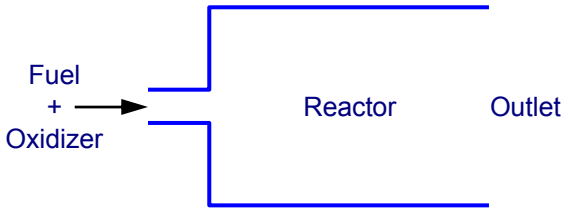
Eddy Dissipation Model (EDM)

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Fast chemistry (high Da)
  - Configuration: Premixed / Non-Premixed / Partially Premixed
- Application examples
  - Gas reactions
  - Coal combustion
- Limitations
  - Unreliable when mixing and kinetic time scales are of similar order of magnitude (Da ~ 1).
  - Does not predict kinetically-controlled intermediate species and dissociation effects.
  - Cannot realistically model phenomena which depend on detailed kinetics such as ignition, extinction and low-Da flows.
- Solves species transport equations. Reaction rate is controlled by turbulent mixing.

Premixed Combustion Model

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Fast chemistry (high Da)
  - Configuration: Premixed only



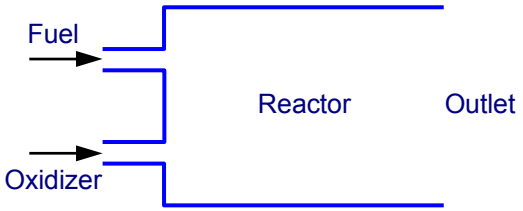
- Application examples
  - Premixed reacting flow systems
  - Lean premixed gas turbine combustion chamber

- Limitations
  - Cannot realistically model phenomena which depend on detailed kinetics (such as ignition, extinction and low-Da flow).

- Uses a reaction progress variable which tracks the position of the flame front (Zimont model).

Non-Premixed Equilibrium Model

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Fast chemistry (high Da), assuming equilibrium conditions
  - Configuration: Non-Premixed only



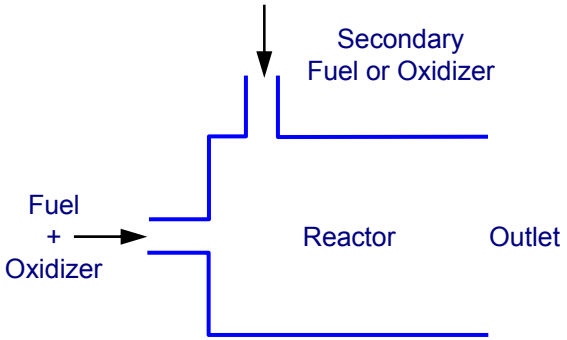
- Application examples
  - Gas reaction (furnaces, burners). This is usually the model of choice if assumptions are valid for gas phase combustion problems Accurate tracking of intermediate species concentration and dissociation effects without requiring knowledge of detailed reaction rates.

- Limitations
  - Unreliable when mixing and kinetic time scales are comparable (Da ~ 1).
  - Cannot realistically model phenomena which depend on detailed kinetics (such as ignition, extinction and low-Da flow).

- Solves transport equations for mixture fraction and mixture fraction variance (instead of the individual species equations).

Partially Premixed Combustion Model

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Equilibrium or moderately non-equilibrium (flamelet)
  - Configuration: Partially premixed only
- Application examples
  - Gas turbine combustor with dilution cooling holes.
  - Systems with both premixed and non-premixed streams



- Limitations
  - Unreliable when mixing and kinetic time scales are comparable (Da ~ 1).
  - Cannot realistically model phenomena which depend on detailed kinetics (such as ignition, extinction and low-Da flow).
- In the partially premixed model, reaction progress variable and mixture fraction approach are combined. Transport equations are solved for reaction progress variable, mixture fraction, and mixture fraction variance.

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Detailed Chemistry Models

- The governing equations for detailed chemistry are generally stiff and difficult to solve.
  - Tens of species
  - Hundreds of reactions
  - Large spread in reaction time scales.
- Detailed kinetics are used to model:
  - Flame ignition and extinction
  - Pollutants (NO_x, CO, UHCs)
  - Slow (non-equilibrium) chemistry
  - Liquid/liquid reactions
- Available Models:
  - Laminar finite rate
  - Eddy Dissipation Concept (EDC) Model
  - PDF transport
  - KINetics model (requires additional license feature)
- CHEMKIN-format reaction mechanisms and thermal properties can be imported directly.
- FLUENT uses the In-Situ Adaptive Tabulation (ISAT) algorithm in order to accelerate calculations (applicable to laminar, EDC, PDF transport models). See the Appendix for details.

Laminar Finite-Rate Model

- Applicability
  - Flow Regime: Laminar flow (low Re)
  - Chemistry: Finite-rate chemistry
  - Configuration: Premixed / Non-Premixed / Partially Premixed
- Application examples
  - Laminar diffusion flames
  - Laminar premixed flames in gas furnaces
- Limitations
  - This approach is CPU-intensive. By default, the ISAT algorithm is used to accelerate calculations (see the Appendix for details).
  - Generally unsuitable for turbulent combustion problems.
- The laminar finite-rate model requires a stiff chemistry solver (available in both the pressure- and density-based solvers).

Eddy Dissipation Concept (EDC) Model

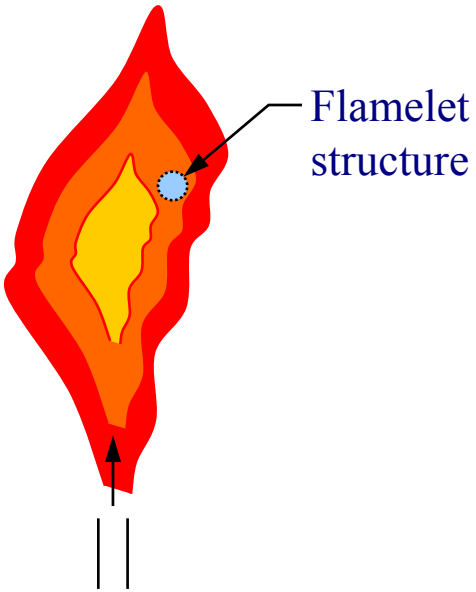
- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Finite-rate chemistry
  - Configuration: Premixed / Non-Premixed / Partially Premixed
- Application examples
  - Prediction of finite rate phenomena in turbulent reacting flows.
  - Slow CO burnout
  - NOx formation
- Limitations
  - This approach is CPU-intensive. By default, the ISAT algorithm is used to accelerate calculations (see the Appendix for details).
- The EDC model is an extension of the eddy dissipation model to account for finite rate chemistry in turbulent flows.

Composition PDF Transport Model

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Finite-rate chemistry
  - Configuration: Premixed / Non-Premixed / Partially Premixed
- Application Examples
  - Prediction of finite-rate phenomena in turbulent reacting/combusting flows such as formation of CO and NOx
  - Liquid/liquid reacting systems
- Limitation
  - The PDF Transport model is very CPU-intensive because it uses a Monte Carlo method. By default, the ISAT algorithm is used to accelerate calculations (see the Appendix for details).
- The composition probability density function (PDF) transport model is used to incorporate finite-rate chemistry in turbulent flames
  - More rigorous than the EDC model
  - Uses a Monte Carlo method.

Steady and Unsteady Flamelet Model

- Applicability
  - Flow Regime: Turbulent flow (high Re)
  - Chemistry: Moderately non-equilibrium due to aerodynamic strain
  - Configuration: Non-Premixed only
- Application examples
  - Prediction of lift off and blow off phenomena in jet flames.
  - Internal combustion engine (Diesel unsteady flamelet submodel only)
  - Liquid/liquid reacting systems (unsteady flamelet submodel)
- Limitations
  - Steady approach cannot realistically model phenomena which depend on detailed kinetics (such as ignition, extinction and low-Da flow).
- In the laminar flamelet model, transport equation for mixture fraction variance is solved. To account for non-equilibrium effects, scalar dissipation (flame strain rate) is calculated.



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Discrete Phase Model (DPM)

- Description
  - Trajectories of particles/droplets/bubbles are computed in a Lagrangian frame.
  - Particles can exchange heat, mass, and momentum with the continuous gas phase.
  - Each trajectory represents a group of particles, each with the same initial properties.
  - Interaction among individual particles is neglected.
  - Discrete phase volume fraction must be less than 10%. Mass loading is not limited.

$$\frac{d\vec{u}_p}{dt} = f_{drag}\left(\vec{u} - \vec{u}_p\right) + g\left(\frac{\rho_p - \rho}{\rho_p}\right) + \frac{\vec{F}}{\rho_p}$$

- Numerous submodels are available.
  - Heating/cooling of the discrete phase
  - Vaporization and boiling of liquid droplets
  - Volatile evolution and char combustion for combusting particles
  - Droplet breakup and coalescence using spray models
  - Erosion/Accretion

- Numerous applications
  - Particle separation and classification, spray drying, aerosol dispersion, bubble sparging of liquids, liquid fuel and coal combustion.

Pollutant Formation Models

- NO_x formation models (predict qualitative trends of NO_x formation).
  - FLUENT contains three mechanisms for calculating NO_x production.
    - Thermal NO_x
    - Prompt NO_x
    - Fuel NO_x
  - NO_x reburning model
  - Selective Non-Catalytic Reduction (SNCR) model
- Soot formation models
  - One step and two steps model
  - Soot affects the radiation absorption (Enable the Soot-Radiation option in the Soot panel)
- SO_x formation models
  - Additional equations for SO_2, H_2S, and, optionally, SO_3 are solved.
  - In general, SO_x prediction is performed as a post-process.

