Modelling Turbulent Non-Premixed Combustion in Industrial Furnaces

Using the Open Source Toolbox OpenFOAM

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August 24, 2015

Overview

Overview

Motivation: Almatis Rotary Kiln

- Cement kiln used for the production of calcium-aluminate cement.
- Fuel used is a mixture of different alkanes (95% CH_4).
- Kiln operates at temperatures upto 1800° C.

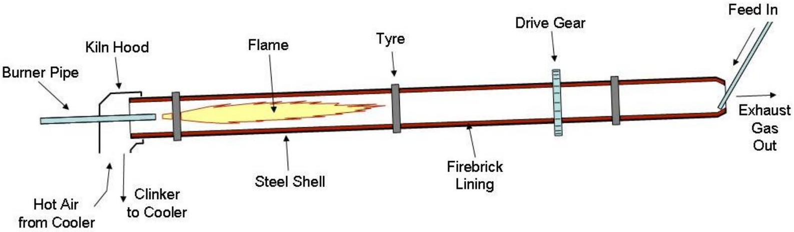
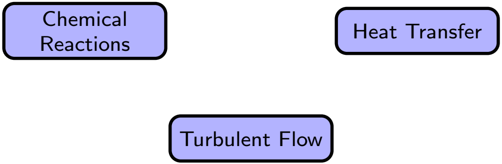


Figure: General layout of a direct fired rotary kiln used in cement manufacturing

Multi-Physics Model of the Kiln



Chemical Reactions

Heat Transfer

Turbulent Flow

Figure: Important physical phenomenon to be incorporated in the model

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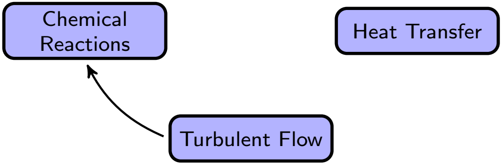

Figure: Important physical phenomenon to be incorporated in the model

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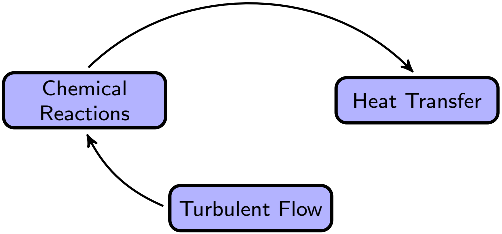
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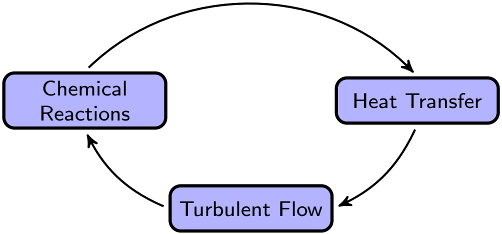

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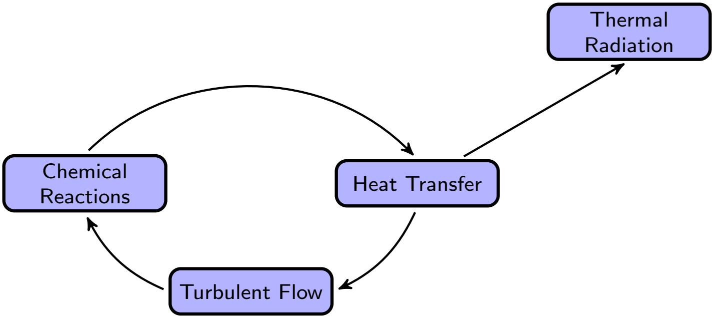
Thermal Radiation

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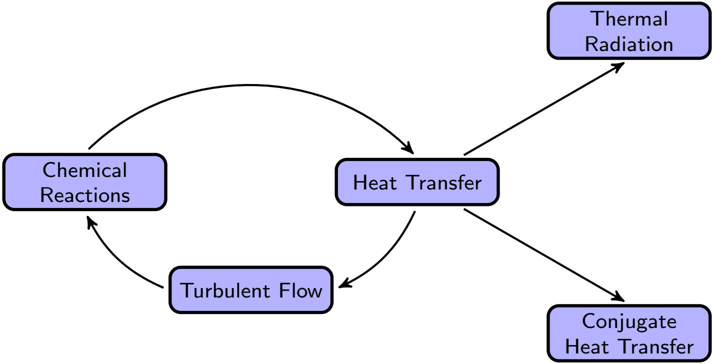

