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Multiprocessor simulations of turbulent diffusion flames

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Content

- Motivation and work objectives
- Experiment and problem statement
- Simulation results
  - Test simulations
  - Comparative analysis of physical models
  - Calculating efficiency of clusters and models
- Conclusions
- Future work

Introduction

- Motivation
  - Computational Combustion is the most difficult area of Computational Fluid Dynamics (CFD)
  - Tight interaction between phenomena of different nature: turbulence, combustion and radiation
  - Wide spectrum of engineering applications: furnaces, turbines, engines, fires
  - Powerful computational software (Ansys Fluent etc.) and multiprocessor computers

Introduction

- Primary aim

  Accurate modeling of real-life problems like fires and industrial combustors using reliable verified models

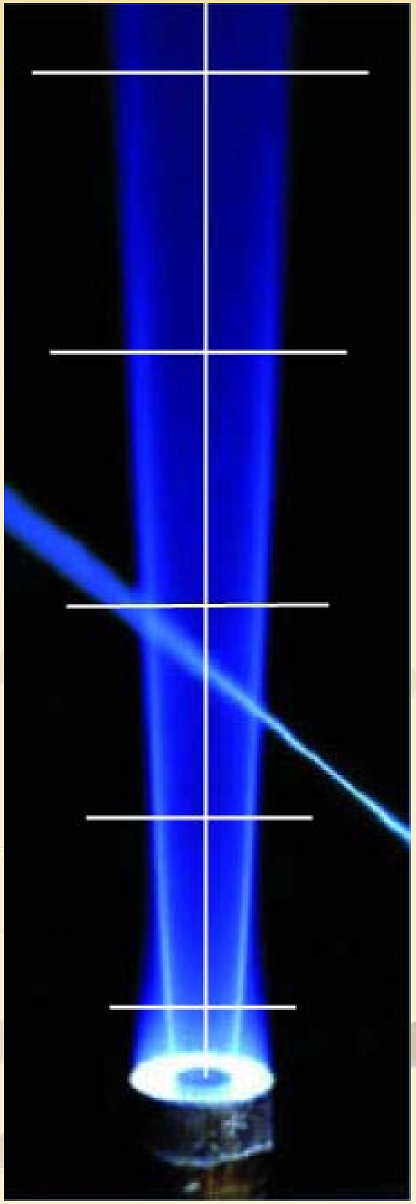
- Objectives
  - Pose model problem (test flame) with detailed statement and experimental data
  - Examine conventional engineering models
  - Research capabilities of advances chemistry models like slow chemistry and pollutant emissions
  - Research capabilities of large eddy simulation turbulence model

Problem description

- Object of research

  Sandia Flame D (*Sandia National Laboratories, CA, USA*)

- Experimental data
  - High-precision laser measurements
  - Mean and root-mean-square (RMS) profiles of temperature, velocity components, concentrations of 9 major species
  - Axial and 8 radial profiles



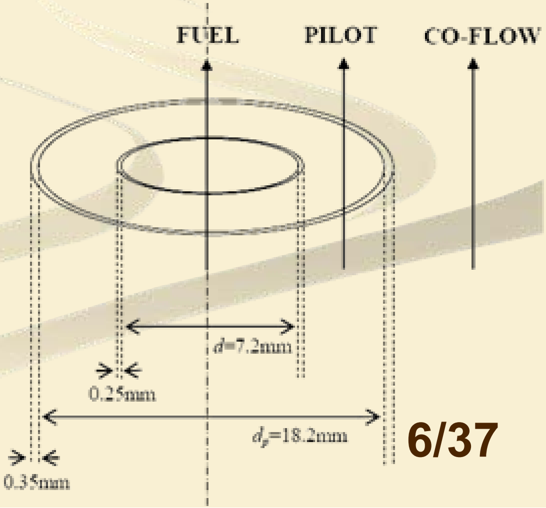
Problem description

Sandia Flame D

- Jet flame with pilot-stabilizer
- Premixed methane-air mixture
  - Highly reduced pollutant formation
  - Accurate experimental measurement
  - Avoiding flame extinction
- Fully developed turbulence

  Reynolds number, based on jet speed

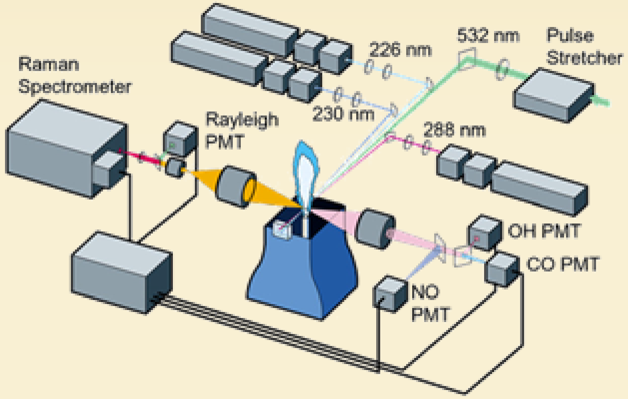
  Re=22400



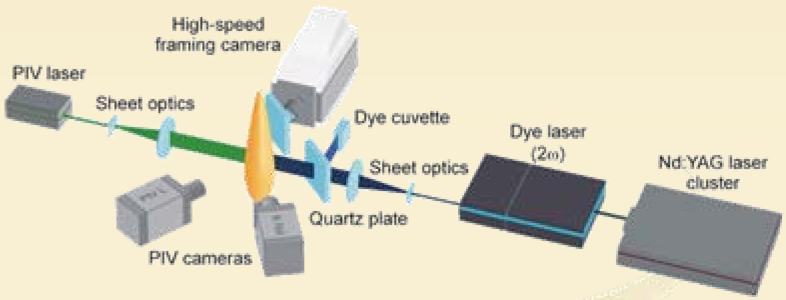
Problem description

High-precision laser measurements

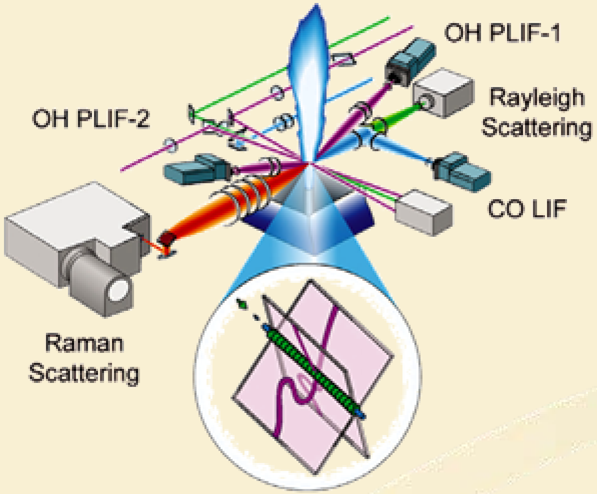
Raman spectrometry



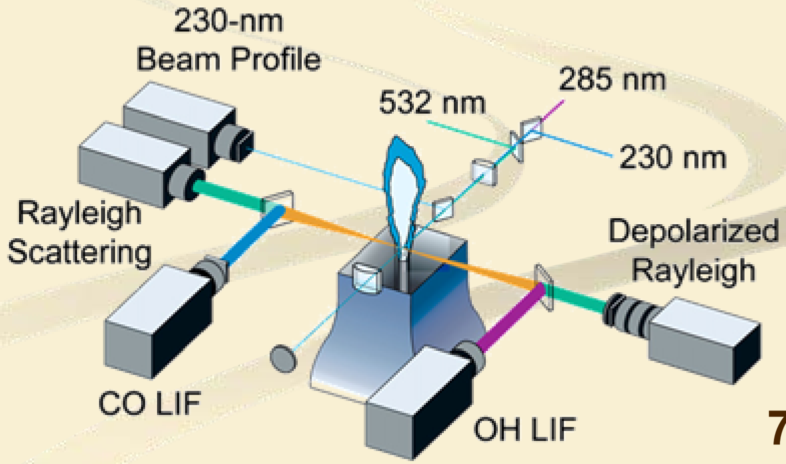
PIV measurements



LIF & PLIF spectrometry

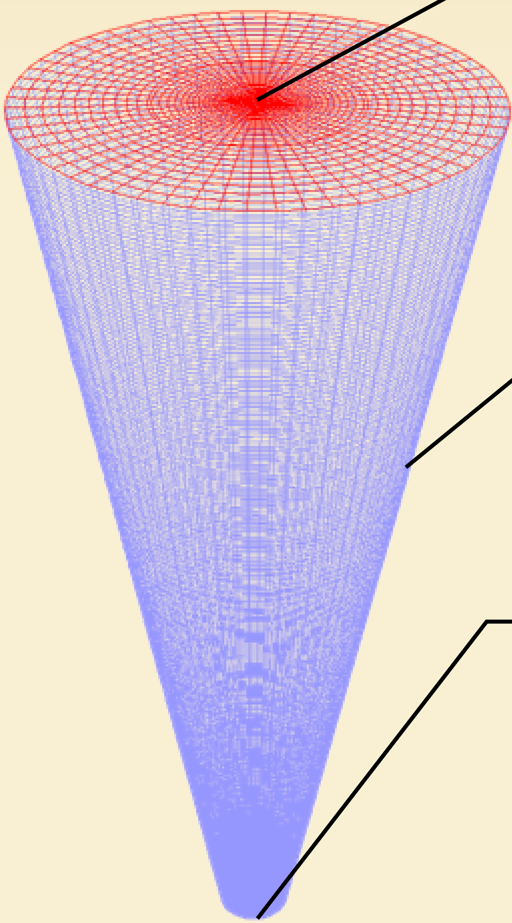


CO, OH LIF measurements



Problem statement

Problem domain and boundary conditions



Defined:
- Pressure
- Backflow parameters

Defined:
- Velocity
- Temperature
- Turbulence
- Mixture composition

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- Velocity
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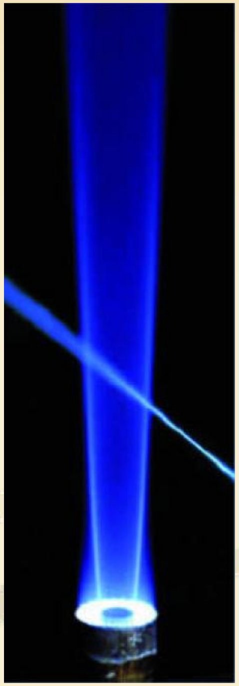

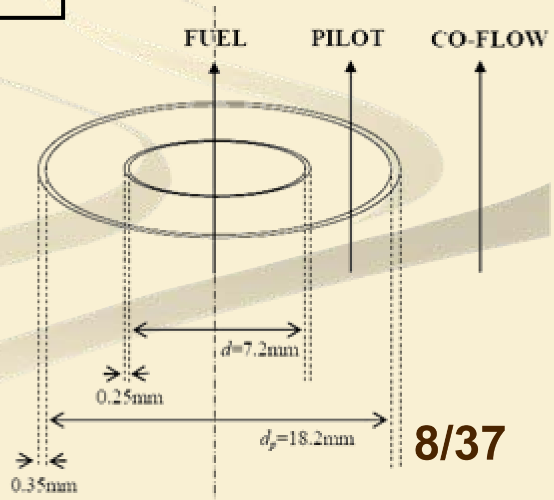

Mathematical model

Favre-average (filtered) Navier-Stokes equations for multicomponent reacting medium

Continuity equation:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j} = 0$$

Momentum transport equation:

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{u}_i}{\partial x_j} = -\frac{\partial \bar{\rho}\widetilde{u''_j u''_i}}{\partial x_j} - \frac{\partial \bar{P}}{\partial x_j} - \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \bar{\rho} g_i$$

Species transport equation:

$$\frac{\partial \bar{\rho}\tilde{Y}_\alpha}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{Y}_\alpha}{\partial x_j} = -\frac{\partial \bar{\rho}\widetilde{u''_j Y''_\alpha}}{\partial x_j} - \frac{\partial \bar{F}_{j,\alpha}}{\partial x_j} + \overline{\dot{r}_\alpha}$$

Enthalpy transport equation:

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{h}}{\partial x_j} = \frac{\partial \bar{P}}{\partial t} - \frac{\partial \bar{\rho}\widetilde{u''_j h''}}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\bar{F}_{j,h} + \overline{u_i \tau_{ij}}\right) - \frac{\partial \overline{q_j^r}}{\partial x_j} + \overline{\rho u_i g_i}$$

RANS Turbulence models:

- k-ε Standard
- k-ε RNG
- k-ε Realizable
- k-ω Standard
- k-ω SST
- RSM Linear
- RSM Quadratic
- RSM Low Reynolds