Surface Reactions

- Chemical species deposited onto surfaces are treated as distinct from the same chemical species in the gas.
- Site balance equation is solved for every surface-adsorbed (or "site") species.
  - Detailed surface reaction mechanisms can be considered (any number of reaction steps and any number of gas-phases or/and site species).
  - Surface chemistry mechanism in Surface CHEMKIN format can be imported into FLUENT.
  - Surface reaction can occur at a wall or in porous media.
  - Different surface reaction mechanisms can be specified on different surfaces.
- Application examples
  - Catalytic reactions
  - CVD

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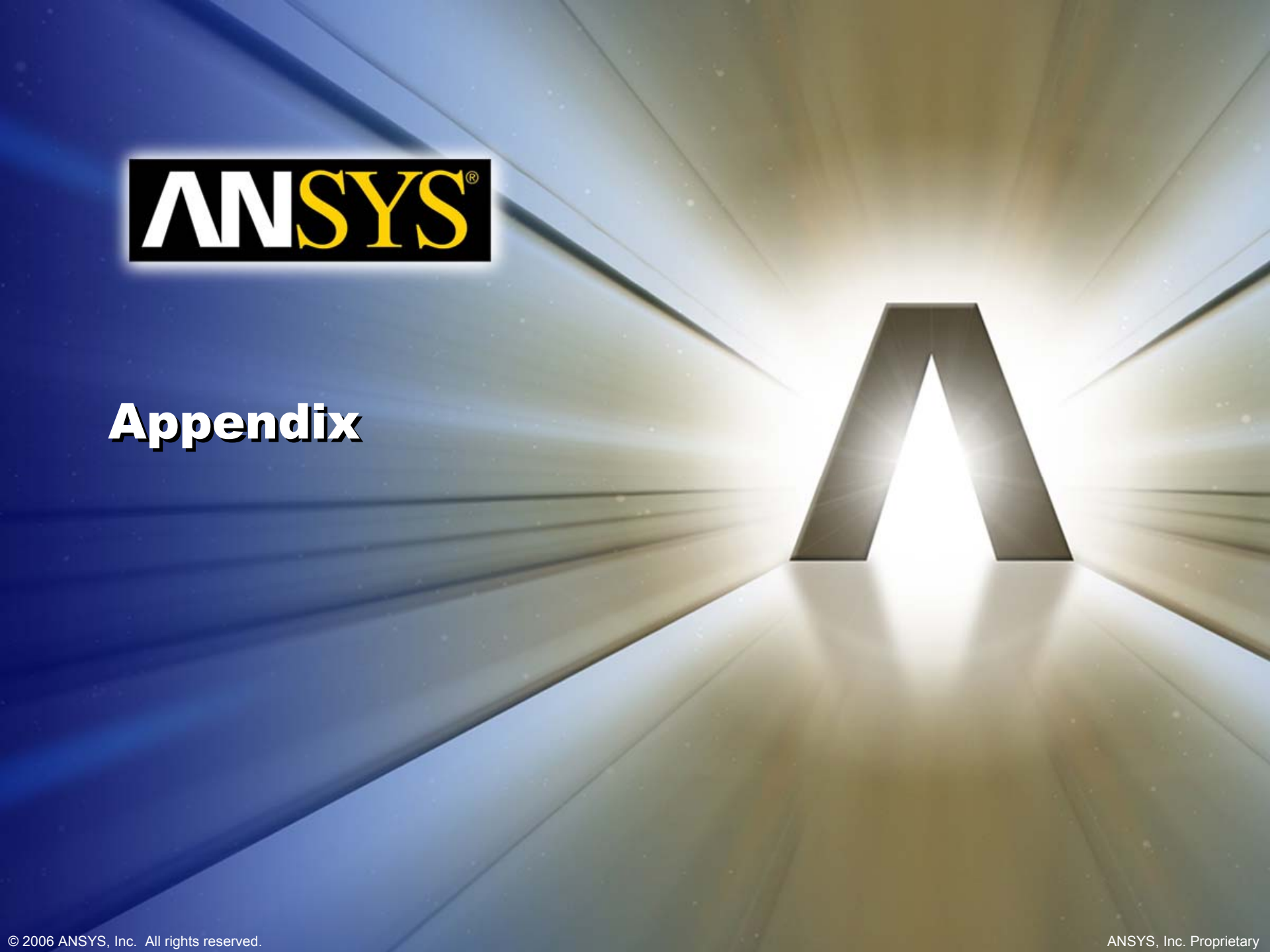
Summary

- There are four introductory level tutorials on reacting flow.
  - Species transport and gas combustion
  - Non-premixed combustion
  - Surface chemistry
  - Evaporating liquid spray
- A number of intermediate and advanced tutorials are also available.
- Other learning resources
  - Advanced training course in reacting flow offered by FLUENT
  - User Service Center, www.fluentusers.com
    - All tutorials and lecture notes
    - Web-based training courses



Appendix

Eddy Dissipation Model (EDM)

- A model for estimating the mean reaction rate (of species k), R_k
- Reaction rate is defined using the eddy-breakup model.
  - Assumes that chemical reactions occur much faster than turbulence can mix reactants into the flame (Da >> 1)
  - Combustion is completely controlled by turbulent mixing rates which are proportional to the large-eddy lifetime scale, k / ε
- Chemical reaction is approximated by the global (1 or 2 step) mechanism
- Reynolds (time) averaged species mass fraction equations for N – 1 species are solved
- Finite-Rate/Eddy Dissipation Option
  - Reaction rate is the lesser of the Arrhenius rate and eddy-dissipation rate.

Non-Premixed Equilibrium Model

- For infinitely fast chemistry in turbulent flow, reaction proceeds to chemical equilibrium instantaneously when the fuel and oxidizer mix (mixing limited).
- The species and enthalpy transport equations collapse into a single conservation equation for mixture fraction, f, under the following assumptions:
  - Species diffusion coefficients are equal
  - Lewis number for each species must equal unity.
  - Moderate Mach number
- Mixture fraction can be directly related to species mass fraction, mixture density, and mixture temperature. These relations are known for instantaneous (not time-averaged) data.
- A probability density function (PDF) is used to relate instantaneous data to time-averaged data (turbulent reacting flow simulations predict time-averaged properties)
  - PDF is assumed to be a beta function (which can describe a wide range of PDF shapes)
  - Requires the variance of volume fraction (based on local turbulence parameters).

Composition PDF Transport Model

- The composition probability density function (PDF) transport model is used to incorporate finite-rate chemistry in turbulent flames
  - More rigorous than the EDC model
  - The PDF represents the fraction of time that the fluid spends at each state

- The mean reaction rate can be calculated from the PDF as:

$$\overline{\dot{w}_k} = \int_0^\infty \int_0^1 \cdots \int_0^1 \dot{w}_k \, P \, dY_N \ldots dY_1 \, dT$$

  - PDF transport equation has very high dimensionality and cannot be solved using the finite-volume method. Instead, a Monte Carlo approach is used to solve the PDF transport equation.

In-Situ Adaptive Tabulation (ISAT) Algorithm

- Motivation
  - When using detailed chemistry models (EDC, Composition PDF, laminar finite rate), the stiff reaction system (a set of ODE's) is solved for each cell (or for each particle) at every iteration.
  - Table look-up method is effective, but the traditional prior tabulation approach is not feasible for a system with a large number of species; moreover, it is inefficient since only a small part of the composition space is accessed during a simulation.
  - We need an efficient way of generating data for only the range of interest in our simulation.
- In-situ adaptive tabulation (ISAT) is a method that can speed up table generation and lookup of reaction data.
  - Instead, the table is built on an as-needed basis.
  - Tabulation error is controlled adaptively via a user-specified tolerance.
- Advantage
  - Avoidance of repeated numerical integration significantly reduces CPU time.
  - Initial iterations are slower (as the table is being built) but accelerate as more retrieval operations take place.
- Application
  - ISAT can be used with PDF-transport, EDC, and laminar finite-rate models

NO_x Models

- NO_x consists primarily of nitric oxide (NO) which is harmful to the environment.
- FLUENT contains three mechanisms for calculating NO_x production.
  - Thermal NO_x
    - Most significant at high temperatures
  - Prompt NO_x
    - Contribution is generally small.
    - Prompt NO_x is significant in fuel rich regions.
  - Fuel NO_x
    - Predominant in coal flames where fuel-bound Nitrogen is high and temperature is generally low.
  - User-defined function
- NO_x reburn chemistry
  - NO can be reduced in fuel-rich zones by reaction with hydrocarbons.
- Selective Non-Catalytic Reduction (SNCR) models exist in FLUENT.
- These models provide qualitative trends of NO_x formation.

Soot Formation Models

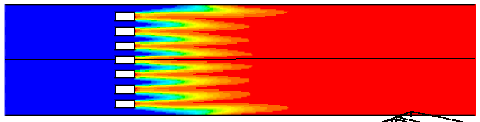
- Soot formation models available in FLUENT:
  - One-step model
    - Single transport equation for soot mass fraction
  - Two-Step model
    - Transport equations for radical nuclei and soot mass fraction concentrations
  - User-defined function
- Soot formation modeled by empirical rate constants

$$\overline{R}_{\text{formation}} = C\, P_f\, \Phi^n\, e^{-\frac{E}{RT}}$$

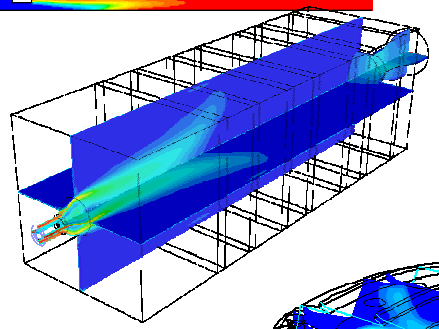
  - C, P_f, and Φ are a model constant, fuel partial pressure and equivalence ratio, respectively
- Soot combustion (destruction) modeled using the Magnussen model
- Soot affects the radiation absorption (Enable the Soot-Radiation option in the Soot panel).