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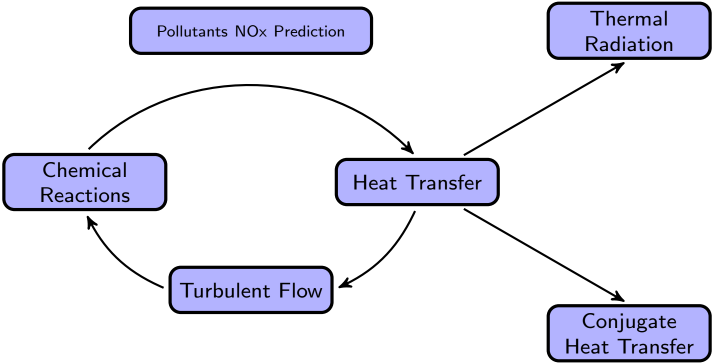

Figure: Important physical phenomenon to be incorporated in the model

Multi-Physics Model for Industrial Furnaces Developed in OpenFOAM

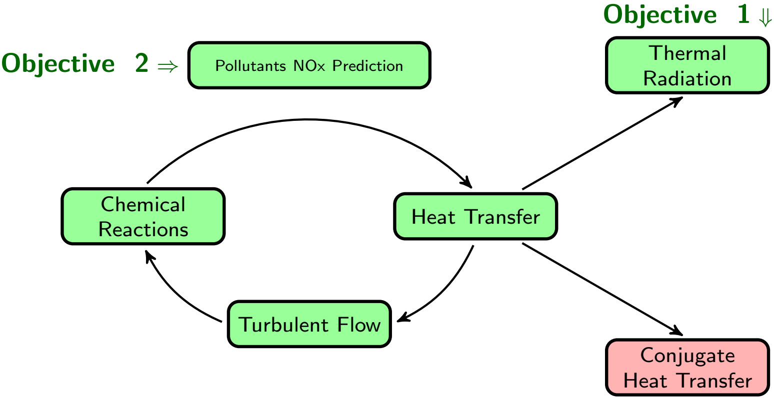

Figure: Important Physical Phenomenon to be Incorporated in the Model

Burner Flow Reactor Test Case

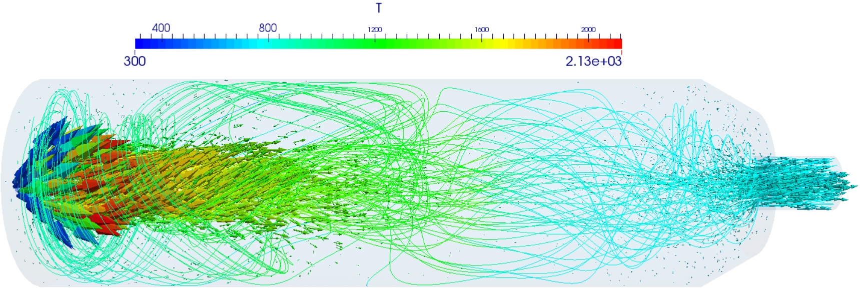

Figure: Stream tracer and glyphs for velocity

Overview

Averaging the Navier Stokes Equations

- Reynolds-averaging

$$\Phi = \underbrace{\overline{\Phi}(x)}_{\substack{time\\averaging}} + \underbrace{\Phi'(x,t)}_{\substack{turbulent\\fluctuations}}, \quad \overline{\Phi} = \lim_{T\to\infty} \frac{1}{T}\int_0^T \Phi(x,t)dt$$

- Favre-averaging

$$\Phi = \underbrace{\tilde{\Phi}(x)}_{\substack{density\\weighted\\averaging}} + \underbrace{\Phi''(x,t)}_{\substack{turbulent\ \ density\\weighted\ \ fluctuations}}, \quad \tilde{\Phi}(x) = \frac{\overline{\rho\Phi(x)}}{\overline{\rho}}$$