LES Smagorinsky

Mathematical model

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Species transport equation:

$$\frac{\partial \bar{\rho}\tilde{Y}_\alpha}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{Y}_\alpha}{\partial x_j} = -\frac{\partial \bar{\rho}\widetilde{u''_j Y''_\alpha}}{\partial x_j} - \frac{\partial \bar{F}_{j,\alpha}}{\partial x_j} + \overline{\dot{r}_\alpha}$$

Enthalpy transport equation:

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Chemistry models:

- **Eddy Break-up model (*EBU*)**
- **Mixture fraction based statistical model (*PDF*)**

Radiation models:

- **Discrete transfer**
- **Discrete ordinates**

Mathematical model

Turbulence models

- Family of *k-ε* turbulence models

  Turbulent kinetic energy and its dissipation rate

- Family of *k-ω* turbulence models

  Turbulent kinetic energy and specific dissipation rate

- Family of Reynolds Stress models

  Six turbulent stresses separately

- Large Eddy Simulation model

  Subgrid turbulence models without additional equations

$$\frac{\partial \overline{\rho}(\cdot)}{\partial t} + \frac{\partial \overline{\rho}\tilde{u}_j(\cdot)}{\partial x_j} = \underbrace{\frac{\partial}{\partial x_j}(\ldots)}_{Diffusion} - \underbrace{(\ldots\ldots)}_{Production} - \underbrace{(\ldots\ldots)}_{Dissipation}$$

Mathematical model

Chemistry models

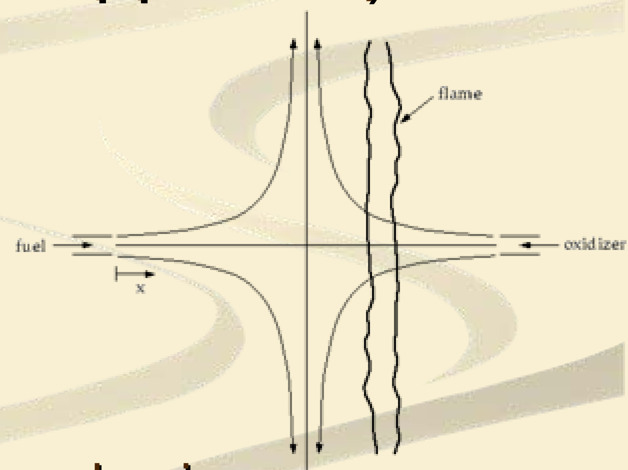
- Eddy Break-up model

  Fast chemistry assumption (infinitely fast reactions)

$$\tilde{\dot{r}}_\alpha = A\overline{\rho}\frac{\varepsilon}{k}\min\left(\tilde{Y}_{fuel}, \frac{\tilde{Y}_{ox}}{s_{ox}}, B\frac{\tilde{Y}_{prod}}{1+s_{ox}}\right)$$

- Statistical model (mixture fraction approach)
  - Equilibrium chemistry

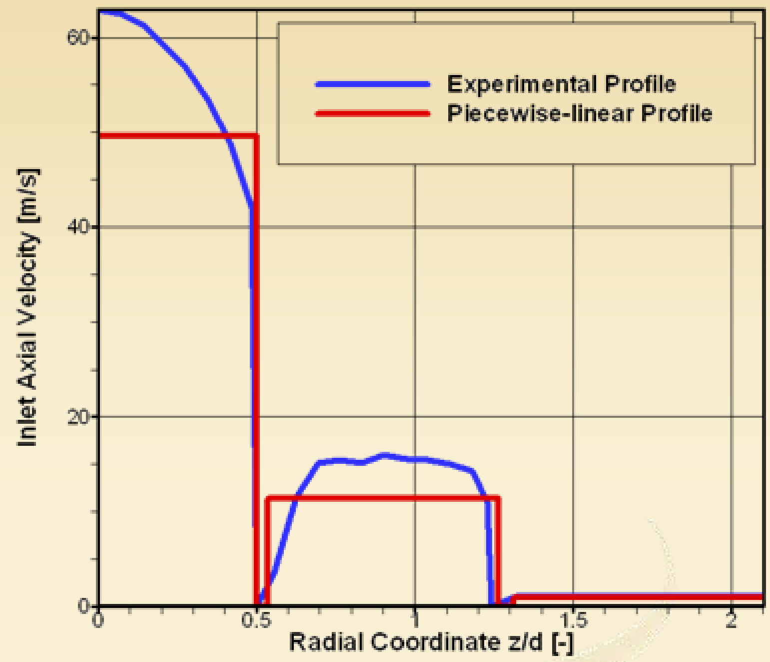
    Incapability of predicting slow chemistry
  - Flamelet models
    - Thin flame assumption
    - Large-scale curvature of flame
    - Capability of using detailed chemistry mechanisms

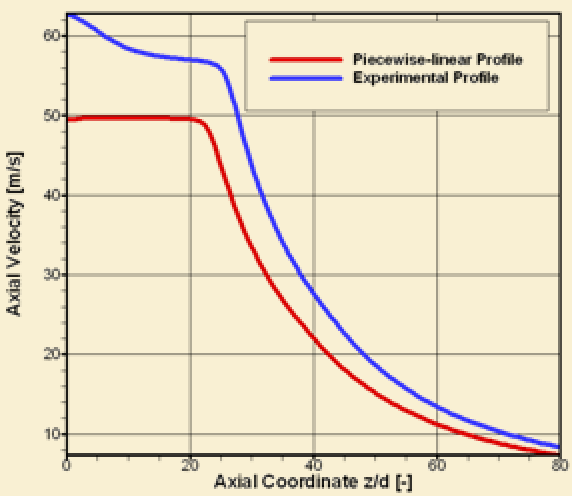


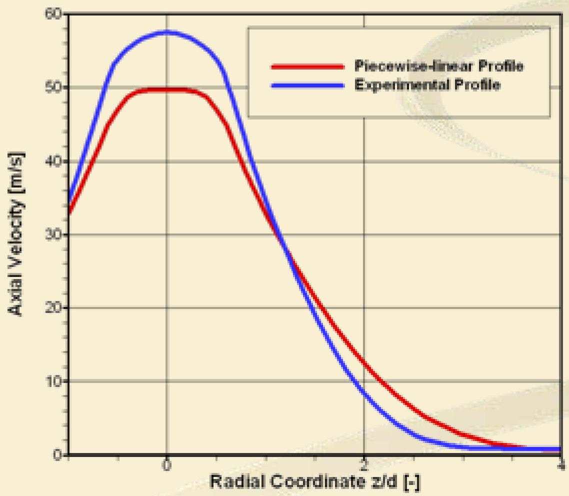
Test simulations

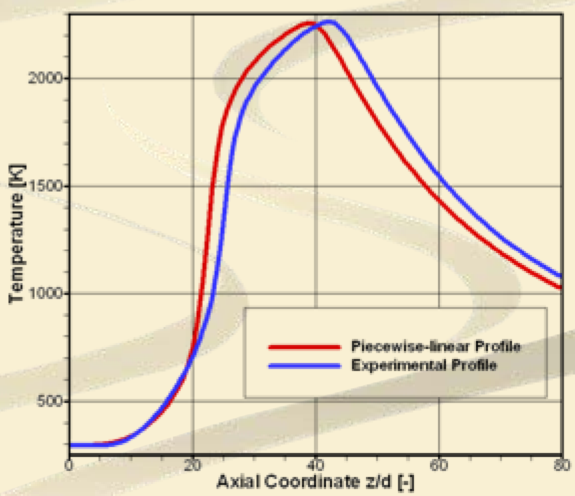
Inlet boundary profile impact

- Velocity experimental profile seriously affects the flame
- Scalar experimental boundary profile impact on the flame is negligible