Case Studies

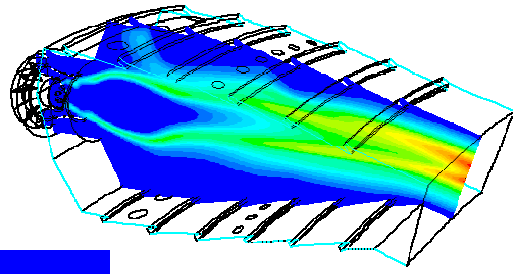
- Lean, Premixed Flame
  - Eddy Dissipation Concept
  - PDF transport
  - Laminar finite-rate



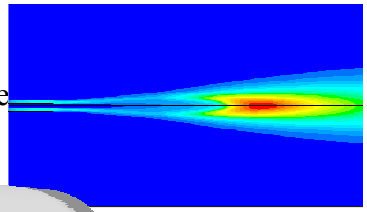
- IFRF Swirling Pulverized Coal Flame
  - Detailed chemistry
  - DPM
  - Radiation



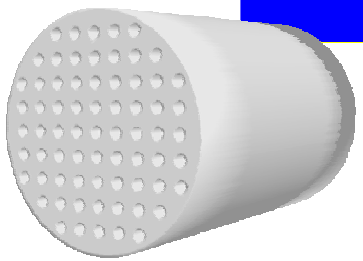
- GE LM-1600 Gas Turbine Combustor
  - Non-Premixed, laminar flamelet
  - Thermal and fuel NO_x prediction



- Sandia Flame D
  - Non-premixed turbulent diffusion flame
  - EDC / PDF transport comparison

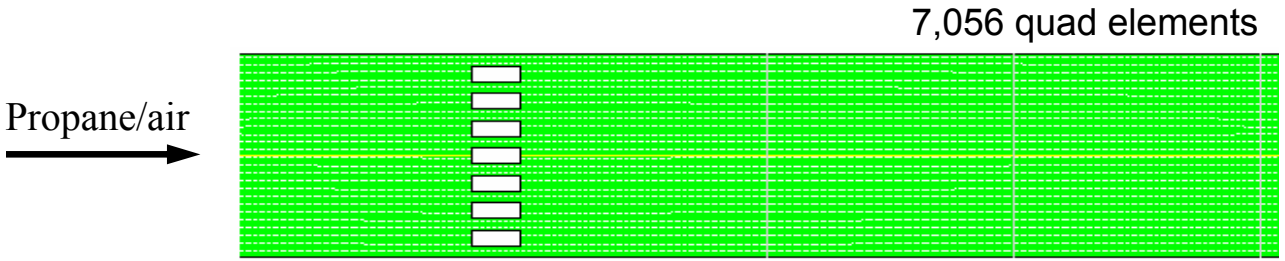


- Catalytic combustion
  - Surface reaction
  - Porous media



Case Study: Lean Premixed Flame

- Lean premixed pre-vaporized (LPP) propane/air flame
  - Reduction of the emissions of combustion pollutants (CO and NO_x)
  - Measurement of CO and NO_x emissions*
- Axisymmetric flame tube
  - Geometry d = 10.25 cm, L = 42.92 cm
  - Propane/air mixture V = 25 m/s, T = 800 K
  - Flame holder 51% open area



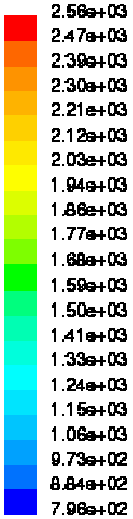
* D.N. Anderson, NASA Lewis Research Center, NASA-TM-X-71592, March 1975.

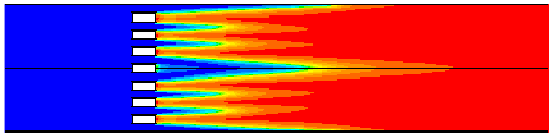
Lean Premixed Flame (cont'd)

- Weak turbulence-chemistry interaction
  - Perfectly premixed
  - Thin flame zone
  - Chemical reactions occur right behind the flame front
- Propane detailed chemical mechanism
  - Kundu mechanism with NO and N_2O formation*
    - 17 species and 23 step reactions
- Finite-rate chemistry combustion models
  - Laminar finite-rate model
    - Fully ignoring turbulence-chemistry interactions
  - EDC model
    - Might lead to under-prediction of NO_x formation – the reaction occurs quickly and NO_x has less time to accumulate.
  - Composition PDF transport
    - Accurately capturing the turbulence-chemistry interaction

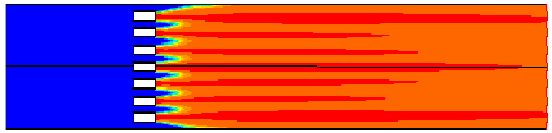
* K.P. Kundu et al., NASA Lewis Research Center, AIAA Paper No. 98-3986, July 1998

Lean Premixed Flame – Temperature Contours

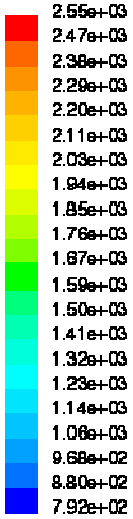


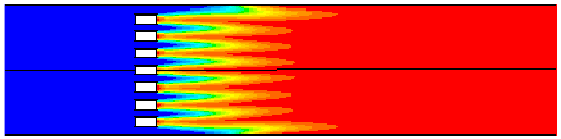


EDC model



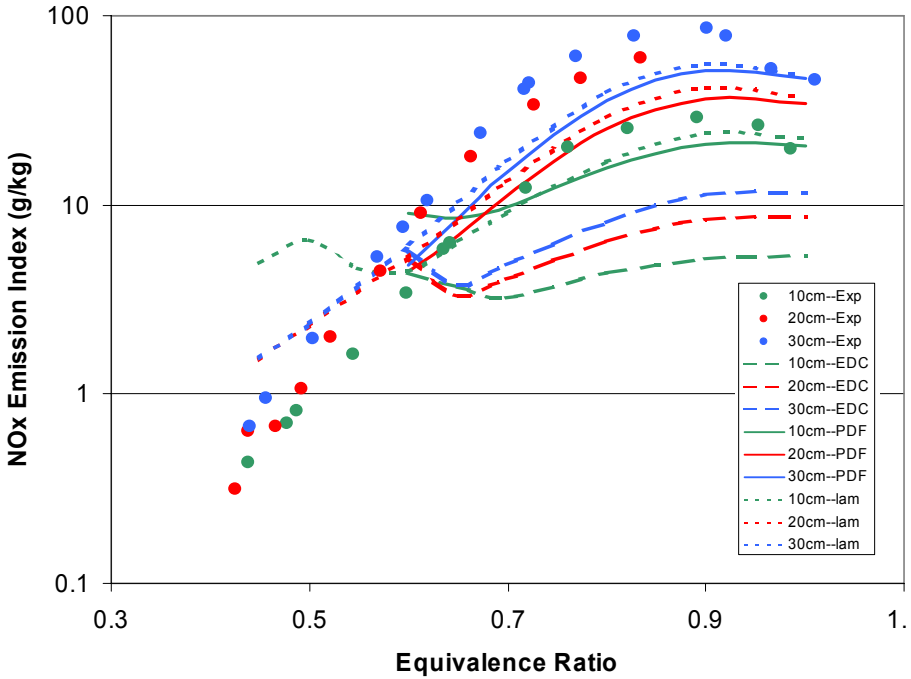
Laminar Finite-Rate Model

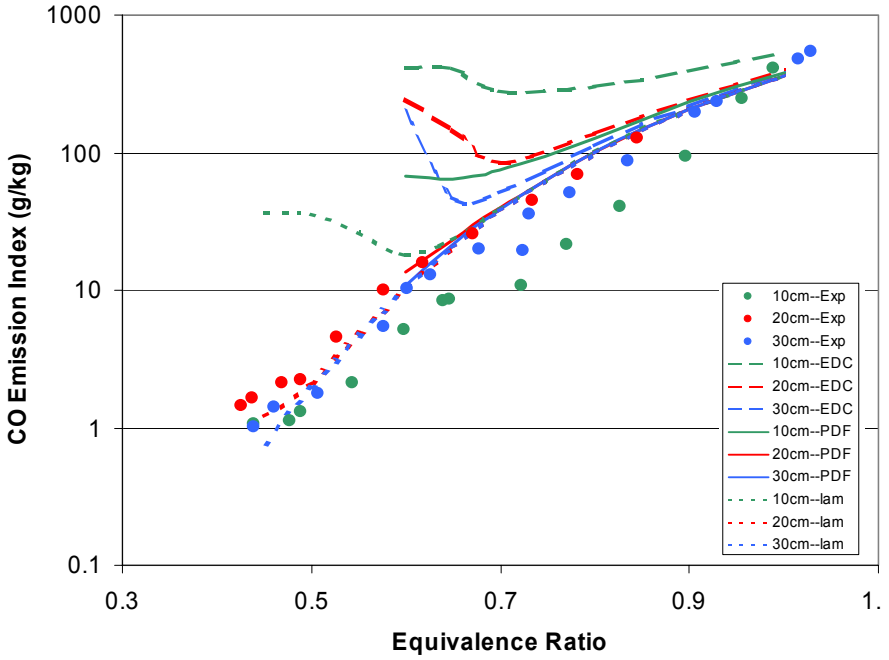




PDF model

Lean Premixed Flame (cont'd)

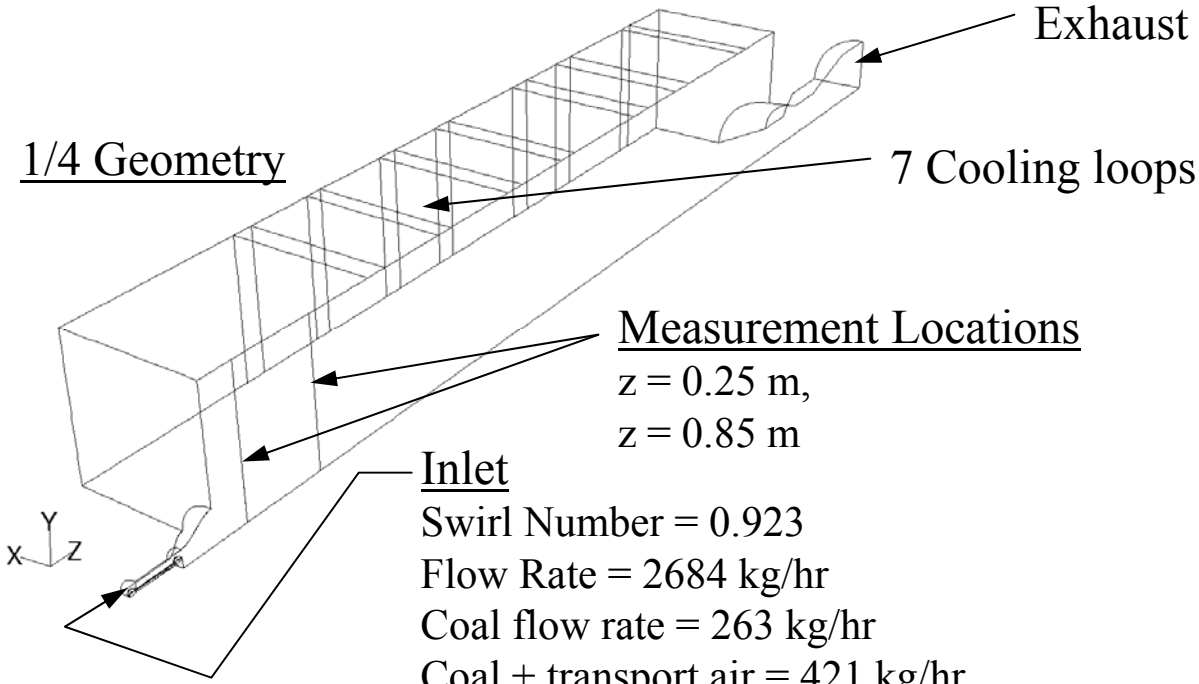




$$\text{Emission Index} = \frac{\dot{m}_{\text{pollutant}}}{\dot{m}_{\text{fuel}}}$$