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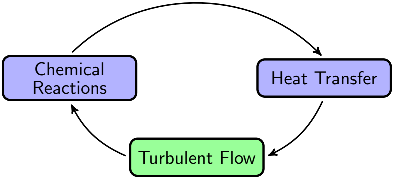
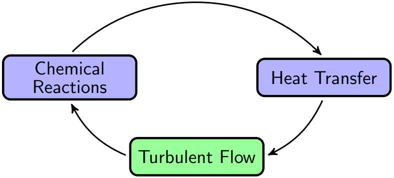
Favre-averaged Continuity Equation



$$\underbrace{\frac{\partial\overline{\rho}}{\partial t}}_{Transient\ \ term} + \underbrace{\frac{\partial}{\partial x_j}(\overline{\rho}\tilde{u}_j)}_{Convection\ \ term} = 0$$

Favre-averaged Momentum Equations


Chemical Reactions

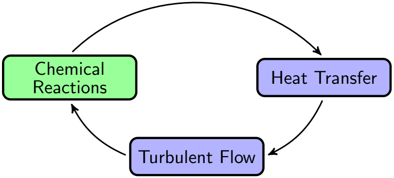
Heat Transfer

Turbulent Flow

$$\underbrace{\frac{\partial}{\partial t}(\overline{\rho}\tilde{u}_i)}_{\substack{\textit{Transient}\\ \textit{term}}} + \underbrace{\frac{\partial}{\partial x_j}(\overline{\rho}\tilde{u}_i\tilde{u}_j)}_{\substack{\textit{Convection}\\ \textit{term}}} = - \underbrace{\frac{\partial \overline{p}}{\partial x_i}}_{\substack{\textit{Pressure}\\ \textit{term}}} + \frac{\partial}{\partial x_j}\left(\overline{\tau_{ij}} - \underbrace{\overline{\rho u_i'' u_j''}}_{\substack{\textit{Reynolds}\\ \textit{Stresses}}}\right)$$

$\Rightarrow$ *Turbulence Models*

Favre-averaged Species Transport Equations



Chemical Reactions

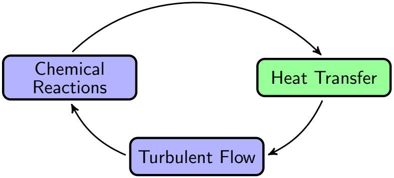
Heat Transfer

Turbulent Flow

$$\underbrace{\frac{\partial}{\partial t}(\overline{\rho}\tilde{Y}_s)}_{\substack{\textit{Transient}\\ \textit{term}}} + \underbrace{\frac{\partial}{\partial x_j}(\overline{\rho}\tilde{Y}_s\tilde{u}_j)}_{\substack{\textit{Convection}\\ \textit{term}}} = \underbrace{\frac{\partial}{\partial x_j}\left(\Gamma_s\frac{\partial \tilde{Y}_s}{\partial x_j}\right)}_{\substack{\textit{Diffusion}\\ \textit{term}}} + \underbrace{\tilde{\dot{\omega}}_s}_{\substack{\textit{Mean}\\ \textit{Reaction Rate}}} \qquad s = 1, 2 \ldots m$$

$\Rightarrow$ *Combustion Models*

Favre-averaged Enthalpy Transport Equation



$$\underbrace{\frac{\partial}{\partial t}(\overline{\rho}\tilde{h})}_{\substack{\text{Transient}\\ \text{term}}} + \underbrace{\frac{\partial}{\partial x_j}(\overline{\rho}\tilde{h}\tilde{u}_j)}_{\substack{\text{Convection}\\ \text{term}}} = \underbrace{\frac{\partial}{\partial x_j}\left(\overline{\rho}\alpha\frac{\partial\tilde{h}}{\partial x_j} - \overline{\rho h'' u_j''}\right)}_{\substack{\text{Diffusion}\\ \text{term}}} + \underbrace{\overline{S_h}}_{\substack{\text{Combustion}\\ \text{Source}\\ \text{Term}}} + \underbrace{\overline{S_{rad}}}_{\substack{\text{Radiation}\\ \text{Source Term}}}$$

$\Rightarrow$ *Radiation Models*

Overview

OpenFOAM (Open Field Operation and Manipulation)

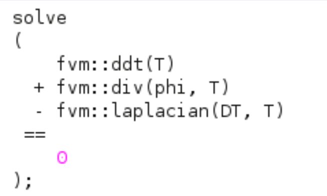
- Open source CFD toolbox written in C++.
- Not a point and click CFD software.
- OpenFOAM employs collocated FVM discretisation for solving PDE's.

OpenFOAM structure

Convection-diffusion equation in the incompressible form.