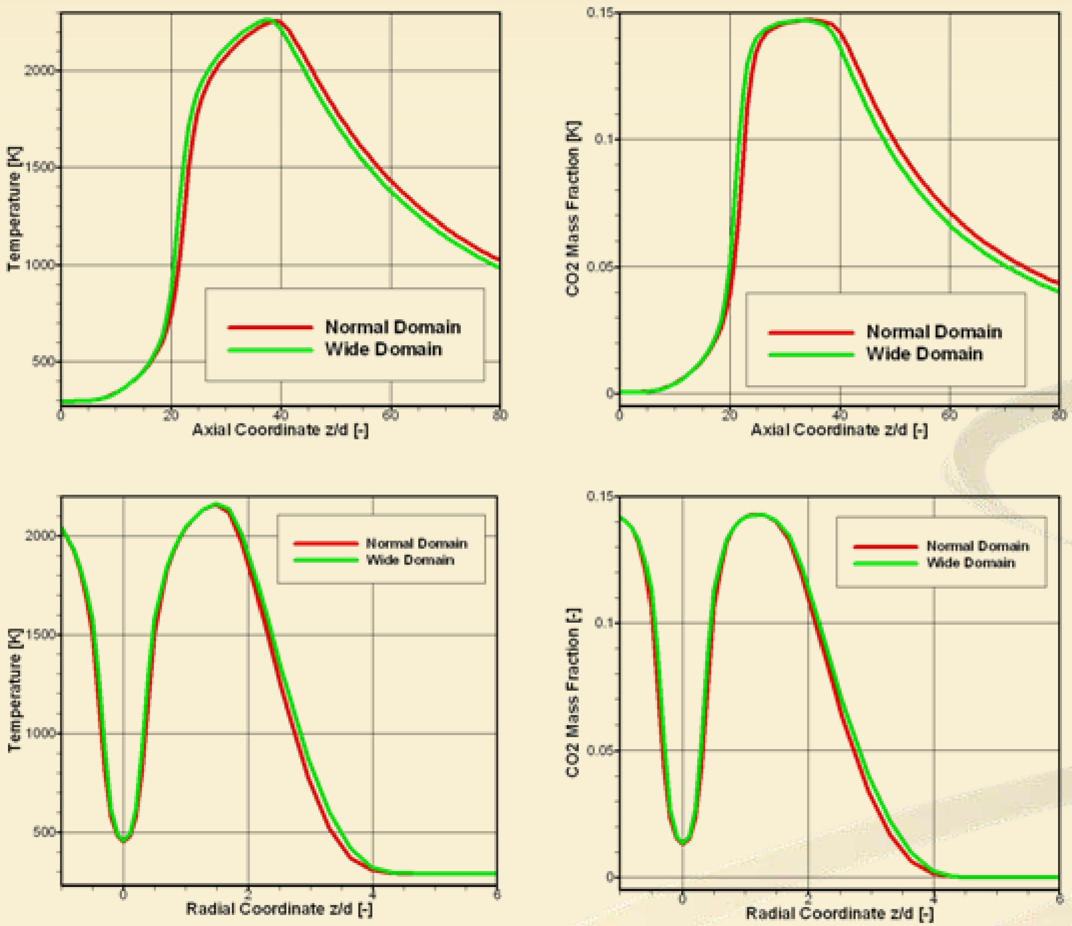


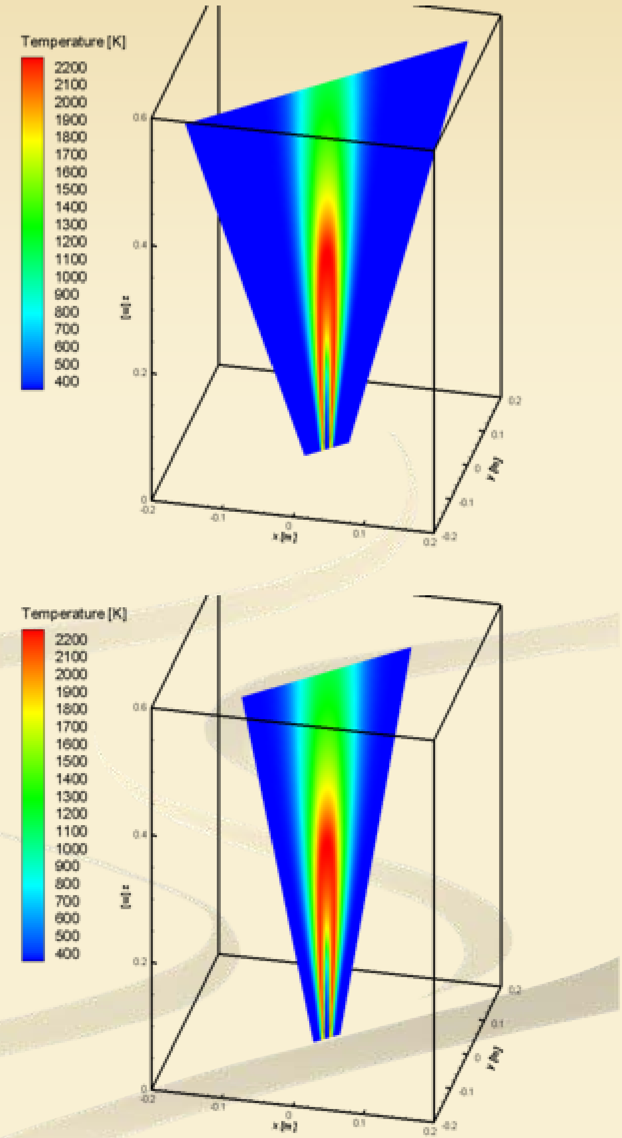


Test simulations

Domain dimensions impact

- Domain widening is unreasonable

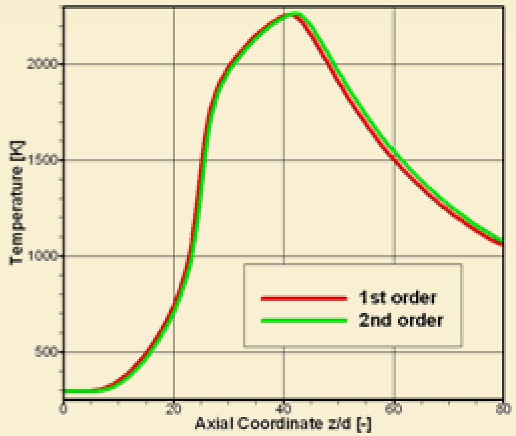


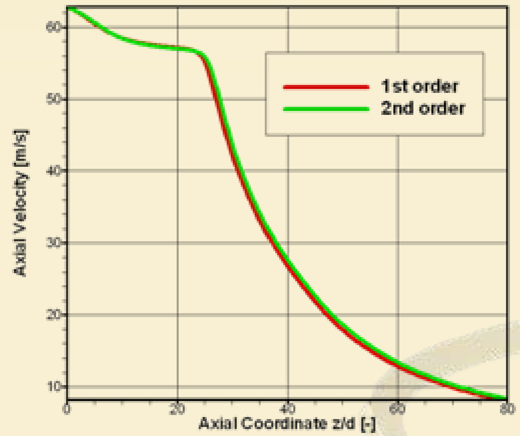


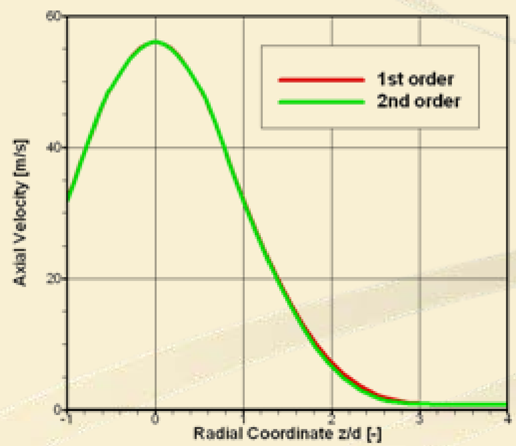
Test simulations

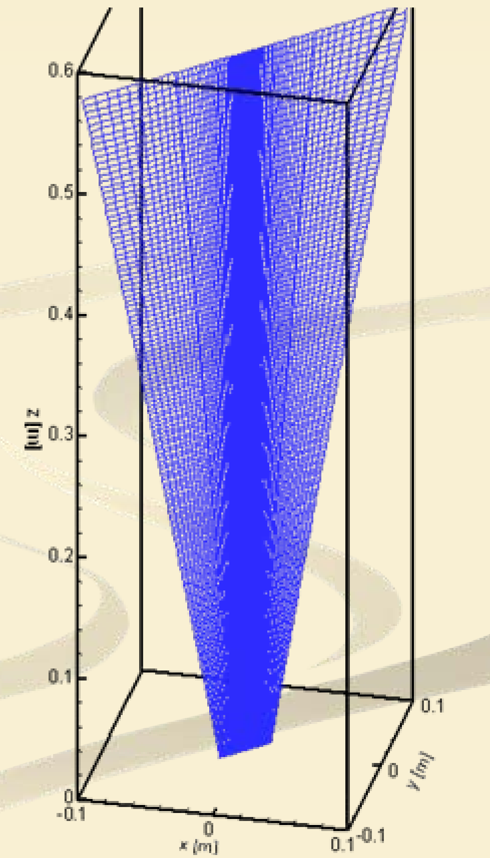
Approximation order impact

- Discretization order does not seriously affect physical fields
- Still 2-nd order discretization will be used further





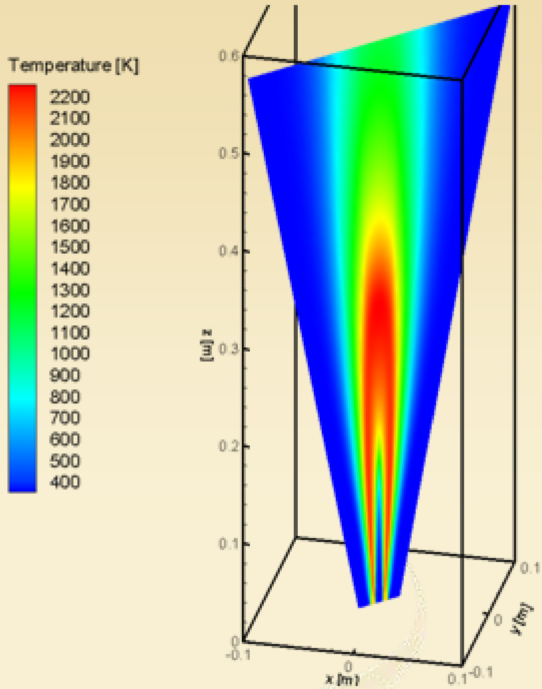


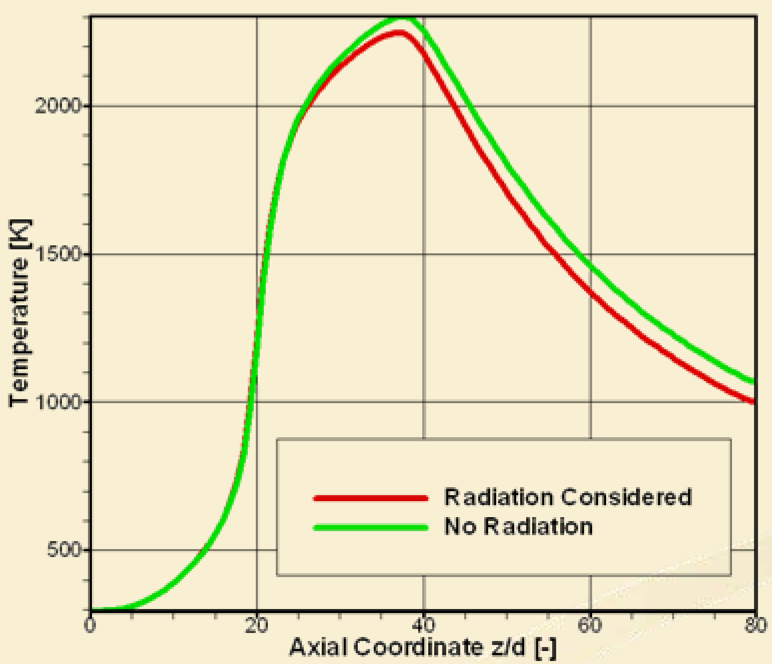


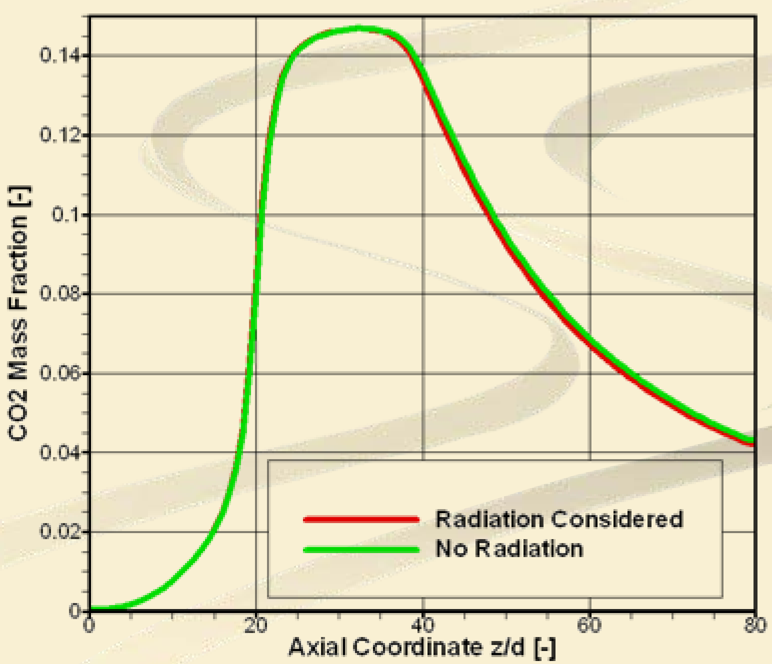
Test simulations

Radiation impact

- Radiation consideration affects only temperature field (*100 K* higher peak value)
- Scalar fields are not seriously affected by radiation
- Radiation was considered in all simulations







Simulation results

Turbulence and chemistry modeling strategies:

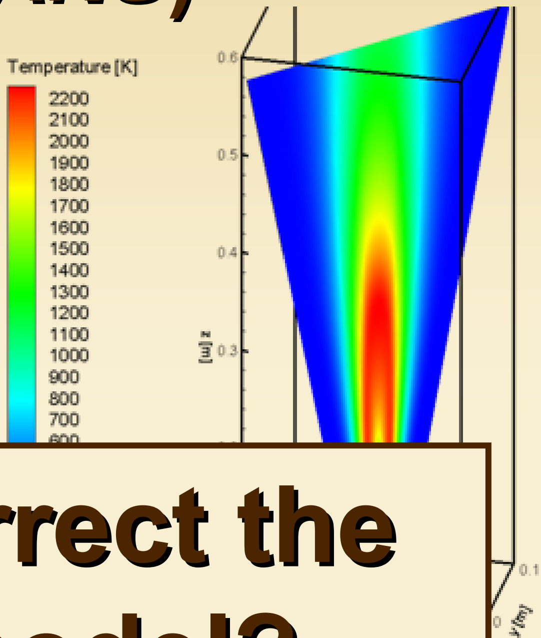
	Favre time-averaging (*RANS*)	Large eddy simulation (*LES*)
Eddy break-up model (*EBU*)	☑ (8x2)	☑ (1x1)
Statistical model (*PDF*)	☑ (8x4)	☑ (1x1)

\+ Accounting for radiation

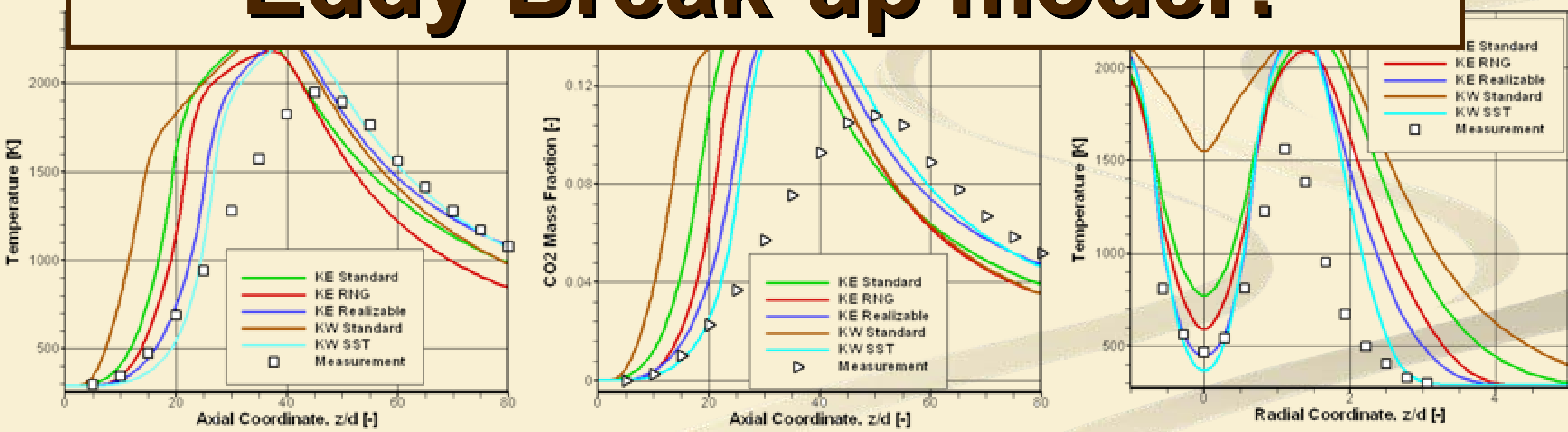
Reynolds time-averaging (*RANS*)

Chemistry: Eddy Break-up model

- Peak temperatures are greatly overestimated (about *300 K*)
- Peak concentrations of reaction products are greatly overestimated (about *15-40%*)
- S



Is it possible to correct the Eddy Break-up model?