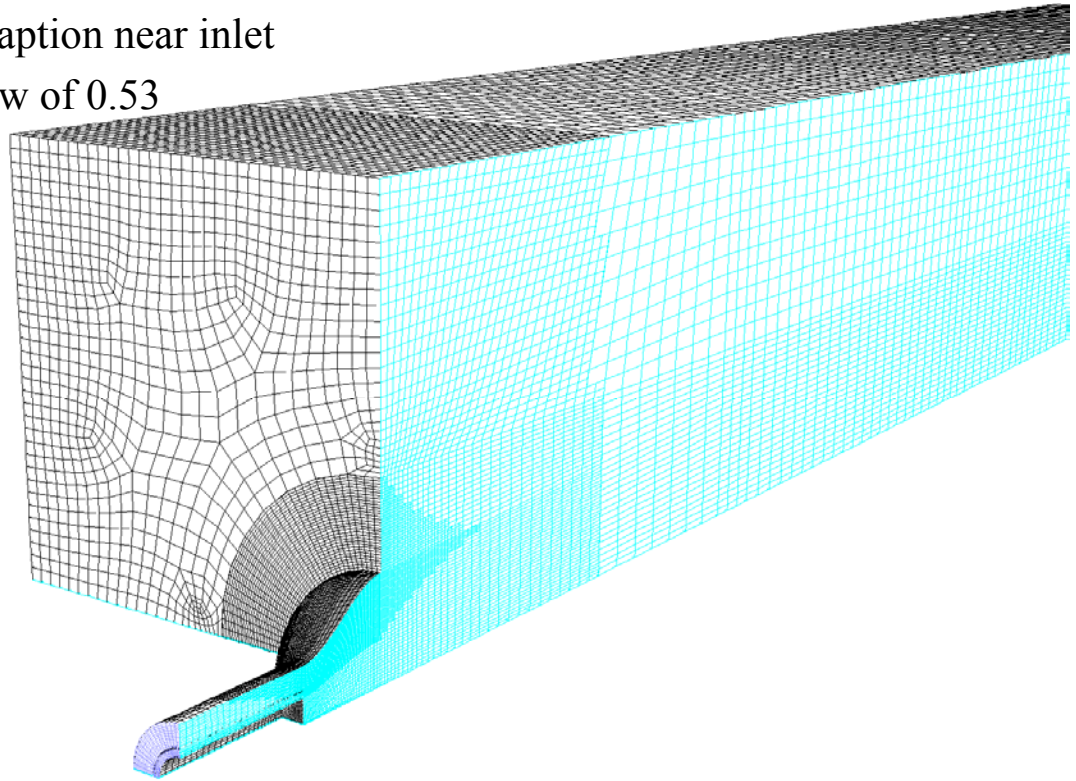
IFRF Swirling Pulverized Coal Flame

- IFRF industrial scale furnace
- Built on simulation by Peters and Weber (1997), "Mathematical Modeling of a 2.4 MW Swirling Pulverized Coal Flame," Combustion Science and Technology, **122**, 131 [Ref. 1]

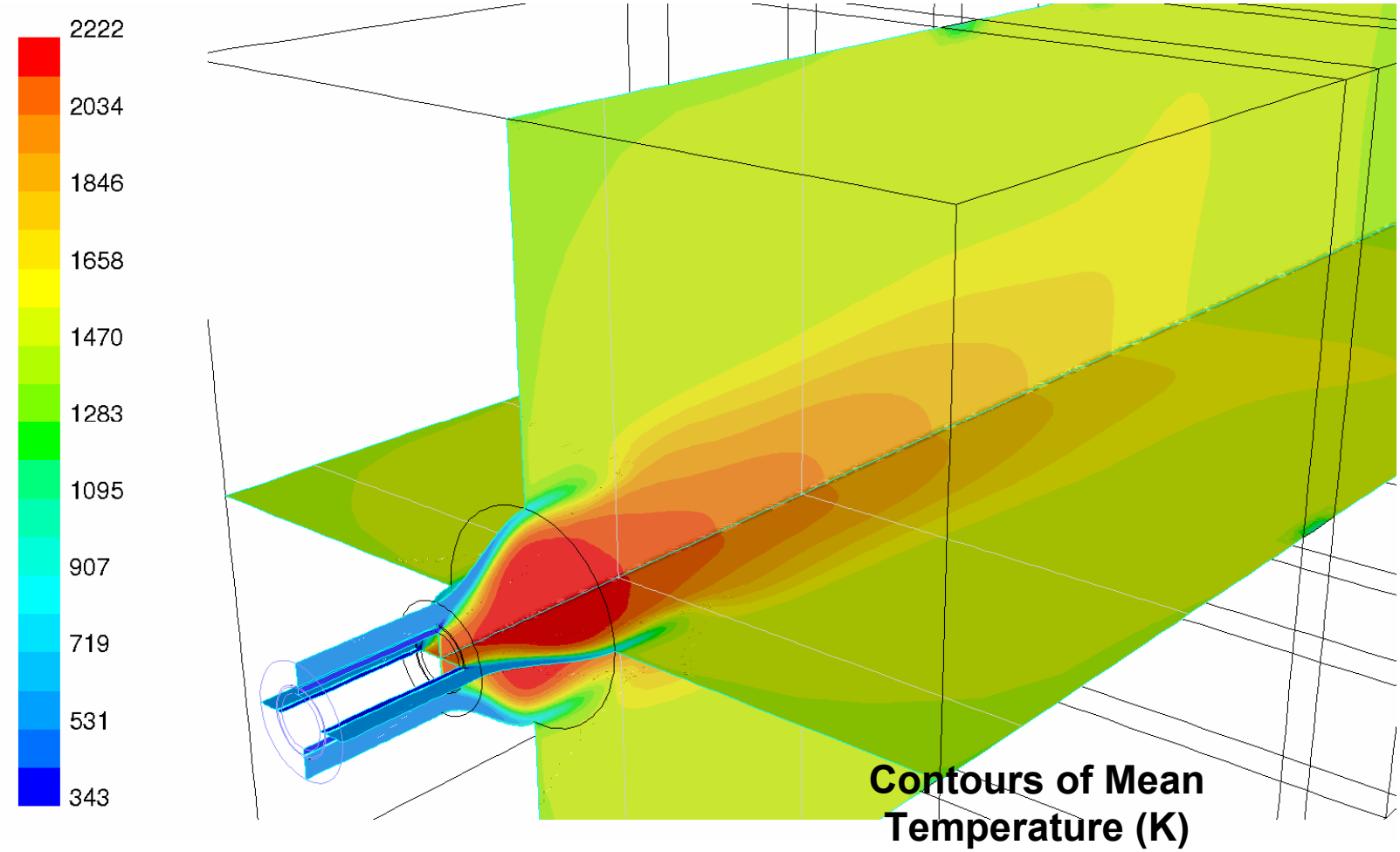


Grid

- 3D, one quarter geometry model due to periodicity
- Unstructured hexahedral mesh
  - 70k cells before adaption
  - 260k cells after region adaption near inlet
  - Maximum equi-angle skew of 0.53



Gas Phase Combustion Modeling (2)

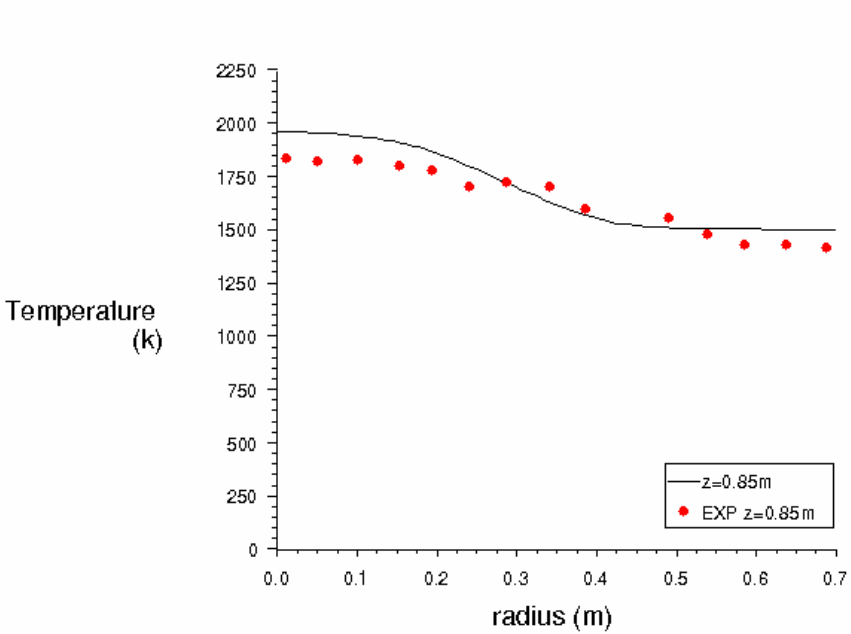


Discrete Phase Modeling (1)