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{U} T) - \nabla^2 (\mathcal{D}_{\mathrm{T}} T) = 0 \tag{1}$$

Representation in OpenFOAM



```
solve
(
    fvm::ddt(T)
  + fvm::div(phi, T)
  - fvm::laplacian(DT, T)
 ==
    0
);
```

Why OpenFOAM ! ?

Open Source

- No license costs!.
- Complete access to the source code.
- Offers great scope for custom development.

Reliability

- First stable release: Dec 2004.
- Detailed validation and verification studies for several benchmark problems.
- Large user community across commercial and academic organizations. Example NRG, Tata Steel, Dynaflow

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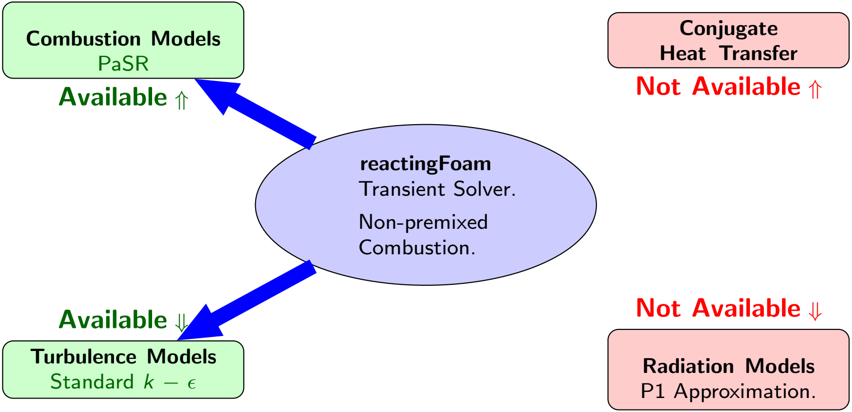
Solver for Turbulent Combustion - **reactingFoam**



Combustion Models
PaSR

Available ⇑

Conjugate Heat Transfer

Not Available ⇑

reactingFoam
Transient Solver.

Non-premixed Combustion.

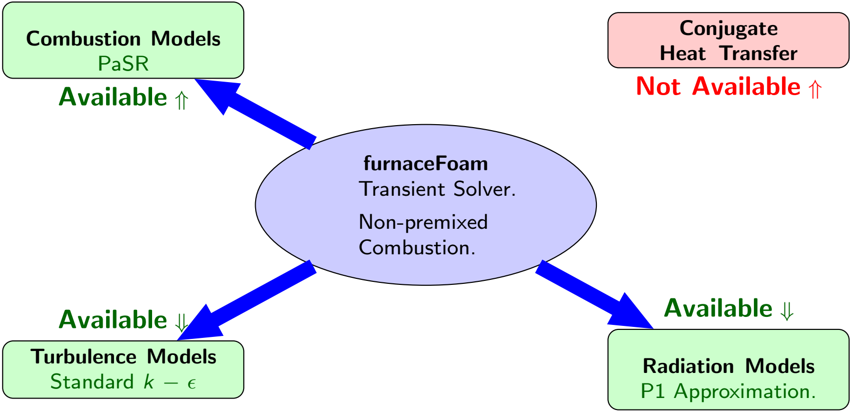
Available ⇓

Turbulence Models
Standard $k - \epsilon$

Not Available ⇓

Radiation Models
P1 Approximation.

Solver for Turbulent Combustion + Radiation = **furnaceFoam**



Combustion Models
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furnaceFoam
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Turbulence Models
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Radiation Models
P1 Approximation.

Overview

1. Motivation: Almatis Rotary Kiln
2. Governing Equations for Turbulent Reacting Flows
3. OpenFOAM.
4. **Sandia Flame D Validation**
5. Combustion Test Case
6. Pollutant NO_x Formation
7. Conclusions and Recommendations

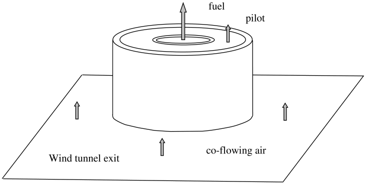
Sandia National Laboratories Flame D

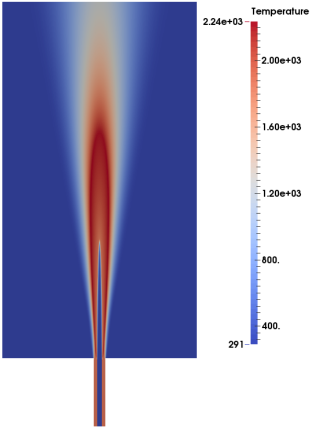
Turbulent piloted methane-air diffusion flame.