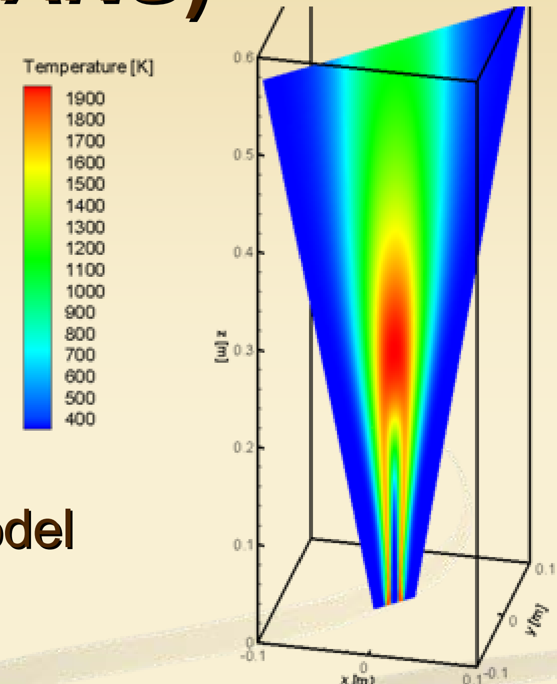
Reynolds time-averaging (*RANS*)

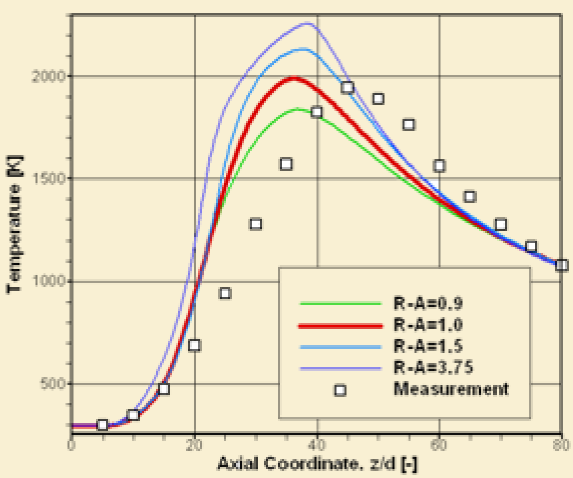
Eddy Break-up model improvement

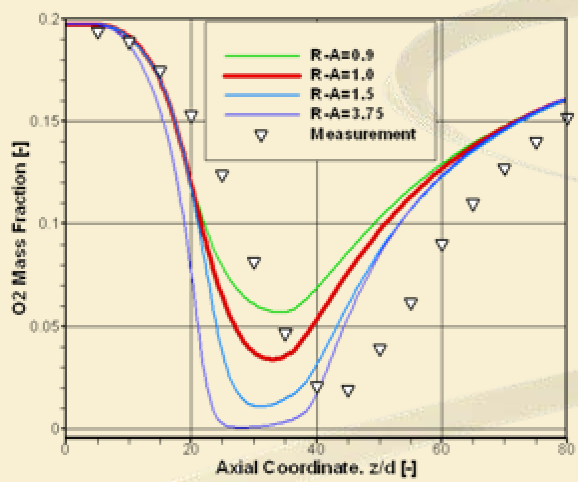
- Generally accepted value of *A*-constant is *4.0*

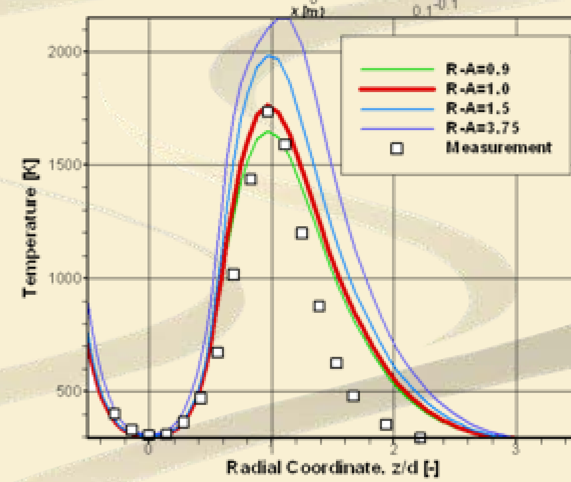
$$\tilde{\dot{r}}_\alpha = \boxed{A}\bar{\rho}\frac{\varepsilon}{k}\min\left(\tilde{Y}_{fuel}, \frac{\tilde{Y}_{ox}}{s_{ox}}, B\frac{\tilde{Y}_{prod}}{1+s_{ox}}\right)$$

- Optimal constant value is *A=1.0*
- Significant variation of constant means poor model adaptability to different types of reacting flows

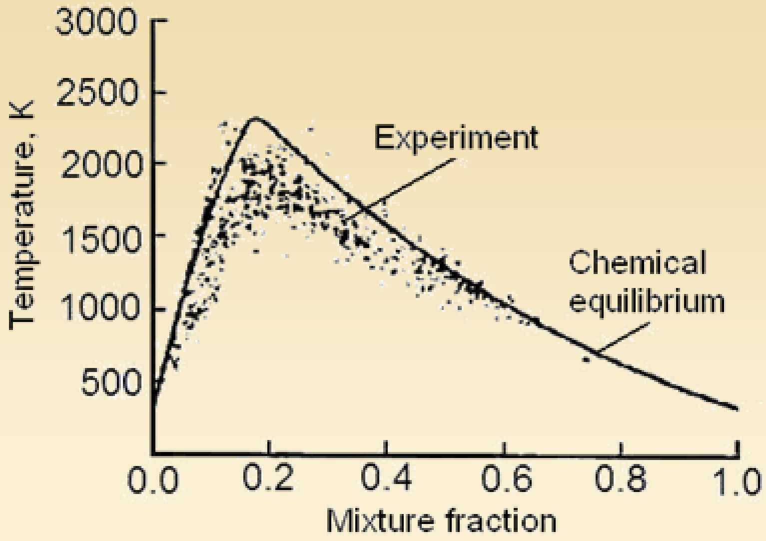








Theory interlude



Chemistry: statistical model

Transport equation for *α*-specie:

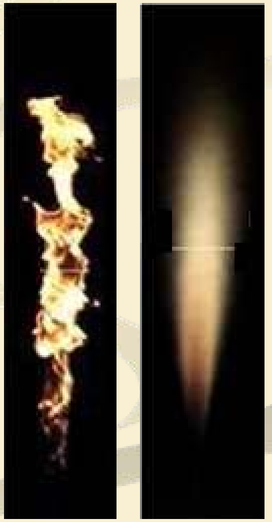
$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho u_j Y_\alpha}{\partial x_j} = -\frac{\partial F_{j,\alpha}}{\partial x_j} + \dot{r}_\alpha$$

Combining different equations:

$$\frac{\partial \rho \left(Y_{fuel} - Y_\alpha / s_\alpha\right)}{\partial t} + \frac{\partial \rho u_j \left(Y_{fuel} - Y_\alpha / s_\alpha\right)}{\partial x_j} - \frac{\partial}{\partial x_j} \rho \mathscr{D}_\alpha \frac{\partial \left(Y_{fuel} - Y_\alpha / s_\alpha\right)}{\partial x_j} = 0$$

Mixture fraction is a concrete conserved scalar:

$$Z = \frac{Y_{fuel} - Y_{ox} / s_{ox} - \left(Y_{fuel}^{air} - Y_{ox}^{air} / s_{ox}\right)}{Y_{fuel}^{fl} - Y_{ox}^{fl} / s_{ox} - \left(Y_{fuel}^{air} - Y_{ox}^{air} / s_{ox}\right)}$$



Using equilibrium dependencies:

$$Y_\alpha = Y_\alpha(Z) \qquad T = T(Z) \qquad \rho = \rho(Z)$$

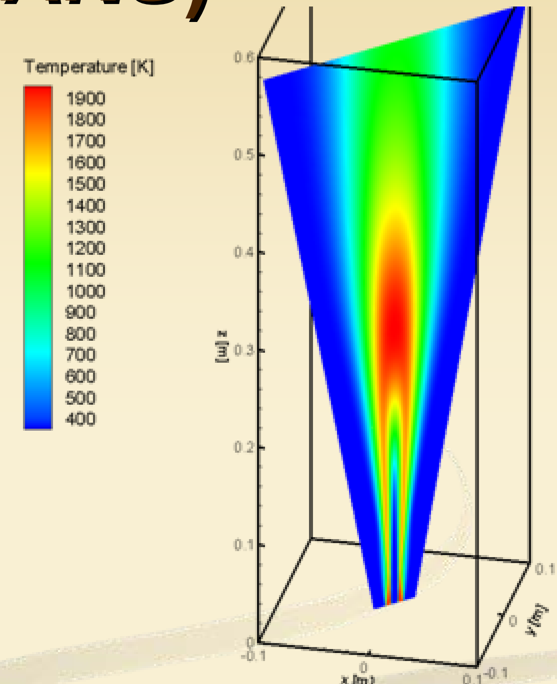
Averaged quantities with *B*-function as density function:

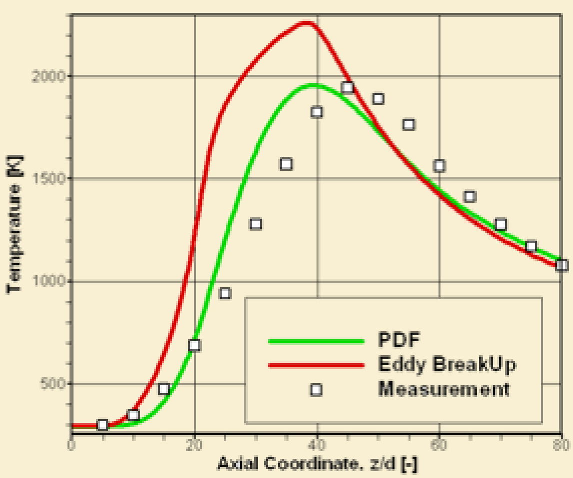
$$\tilde{Y}_\alpha = \int_0^1 Y_\alpha(Z)\tilde{P}(Z)dZ \qquad \tilde{T} = \int_0^1 T(Z)\tilde{P}(Z)dZ \qquad \bar{\rho} = \left(\int_0^1 \rho^{-1}(Z)\tilde{P}(Z)dZ\right)^{-1}$$

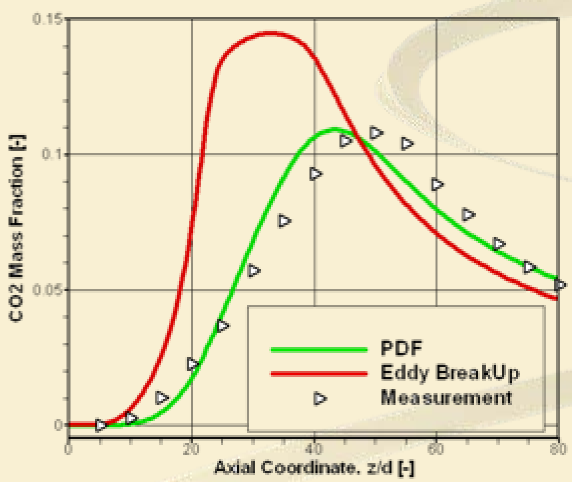
Reynolds time-averaging (*RANS*)

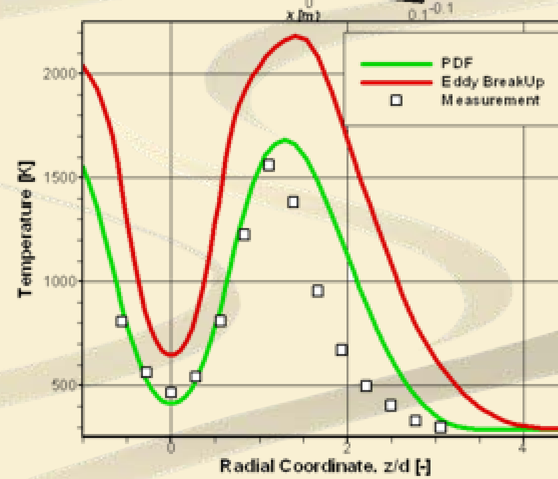
Chemistry: statistical model

- Significantly more accurate flame prediction
- Correct peak values of temperature and reaction products
- More narrow and long flame than in Eddy Break-up model