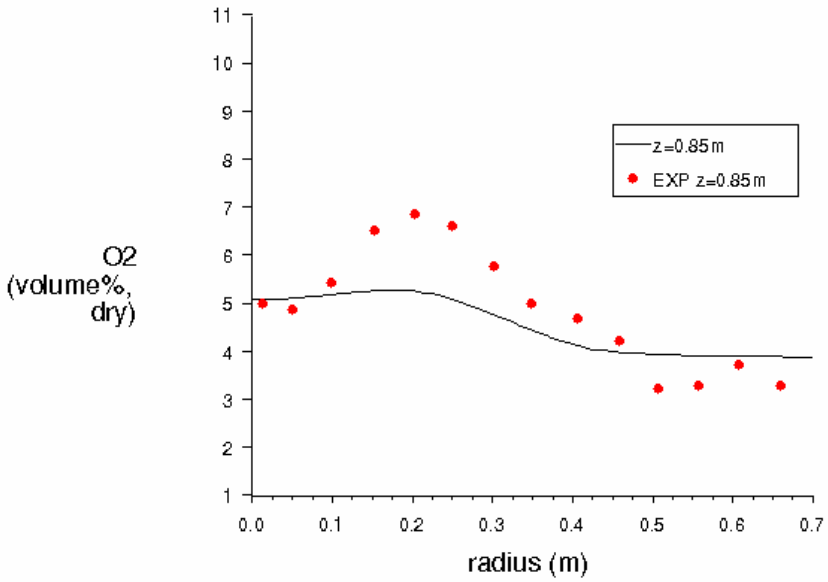
- Gottelborn hvBb coal
  - Proximate (weight %, dry)
    - Volatiles 55.0, Fixed Carbon 36.7, Ash 8.3
  - Ultimate (weight %, daf)
    - 80.36 C, 5.08 H, 1.45 N, 0.94 S, 12.17 O.
  - Lower Calorific Value (LCV, MJ/kg daf)
    - Volatiles 32.3, Char 32.9
- Rosin-Rammler size distribution
  - Smallest 1 μm, Largest 300 μm, Mean 45 μm, Spread 1.36
- Single rate devolatization model
  - $A = 2 \times 10^5\ s^{-1}$
  - $E = 7.4 \times 10^7$ J/kmol
- Kinetics/diffusion-limited surface (char) combustion
- Discrete Random Walk (DRW) model
  - 21600 tracks per DPM iteration, 10 particle sizes
  - 25 gas phase iterations per DPM iteration

Results Temperature/Species Field

- Mean Temperature (K)

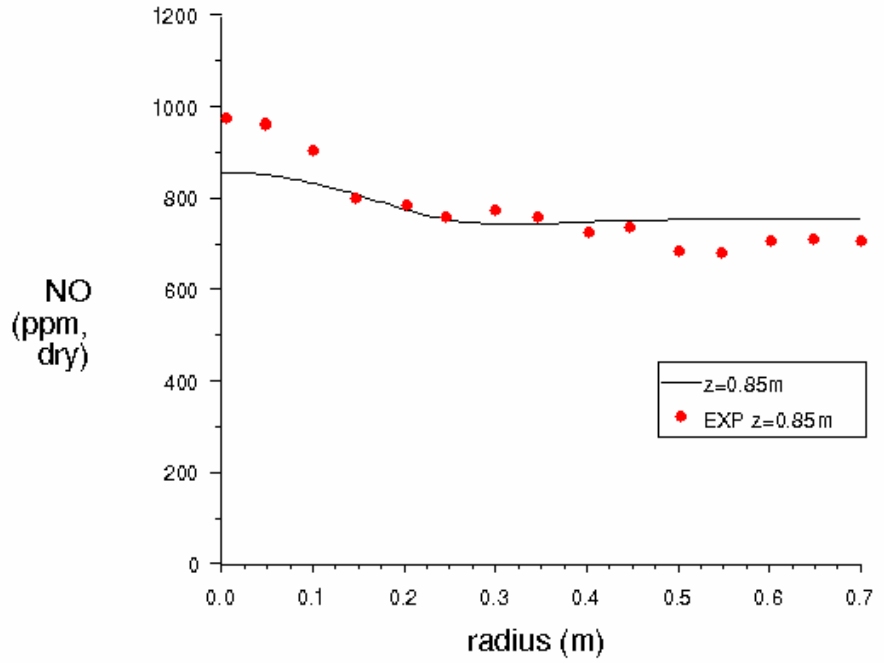


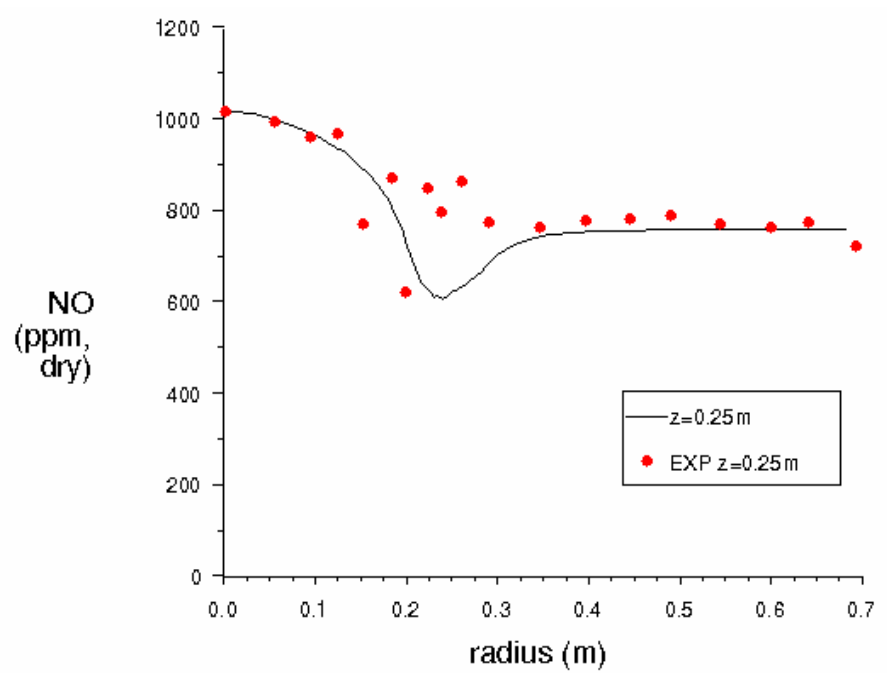
- Mean O_2 (Vol. %, dry).



Results NO_x Field

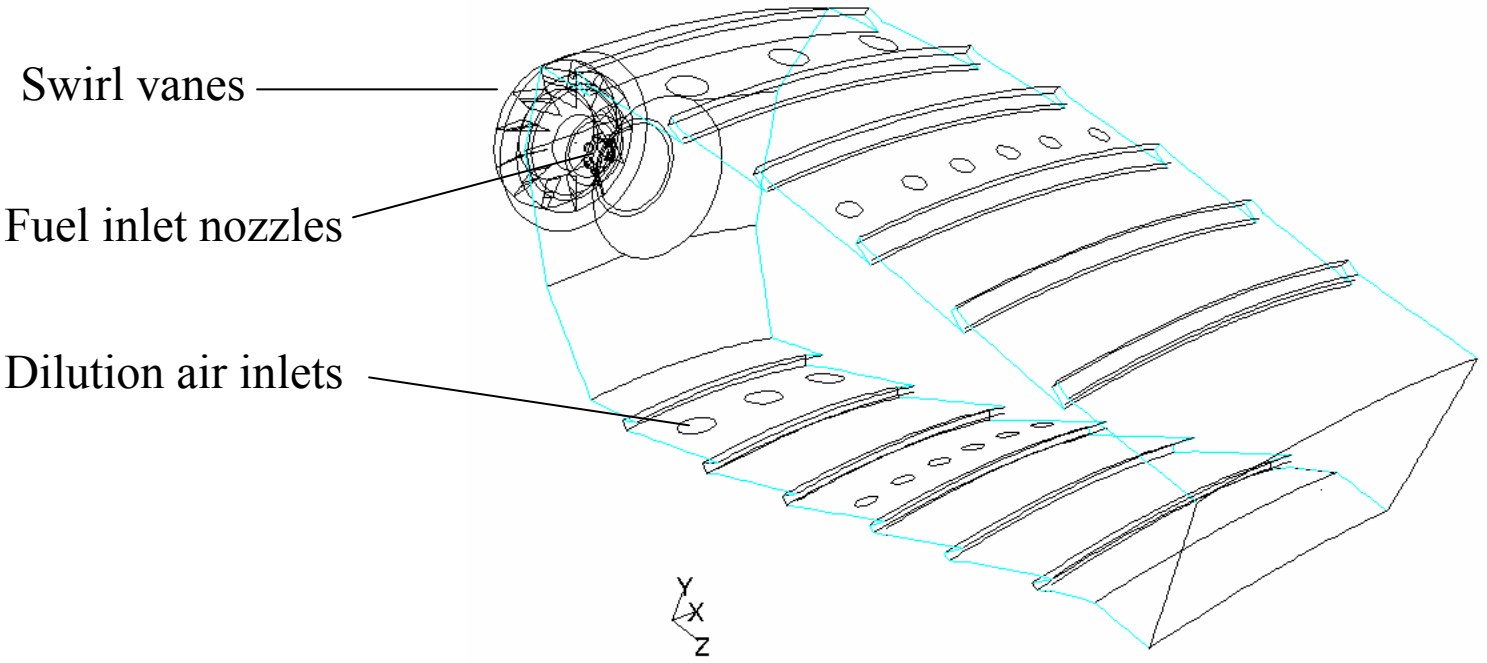
- Mean NO (ppm, dry)