Central fuel jet(49.6 m/s, Re 22400) consists of a 25/75%(by volume) methane-air mixture.

Hot pilot jet(11.4 m/s) surrounding the central fuel jet for stabilisation and ignition.

Slow coflow of air(0.9 m/s) outside.





Computational Domain and Mesh

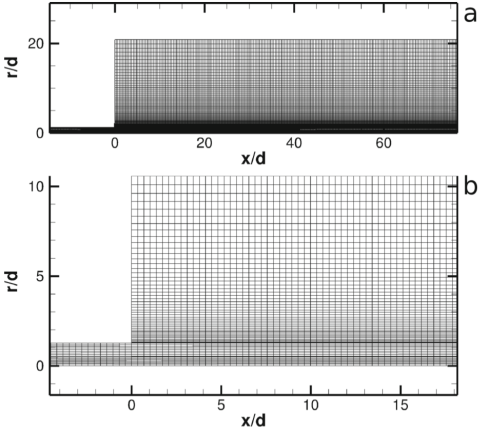
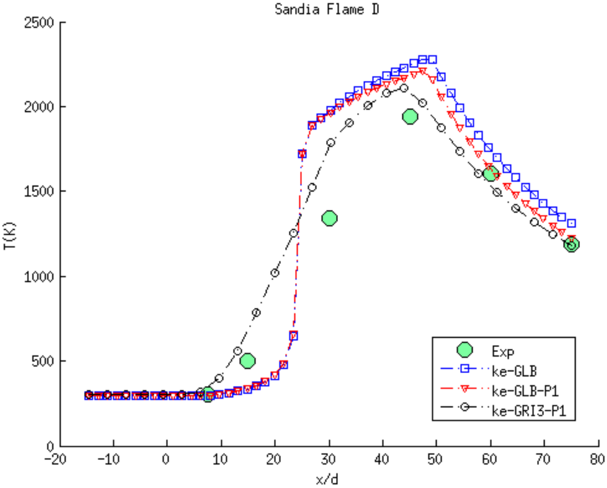
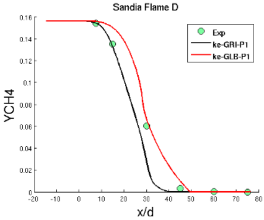


Figure: Computational domain **a** and mesh near the inlet **b**

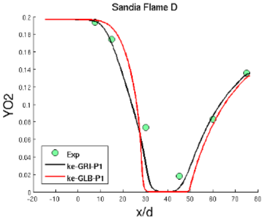
Temperature distribution along the central axis



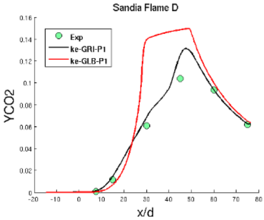
Chemical species concentration along the central axis



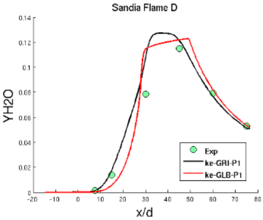
CH_4



O_2



CO_2



H_2O

Run Time (in Hours) on 4 cores using OpenMPI.

Test Case	**Mesh C1(#5835)**	**Mesh R1(#23340)**	**Mesh R2(#45822)**
Global Reaction Mechanism (1-step)	0.62	3.58	16.73
Detailed Reaction Mechanism (325-steps)	59.94	-	-

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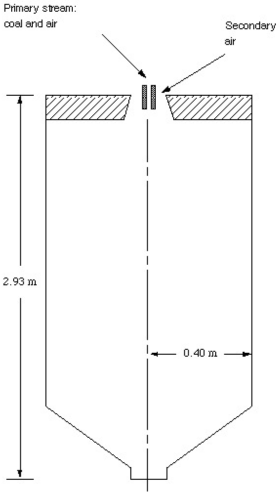
Test Case: Burner Flow Reactor (BFR) Geometry

BFR located at Brigham Young University, USA.

Axi-symmetric, vertical-fired reactor with a swirling flow(9.5°).

Used for validating new CFD code.