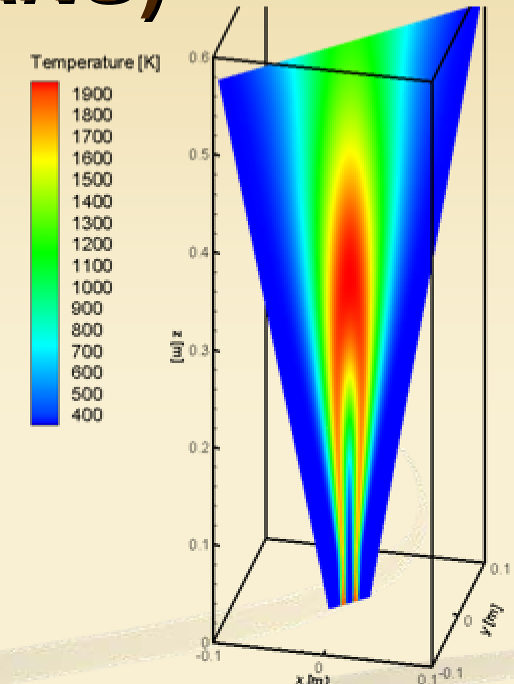






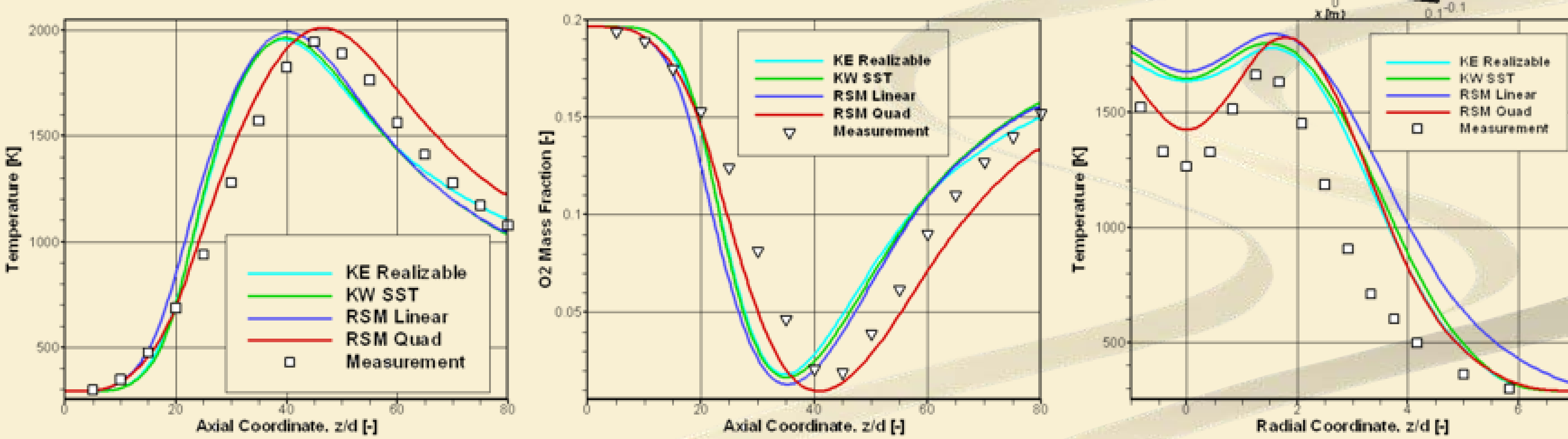


Reynolds time-averaging (*RANS*)



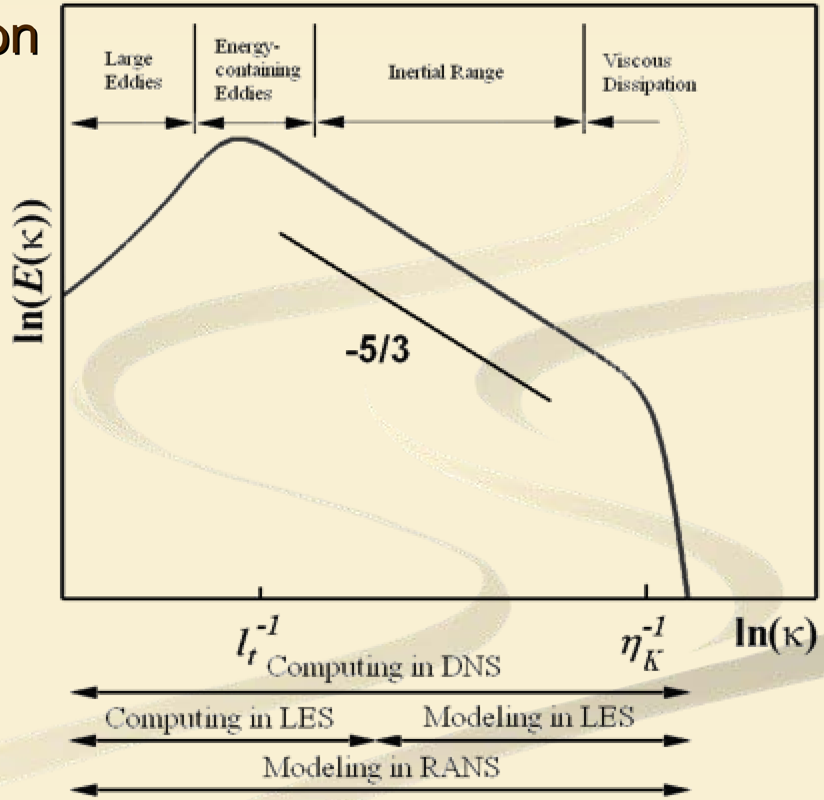
Turbulence models

- Best models with two additional turbulence equations: *k-ε Realizable* and *k-ω SST*
- *Quadratic Reynolds Stress model* (RSM) is the most accurate stationary model
- *k-ε Standard, k-ε RNG, k-ω Standard, RSM LowRe* models are significantly worse

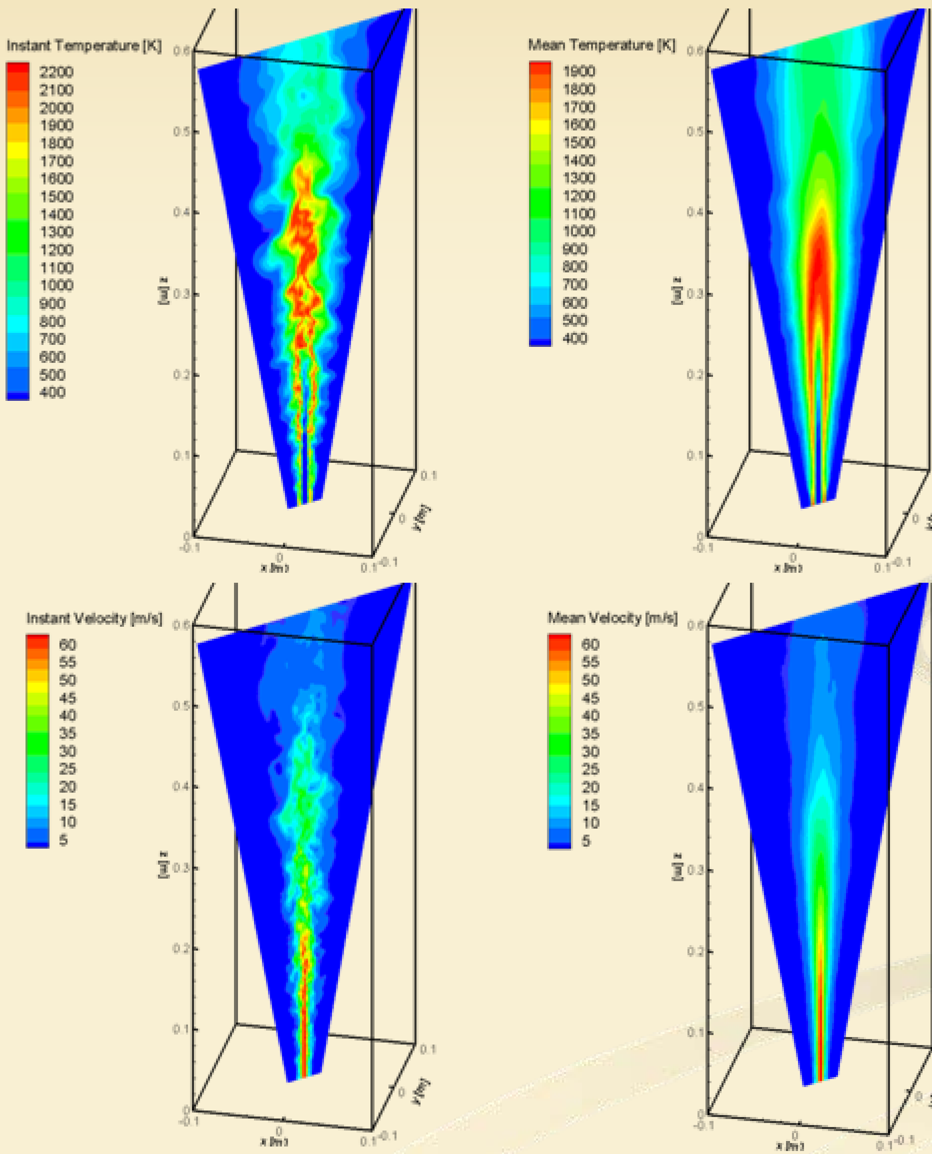


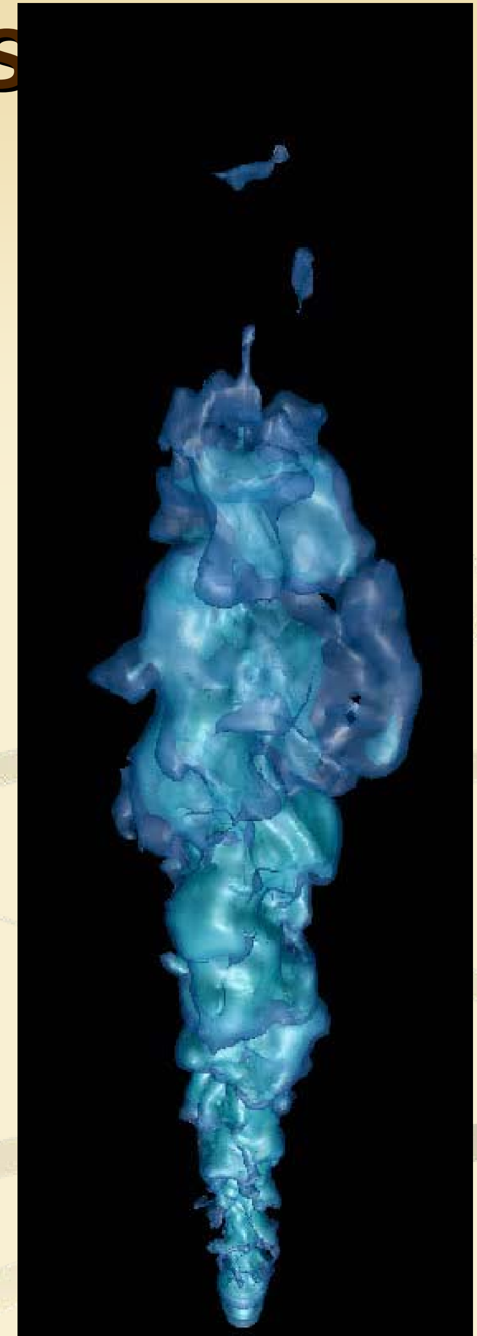
Theory interlude

- Favre time-averaging (*RANS*) is a conventional engineering approach
- Large Eddy Simulation (*LES*) capabilities
  - Less modeling, more calculation
  - Enables explicitly resolve energy-bearing long-wave part of vortex spectrum
  - High computational cost
  - Currently introduces in engineering practice

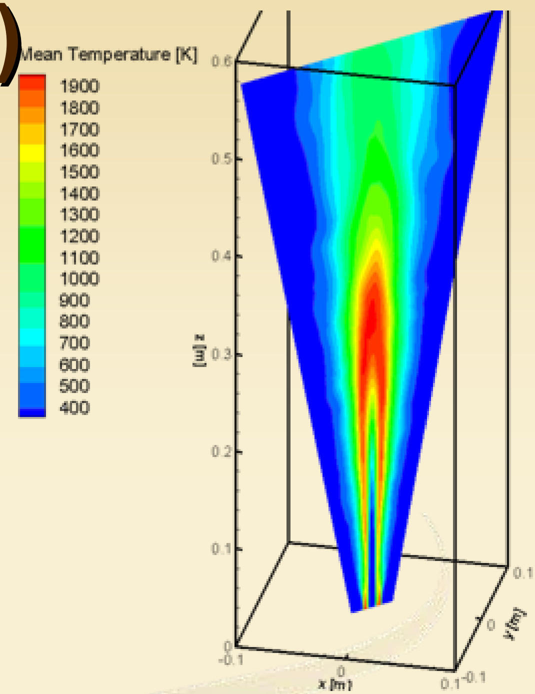


Large Eddy Simulation (*LES*





Large Eddy Simulation (*LES*)