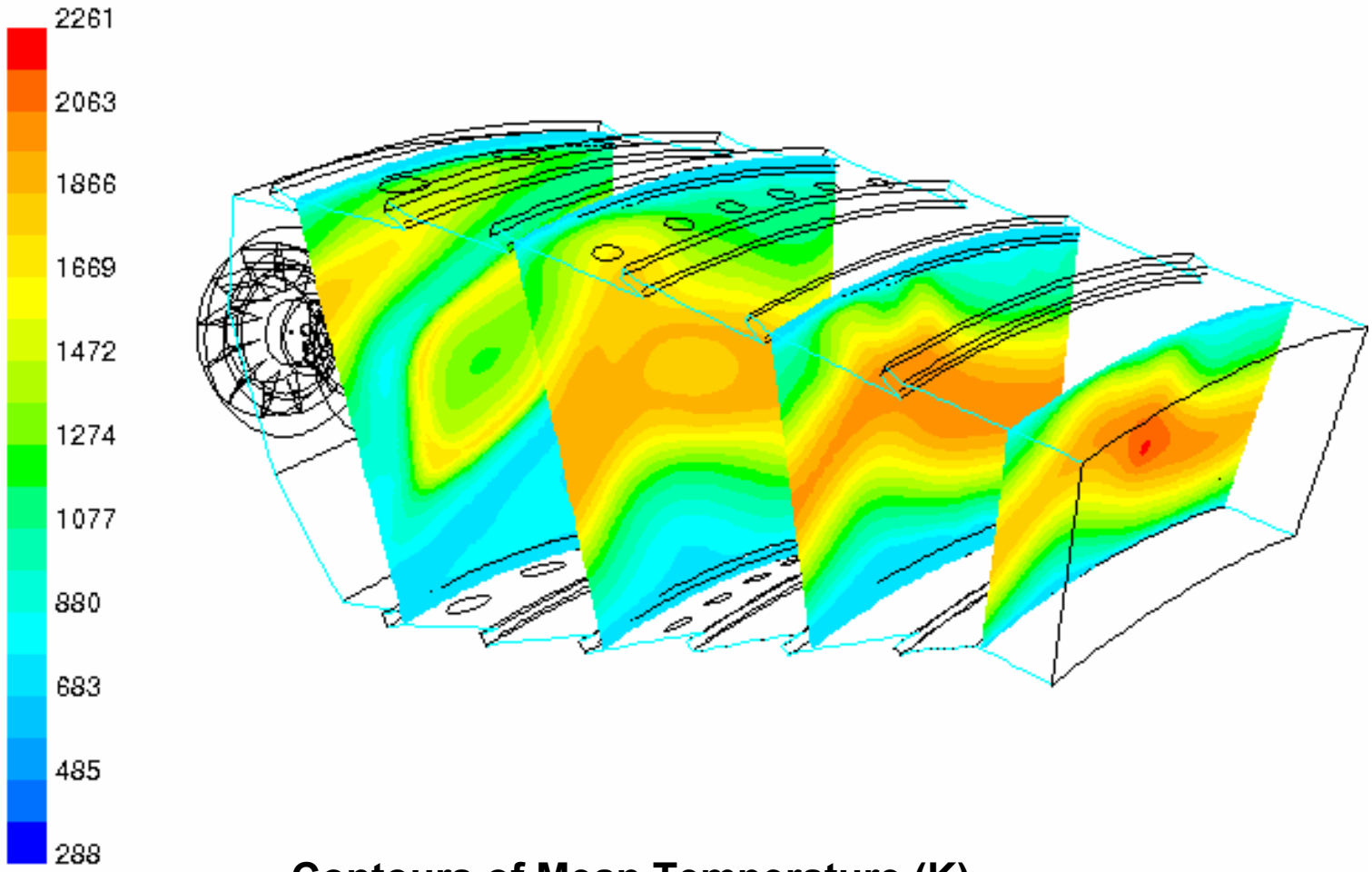


GE LM-1600 Gas Turbine Combustor

- Courtesy Nova Research and Technology Corp., Calgary, Canada
- Non-premixed, natural gas
- 12.8 MW, 19:1 pressure ratio (full load)
- Annular combustion chamber, 18 nozzles



Gas Phase Combustion Modeling (3)

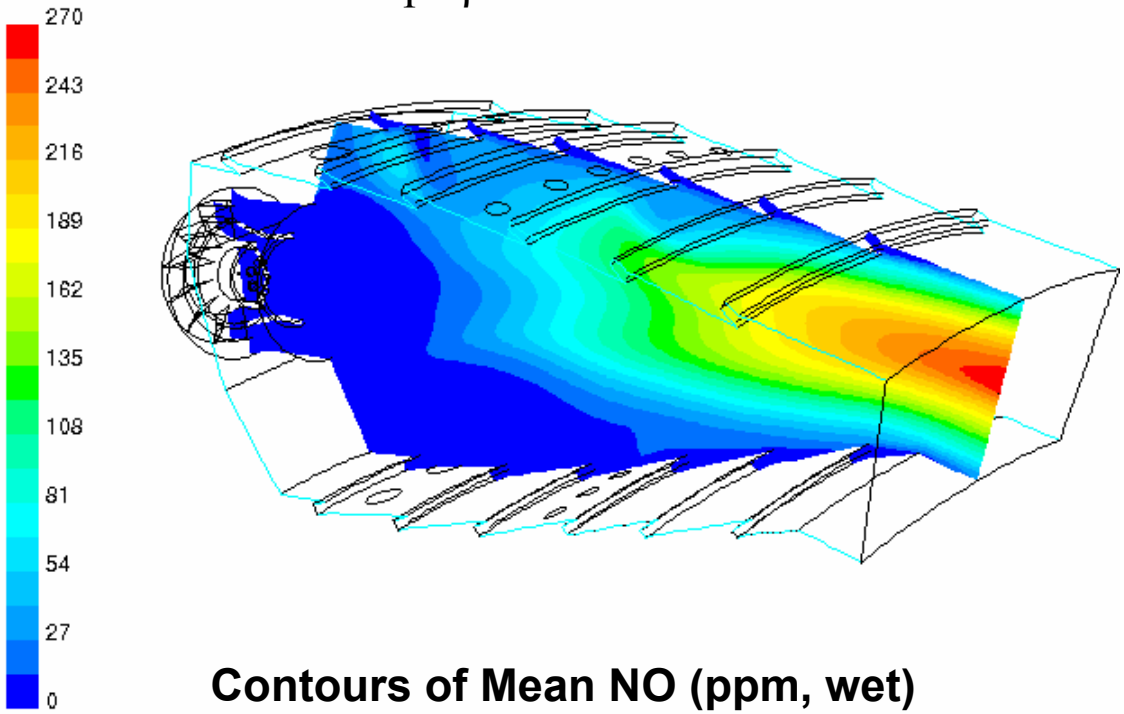


Contours of Mean Temperature (K)

NO_x Modeling (1)

- Thermal and fuel NO_x
  - Zeldovich thermal NO dominant
- [O] from partial equilibrium assumption
- Post-processed: Assumed shape β-PDF.

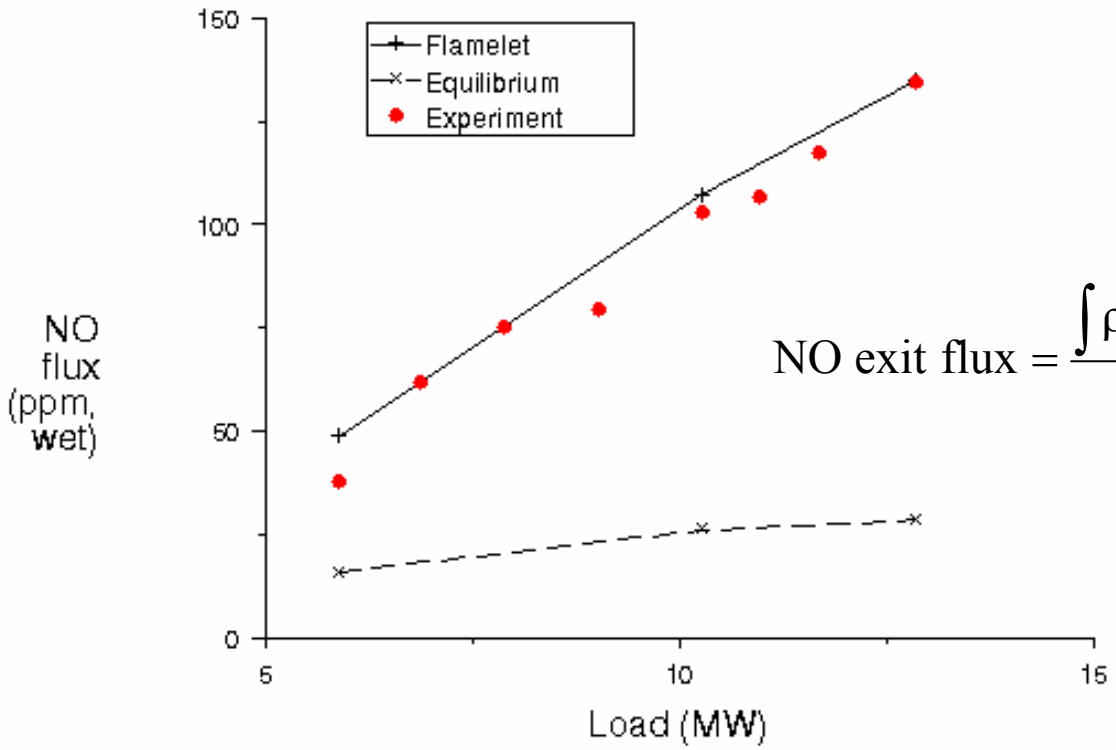
$$\frac{d[\mathrm{NO}]}{dt} = 2Ae^{-E/RT}[\mathrm{O}][\mathrm{N}_2]$$



Contours of Mean NO (ppm, wet)

NO_x Modeling

- Plot of NO flux exiting outlet vs. combustor load

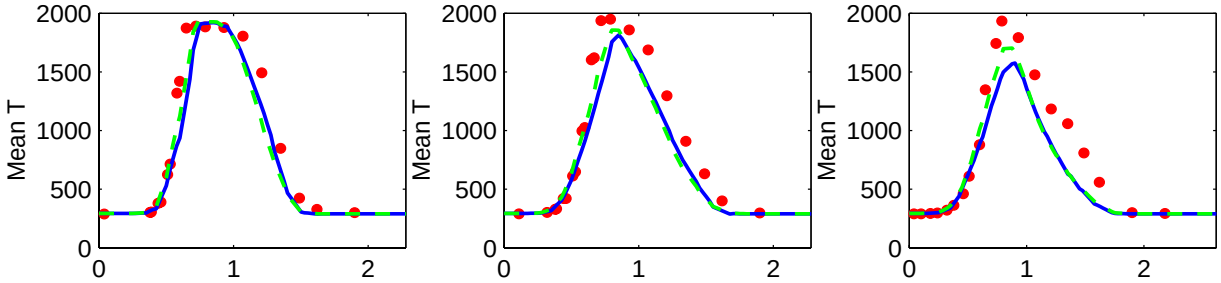


$$\text{NO exit flux} = \frac{\int \rho X_{NO} \mathbf{V} \cdot d\mathbf{A}}{\int \rho \mathbf{V} \cdot d\mathbf{A}} \times 10^6$$