Block Structured Mesh for BFR

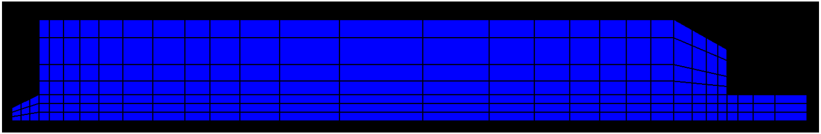


Figure: Orthogonal Mesh C1

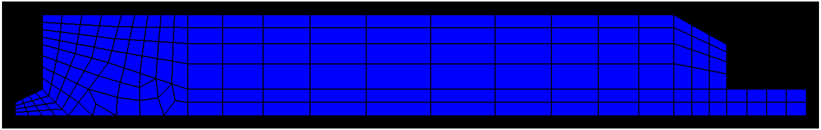
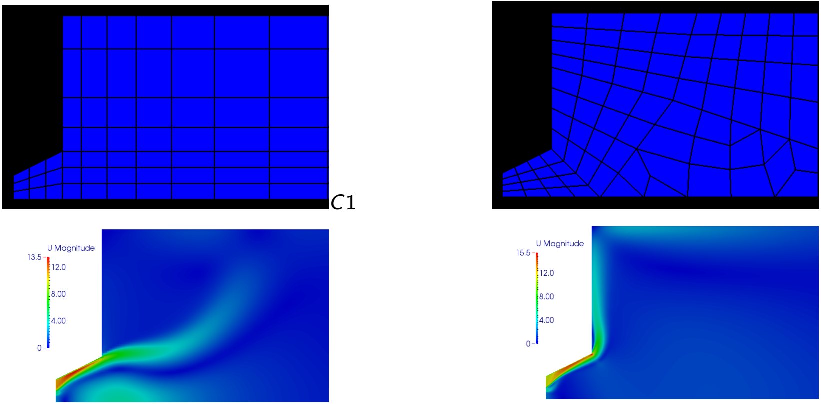


Figure: Non-Orthogonal Mesh N1

Non-Orthogonality Tests - Isothermal Flow



*C*1 *N*1

*C*1 *N*1

Figure: OpenFOAM sensitivity to Mesh Non-Orthogonality.

Contour Plots of Velocity and Temperature - Reacting Flow

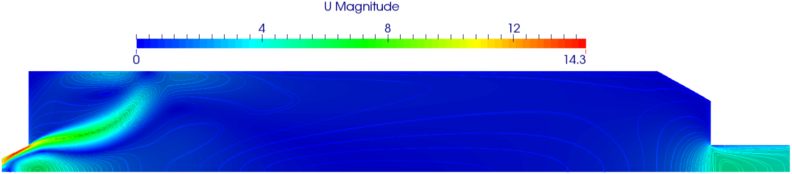


Figure: Contours of velocity magnitude (m/s)

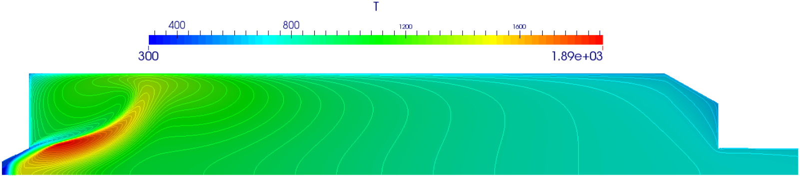
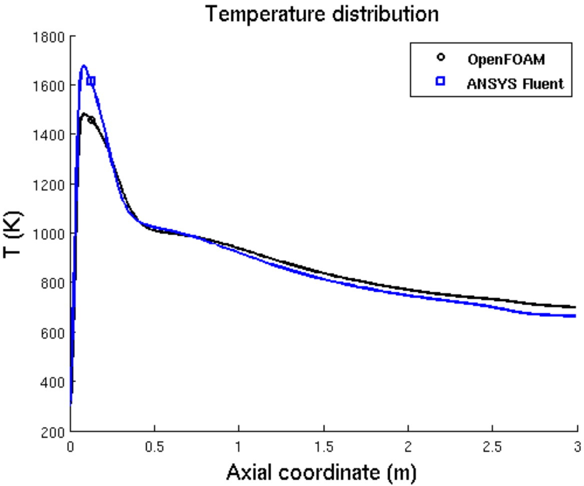


Figure: Contours of temperature (K)