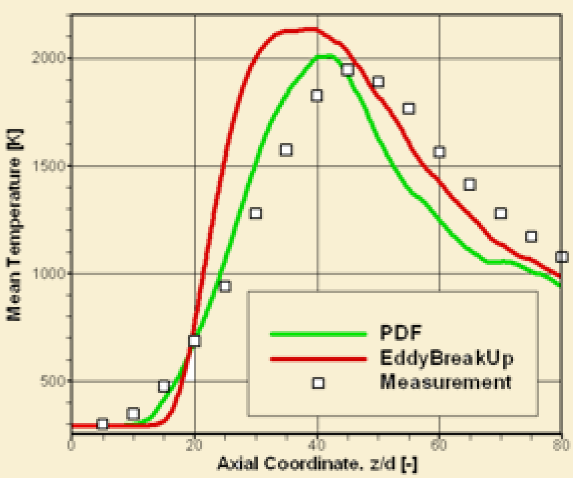


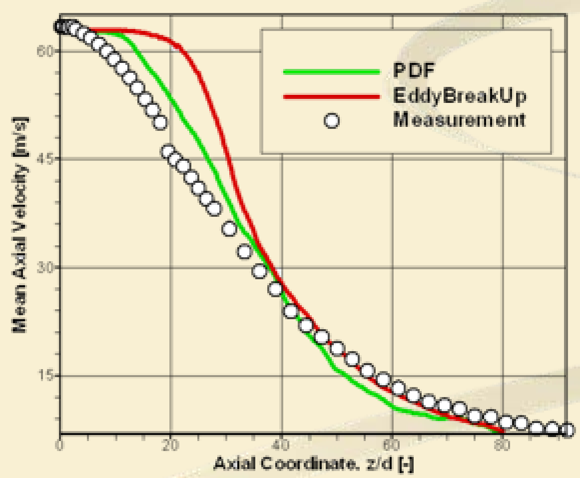
Chemistry model

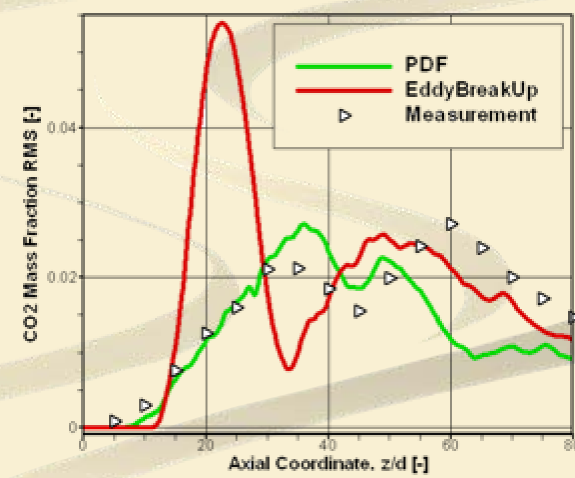
- Eddy Break-up model for *LES* is more accurate than Eddy Break-up model for *RANS*

$$\tilde{\dot{r}}_\alpha = A\bar{\rho}\tau^\gamma \min\left(\tilde{Y}_{fuel}, \frac{\tilde{Y}_{ox}}{s_{ox}}, B\frac{\tilde{Y}_{prod}}{1+s_{ox}}\right) \qquad \tau^r = \left(\sqrt{2S_{ij}S_{ij}}\right)^{-1}$$

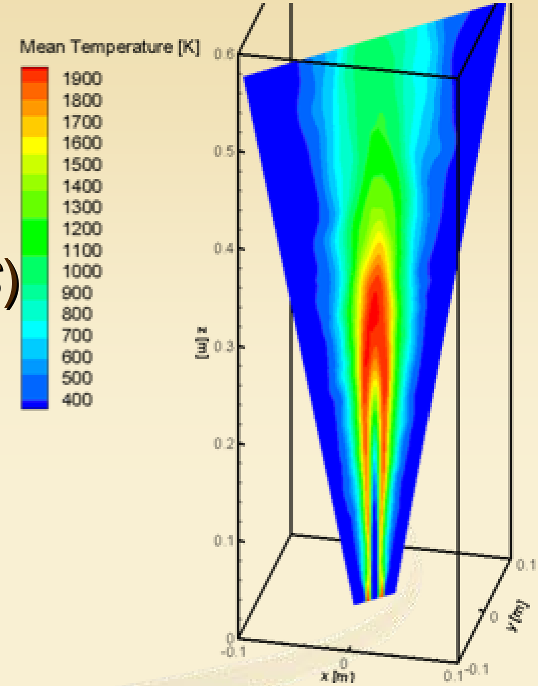
- Statistical model is still preferable
- Good agreement for 2-nd order statistics





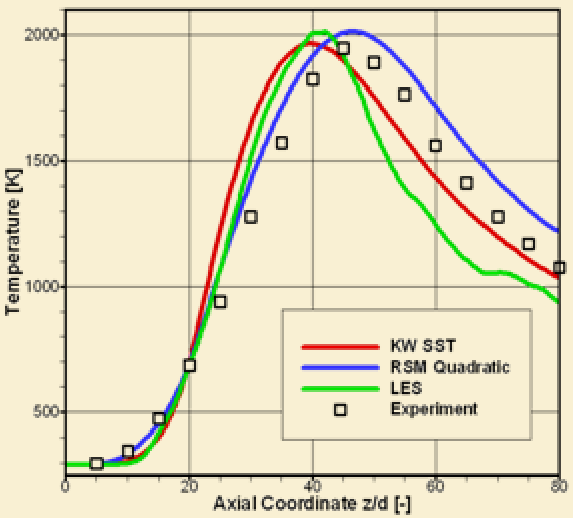


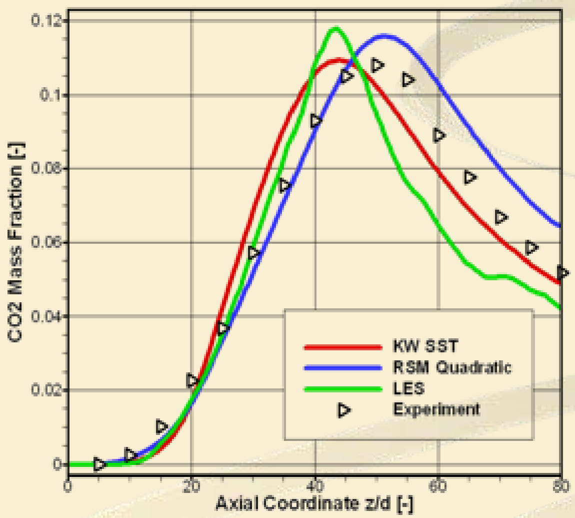
Large Eddy Simulation (*LES*)

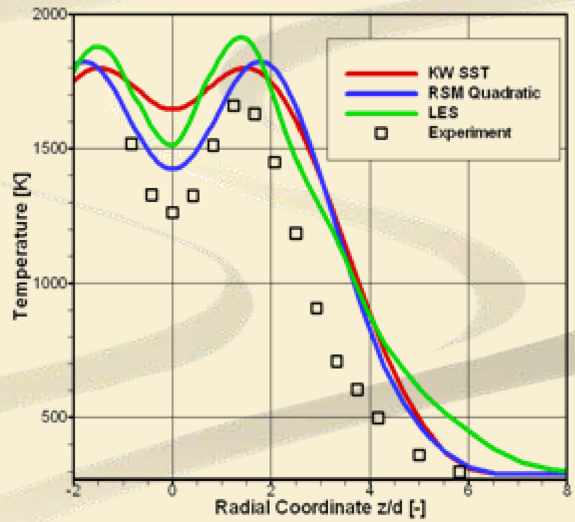


Turbulence comparison

- Perturbations were not generated at inlet (*LES*)
- Good agreement for *LES* up to the peak
- The simplest *LES* model is inferior only to the most comprehensive *RANS* model
- *LES* (as *Quadratic RSM*) predicts correct shape of the flame



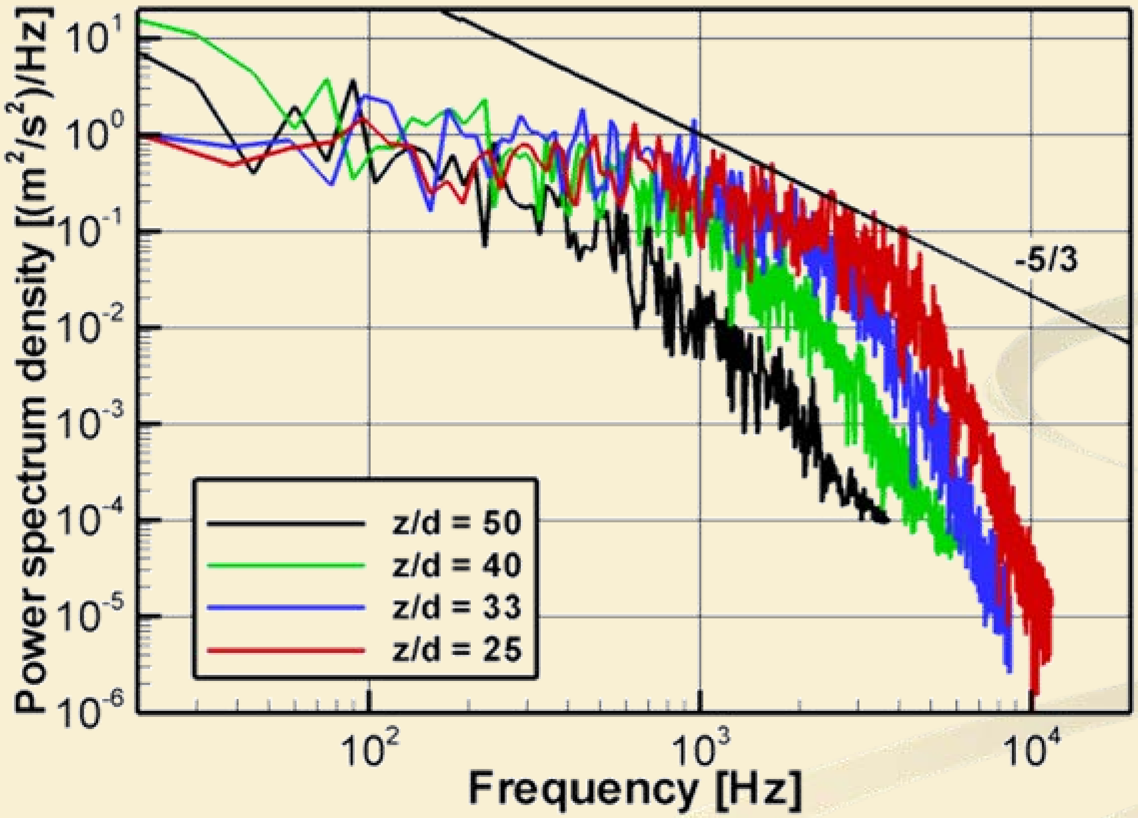


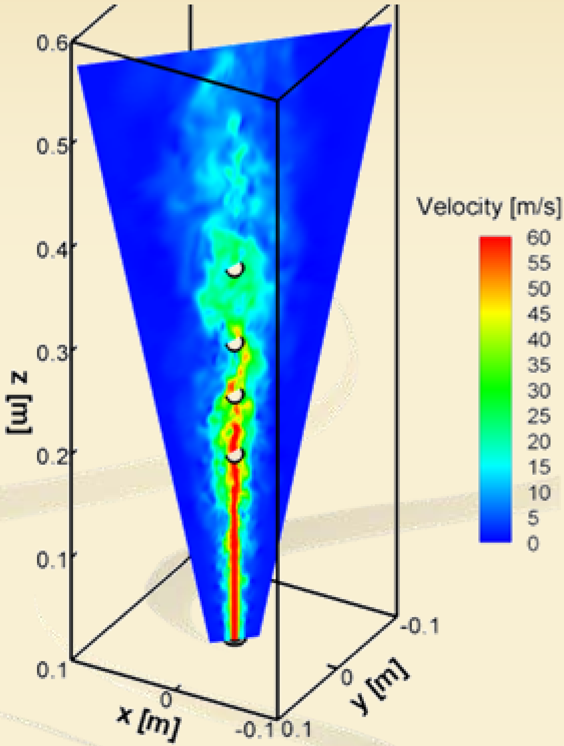


Large Eddy Simulation (*LES*)