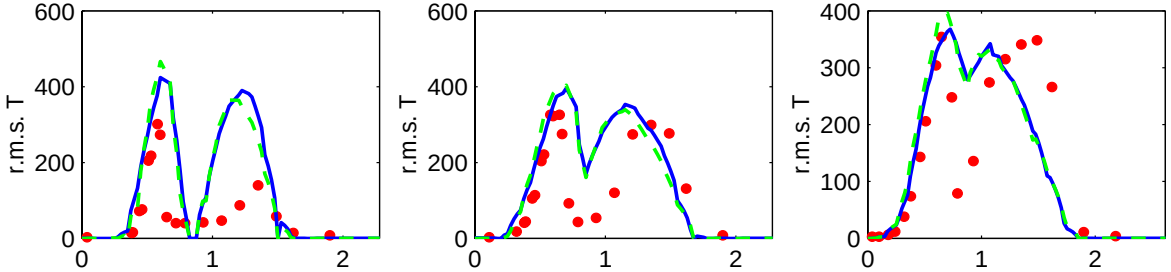
Sandia Flame D - PDF Transport

- Experiment
  - Non-premixed methane, piloted, turbulent diffusion flame
  - Sandia Flame D
- Geometry
  - Axisymmetric grid with 2352 quad cells
- Turbulence
  - Standard k–ε with $C_{\varepsilon 1} = 1.52$, $Sc_T = 1.0$ (Pope correction)
- Mixing
  - IEM and Modified Curl with $C_{\varphi} = 2$
- Chemistry
  - 16 species skeletal mechanism

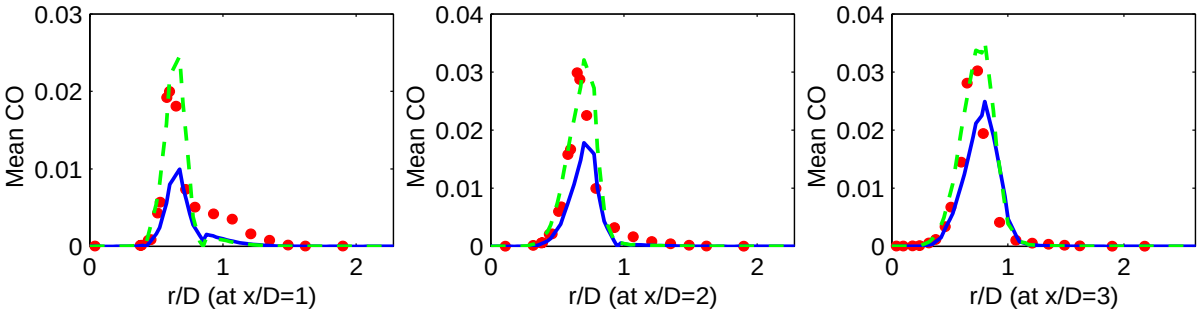
Mean Temperature



RMS Temperature



Mean CO

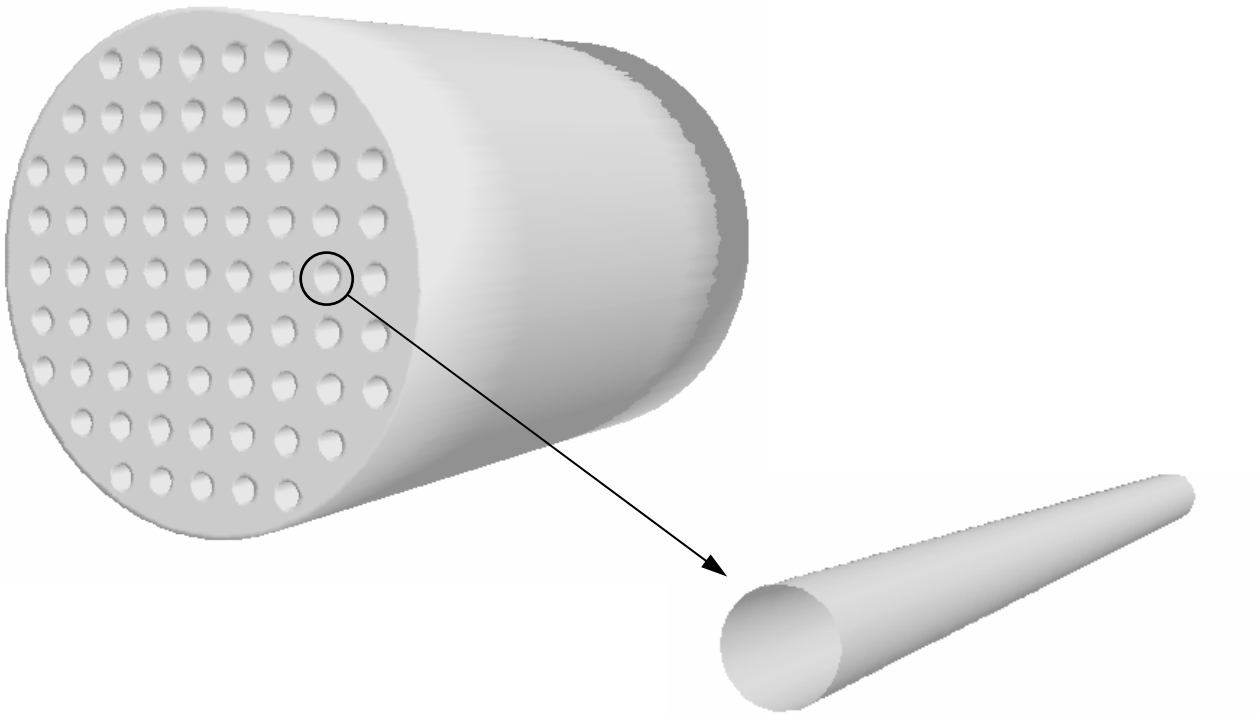


Red symbol: Experiment, Blue solid line: Modified Curl, Green dashed line: IEM

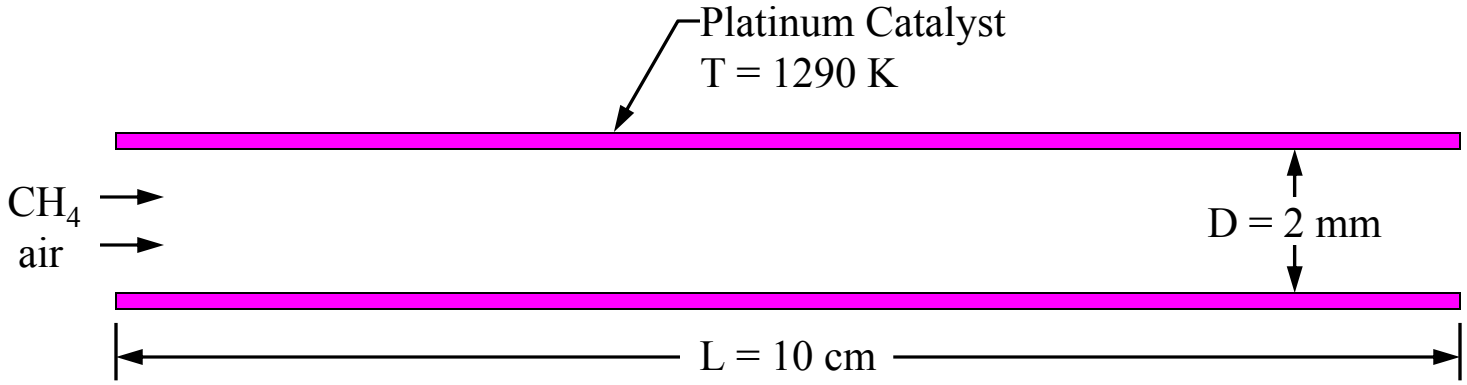
Case Studies: Catalytic combustion

- Single channel modeling:
  - Reaction is occurring at the wall
  - 2d axisymmetric geometry
- Full monolith modeling:
  - The monolith is treated as porous media
  - Pressure drop and fluid acceleration is accounted for in the porous media
  - Reaction is occurring in the porous media (specifying a surface-volume ratio)
  - 2d axisymmetric geometry

Honeycomb Monolith Catalyst – Single Channel



Model Setup – Single Channel

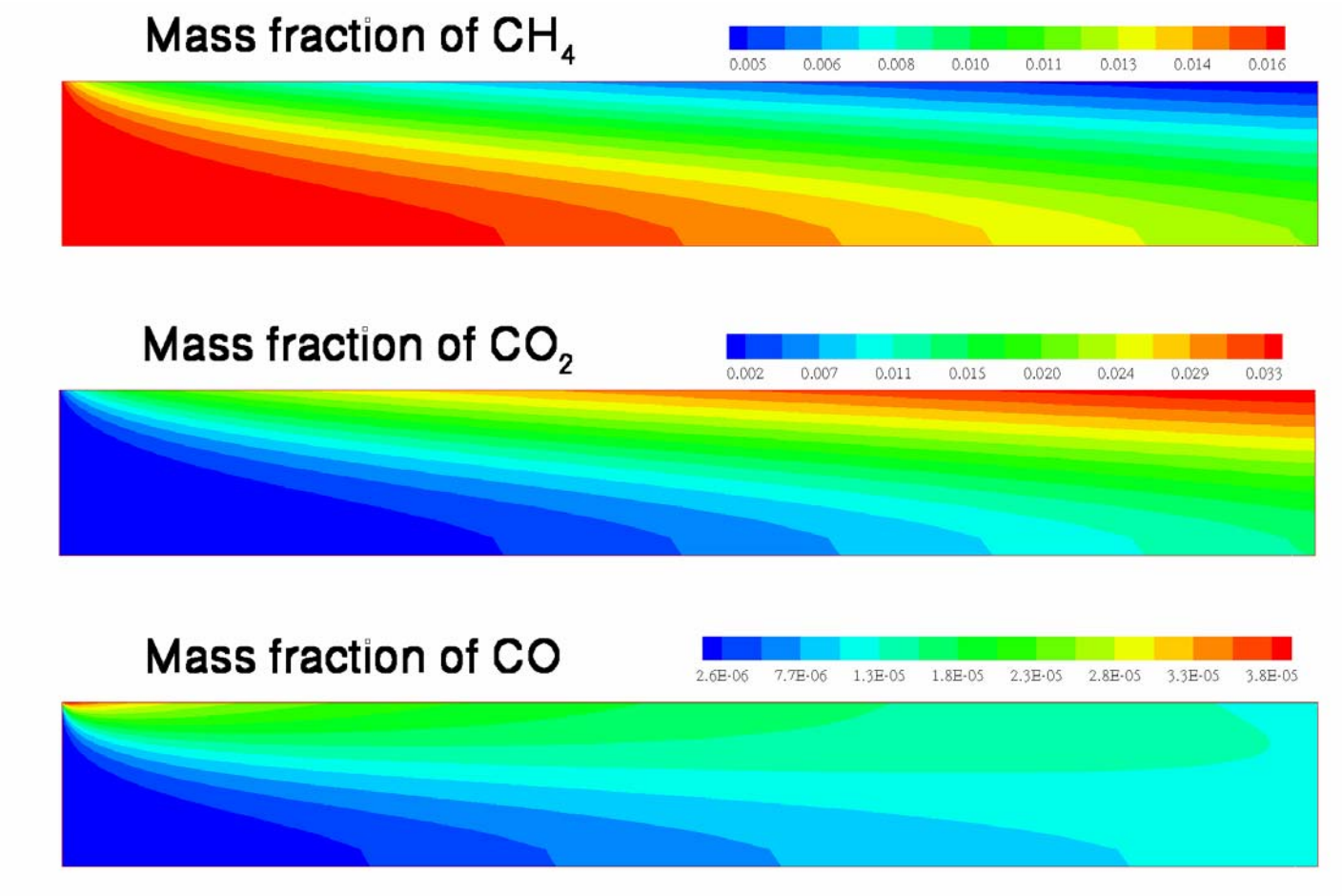


- Boundary Conditions:
  - Volume Fraction: 3% CH4
  - Inlet velocity: 5 m/s
  - Inlet temperature: 600 K
- Gas species:

  CH_4, O_2, H_2, H_2O, CO, CO_2, N_2, OH
- Surface species:

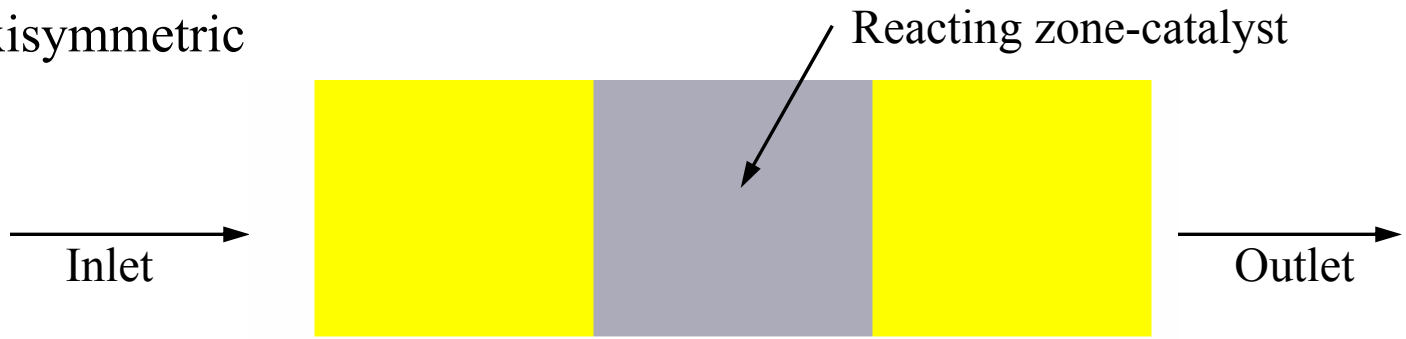
  Pt(s), H(s), O(s), OH(s), H_2O(s), H_3(s), CH_2(s), CH(s), C(s), CO(s), CO_2(s)

Contours of Mass Fraction of Major Gas Species

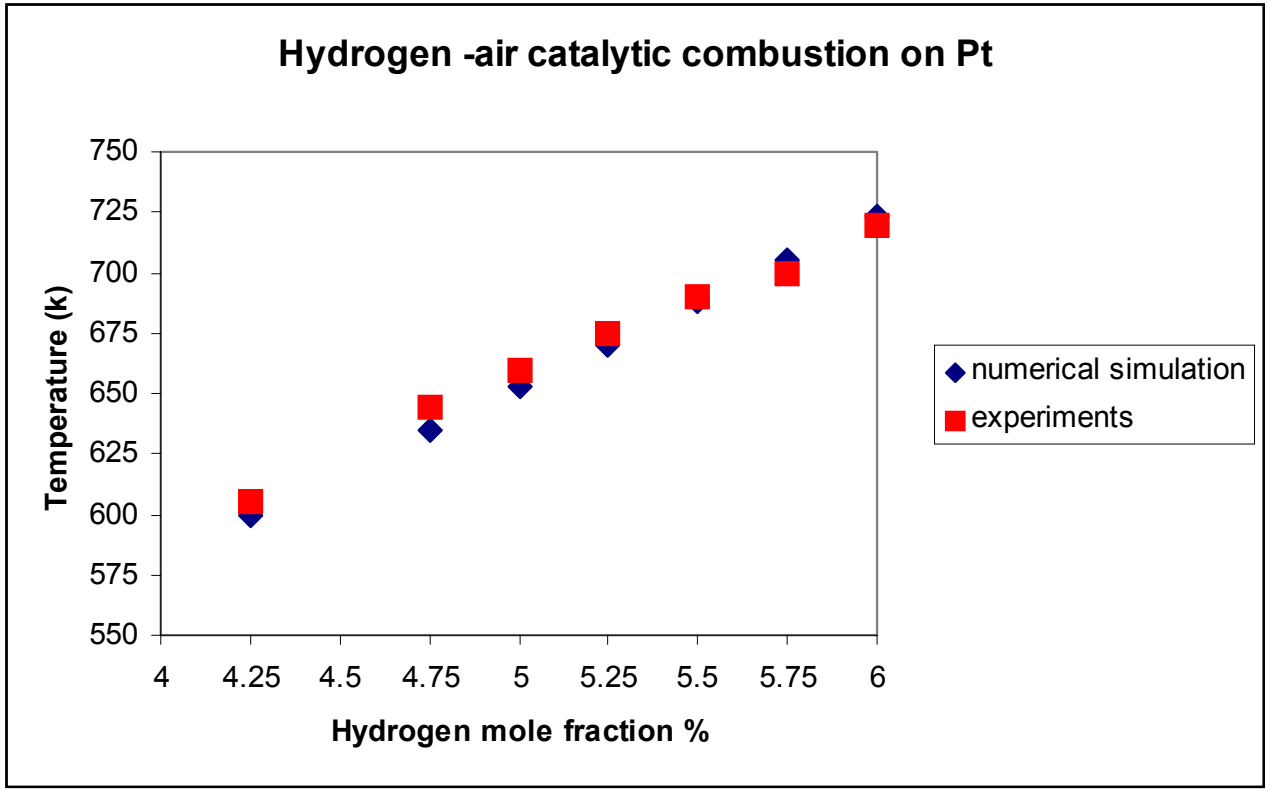


Surface Reactions in Porous Media (Multiple Channels)

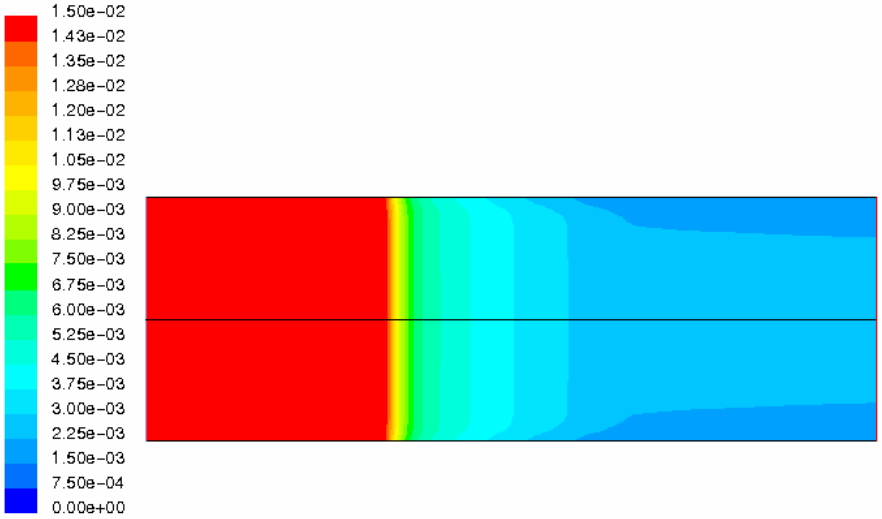
- H_2 / CH_4 catalytic combustion
- Boundary Conditions:
  - Inlet feed — Air / CH_4 / H_2 mixture
  - Inlet velocity — 0.8 m/s
  - Inlet temperature — 300K
- 10 gas species and 12 site species
- Adiabatic boundary conditions
- 2D axisymmetric



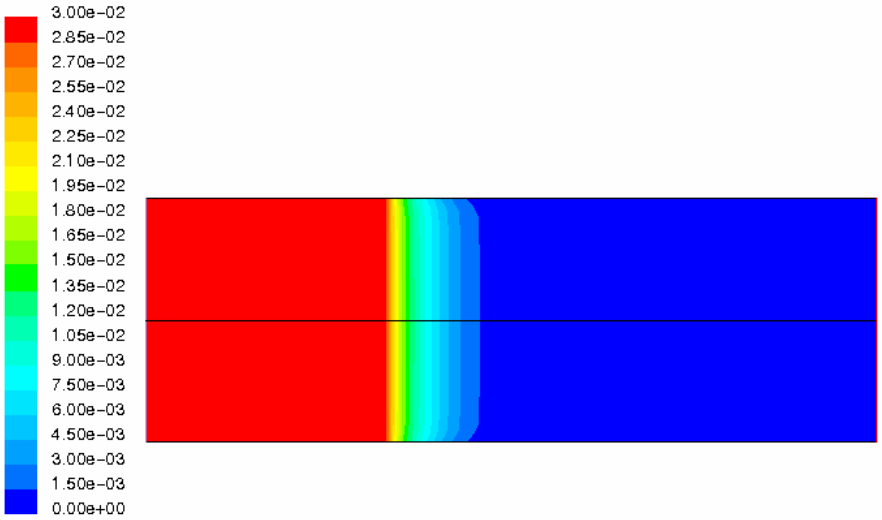
Temperature vs. Mole fraction



CH_4 Ignition Inlet – 6% Hydrogen Feed



Inlet methane feed 1.5 %
CH_4 mole fraction contour



Inlet methane feed 3.0 %
CH_4 mole fraction contour