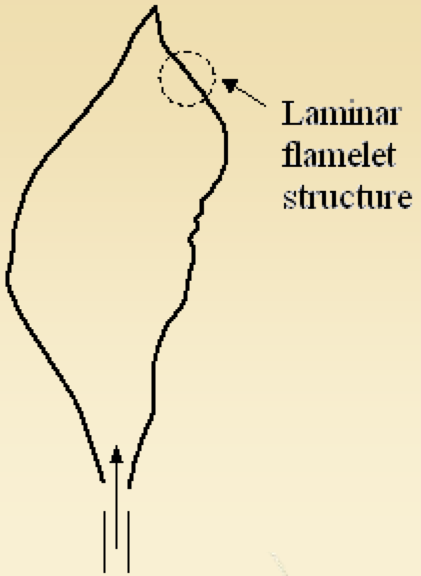
Velocity spectrum

- The spectrum -5/3 region is captured quite well





Theory interlude



Chemistry: flamelet model

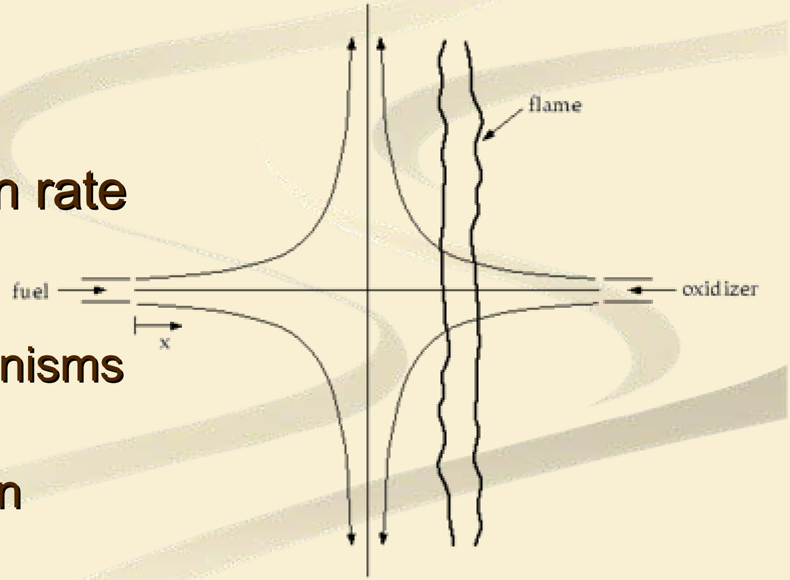
Statistical model complication - flame structure in mixture fraction space

$$\frac{\partial Y_\alpha}{\partial t} = \dot{r}_\alpha\left(Y_\alpha, T\right) + \frac{1}{2}\chi\frac{\partial^2 Y_\alpha}{\partial Z^2}$$

χ - scalar dissipation (parameter)

$$\chi = 2\mathscr{D}\left[\left(\frac{\partial Z}{\partial x_1}\right)^2 + \left(\frac{\partial Z}{\partial x_2}\right)^2 + \left(\frac{\partial Z}{\partial x_3}\right)^2\right]$$

Scalar dissipation is proportional to strain rate



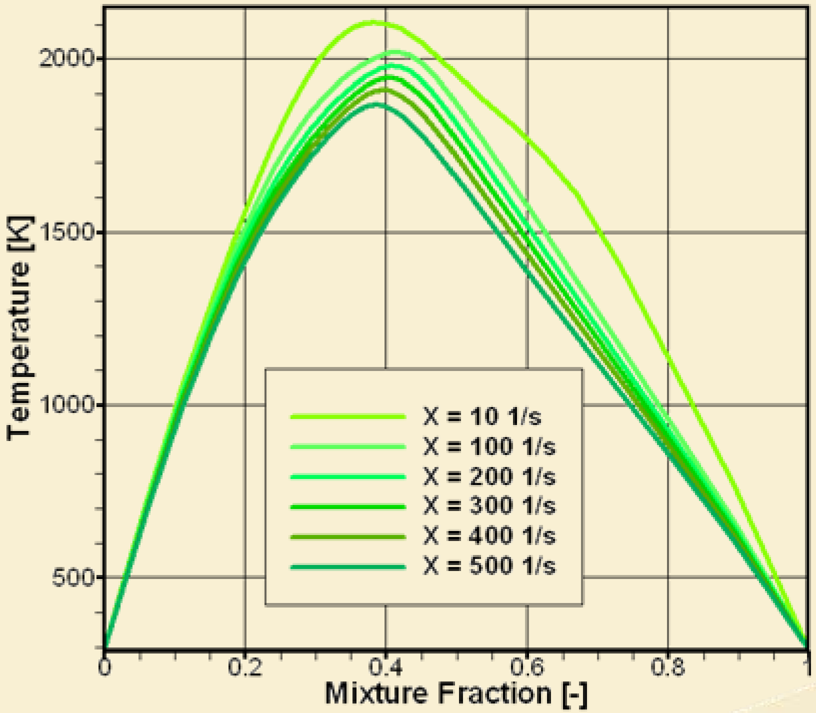
Characteristics:

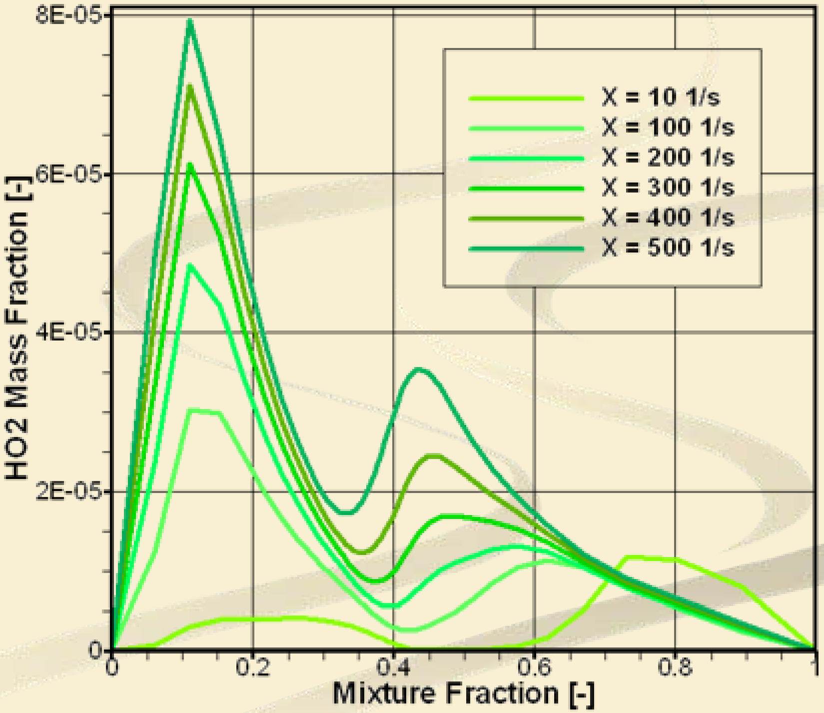
- Capability of using detailed chemistry mechanisms
- Thin flame front assumption
- Fast flame adaptation to flow field assumption

Statistical chemistry

Flamelet construction

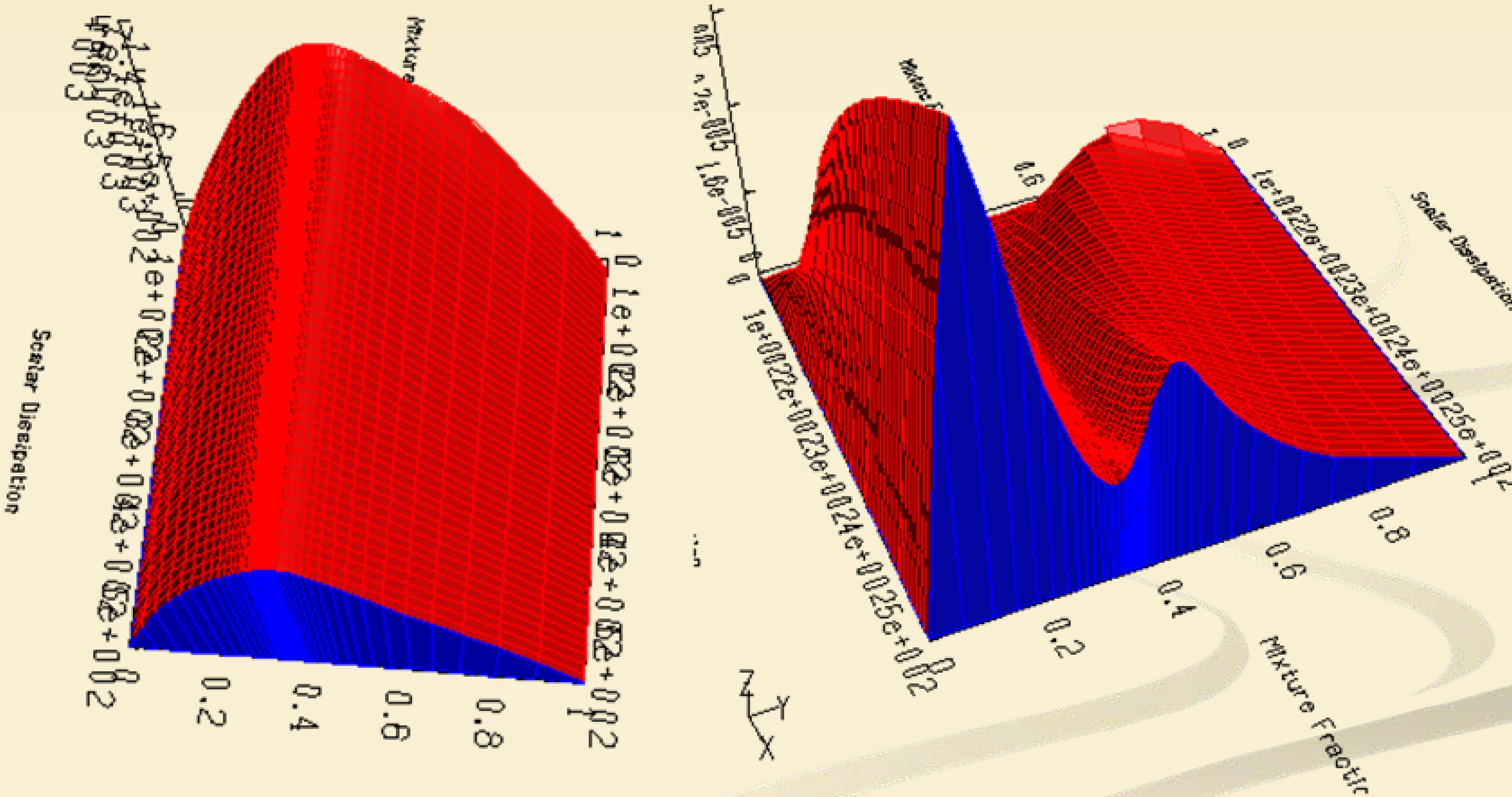
- Scalar dissipation does not affect temperature and major species
- Intermediate species are highly scalar-dissipation-dependent
- Still some serious numerical deviations near $\chi = 0$





Statistical chemistry

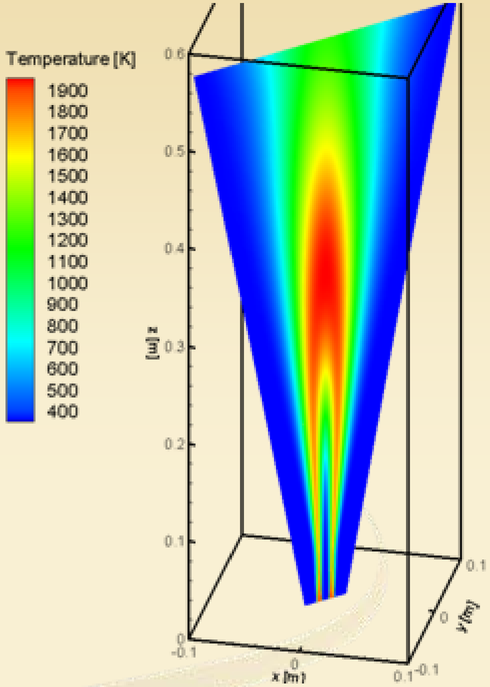
Flamelet construction

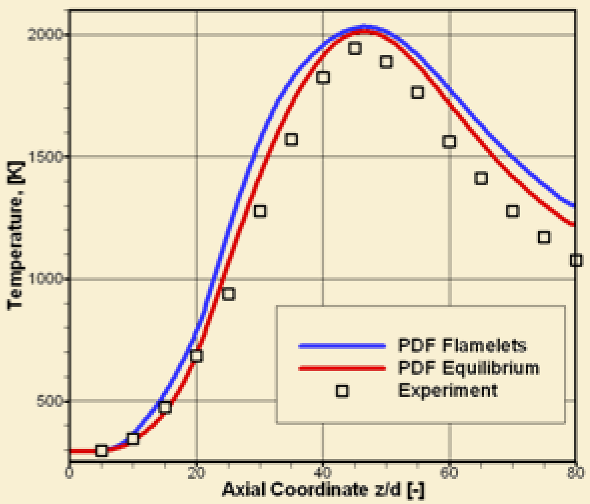


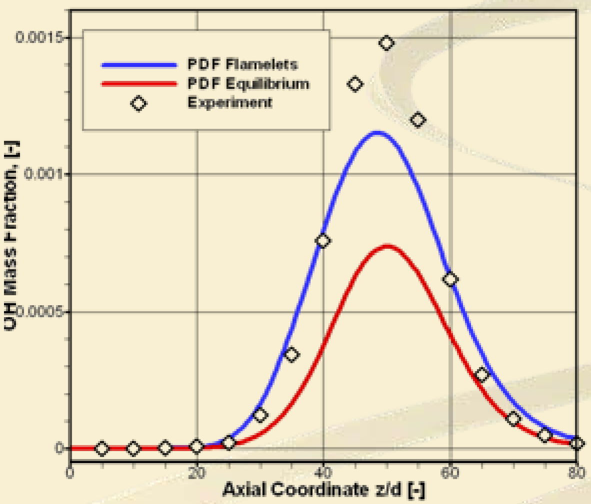
Statistical chemistry

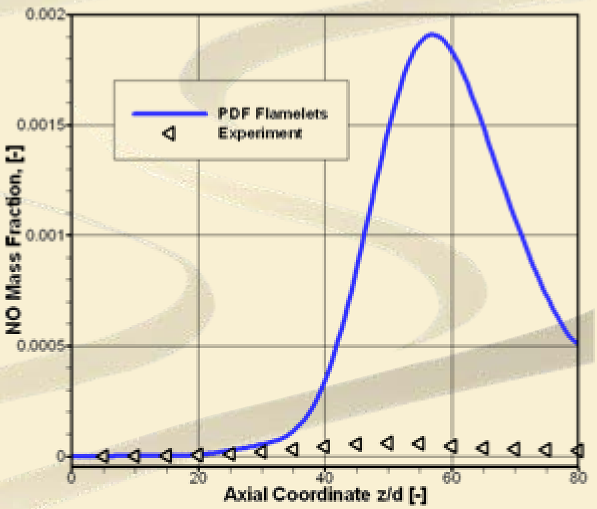
Flamelet model

- Flow, scalar and major species fields are quite the same as in Equilibrium chemistry
- Intermediate species fields are significantly improved
- Bad NO field prediction due to specific processes of NO formation









Computational resources

Laboratory of Applied Mathematics and Mechanics

- λ cluster

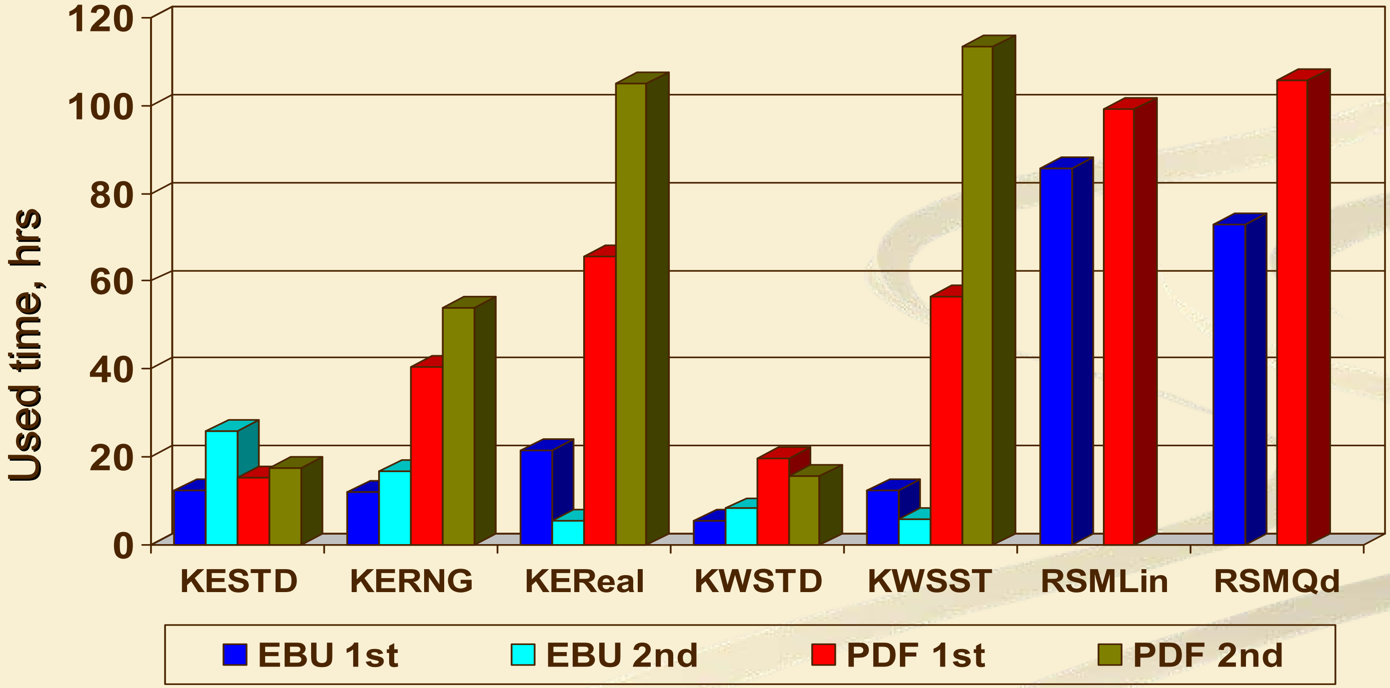
Cores count:	256 (64 nodes)
Processors:	AMD Opteron 280
Memory:	512 Gb
Network connection:	Infiniband
Peak performance:	1035 GFLOPS
Operating system:	SUSE Linux

- ε cluster

Cores count:	16 (4 nodes)
Processors:	AMD Opteron 265
Memory:	8 Gb
Network connection:	Gigabit Ethernet
Peak performance:	35 GFLOPS
Operating system:	Windows CCS

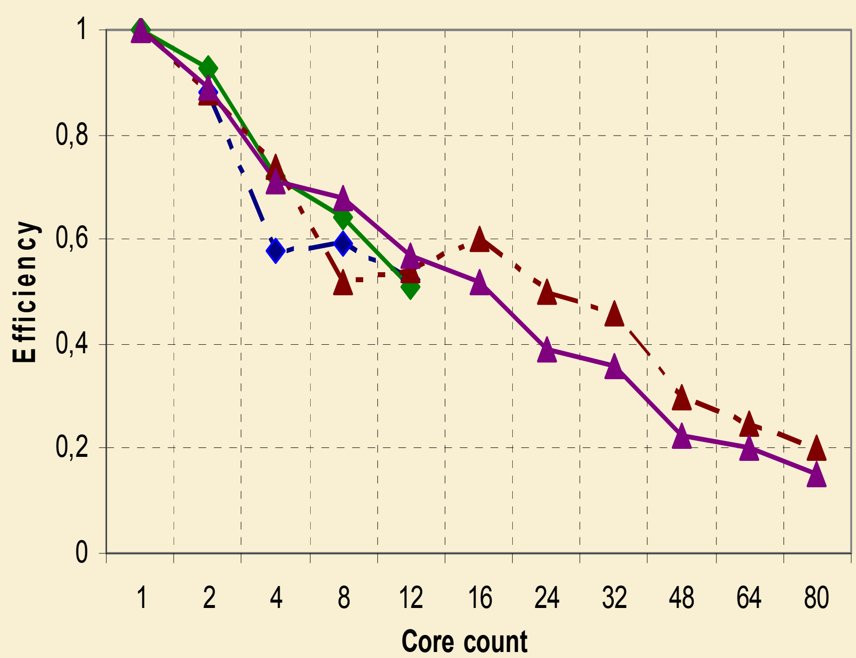
Models computational efficiency

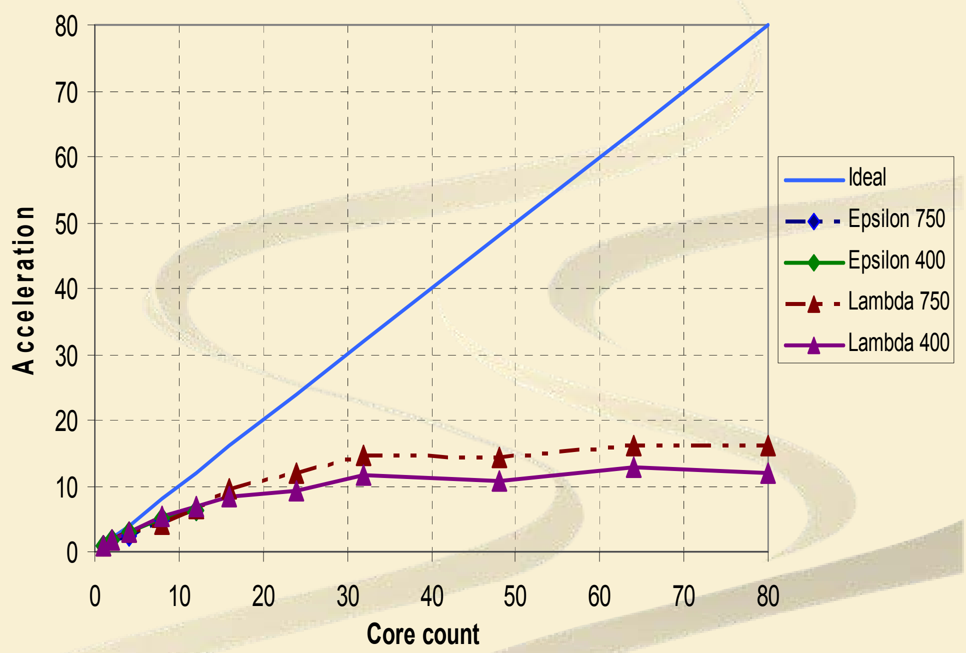
- Chemistry: Eddy Break-up model is significantly faster than statistical model (PDF)
- Turbulence: RSM Quadratic Model is optimal stationary model
- In general: More accurate model requires more calculation time



Cluster computational efficiency

- *Windows CCS* and *Linux SUSE* have equal paralleling efficiency in this type of simulations
- ε cluster capabilities are insufficient for Large Eddy Simulations LES
- Computational time on λ-cluster: 5 weeks on 48 cores





Code efficiency

Fluent simulation

- 725 000 computational cells
- 16 (real) processors
- 25 000 time steps
- **840 hours**

Shekli et al.* simulation

- 930 000 computational cells
- 6 processors
- 50 000 time steps
- **110 hours**

$$\tilde{k} = \left(\frac{930000}{725000}\right)^3 \frac{1/6}{1/16} \frac{50000}{25000} \frac{1/110}{1/840} \approx 86$$

General conclusion:

Fluent specific code efficiency is 50 – 200 times poorer than in-house code

* - M.R.H. Sheikhi, T.G. Drozda, P. Givi, F.A. Jaberi, S.B. Pope "Large eddy simulation of a turbulent non-premixed piloted methane jet flame (Sandia Flame D)", Proc. of Comb. Inst., 30, 2005

Conclusions

- Simple turbulence and chemistry models usage leads to severe errors in turbulent flame simulations
- Statistical Chemistry model significantly excels Eddy Break-up model
- RSM Quadratic, k-ε Realizable and k-ω SST stationary turbulence models are recommended
- Large Eddy Simulation provides lots of additional information but requires much computational time
- *Windows CCS* and *Linux SUSE* equals in paralleling efficiency on *Fluent* software

Future work

- Detailed research of flamelet chemistry models and reaction mechanisms
- Inspecting boundary perturbations impact on flame structure in *LES*
- Processors load balancing research
- Accurate pollutant emission models incorporation

Danke schön für Ihre Aufmerksamkeit!