Comparison of Results with Ansys Fluent



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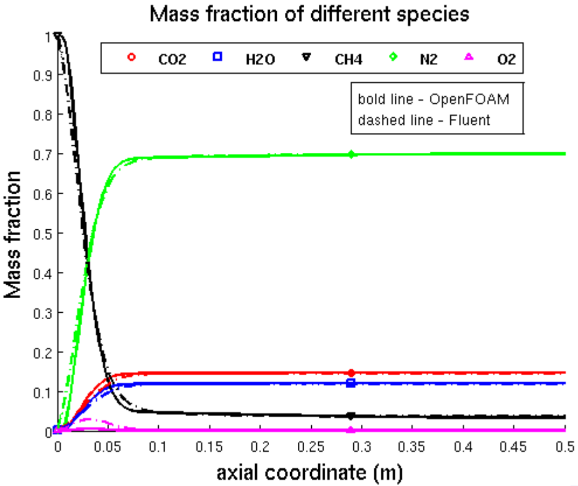

Computational Time (in Hours) on 4 cores using OpenMPI.

	Test Case	**Isothermal Flow**	**Reacting Flow**
ANSYS Fluent	$R2 - GLB - P1$	~ 0.1	~ 3
OpenFOAM	$R2 - GLB - P1$	0.12	32.68
OpenFOAM	$C13D - Inf - fvDOM$	0.83	82.01

R2 . . . . Axi-symmetric mesh with cell count # 46800
C13D. . . . . . 3D mesh with cell count # 421200
GLB . . . . . . Global Reaction Mechanism
Inf . . . . Infinite Fast Chemistry

Overview

Pollutant NOx

NOx = NO + NO2

NO_x causes ⇒

- Ozone depletion
- Acid rain
- Smog formation

Main sources of NO_x ⇒

- Industrial combustion processes
- Automobiles.

NO_x from industrial sources is predominantly Nitric Oxide NO.

Sources of NO

- Thermal NO - Main contribution
- Other Sources - Prompt NO, Fuel NO, NO from N_2O Intermediate.

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Implementation of NO_x Post-Processor in OpenFOAM

NO concentrations generated in combustion systems are very low.

1-way coupling

Flow and Temperature ⇒ NOx Chemistry

Governing convection diffusion equation for Thermal NO transport

$$\underbrace{\frac{\partial \rho Y_{NO}}{\partial t}}_{Transient\ \ term} + \underbrace{\nabla \cdot (\rho \vec{u} Y_{NO})}_{Convection\ \ term} = \underbrace{\nabla \cdot (\rho D_{eff} \nabla Y_{NO})}_{Diffusion\ \ term} + \underbrace{S_{Y_{NO}}}_{Source\ \ Term}$$

$$S_{Y_{NO}} = M_{NO} \quad 1.32 \times 10^{10} \quad \underbrace{e^{-65493/T} \; T^{1/2}}_{Sensitivity\ \ To\ \ Temperature} \quad [O_2]^{1/2} \, [N_2] \; \underbrace{\frac{\left(1 - \frac{k_{b1} \; k_{b2} \; [NO]^2}{k_{f1} \; k_{f2} \; [N_2] \; [O_2]}\right)}{\left(1 + \frac{k_{b1} \; [NO]}{k_{b2} \; [O_2]}\right)}}_{Non-Linear\ \ Term}$$

ρ, $\vec{u}$, D_{eff}, $[O_2]$, $[N_2]$, T → Input from flow calculations.

Validation with ANSYS Fluent

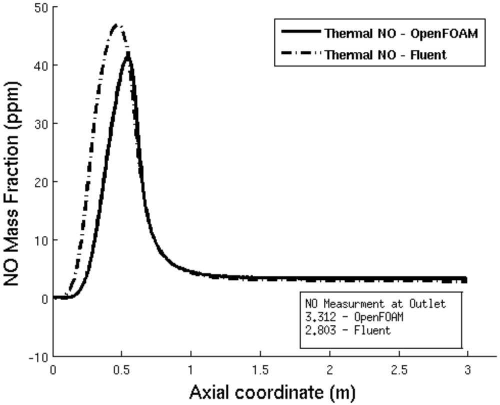

Figure: Thermal NO mass fraction (in ppm) along the central axis of the furnace.

Thermal NO Reduction - Equivalence Ratio Variation

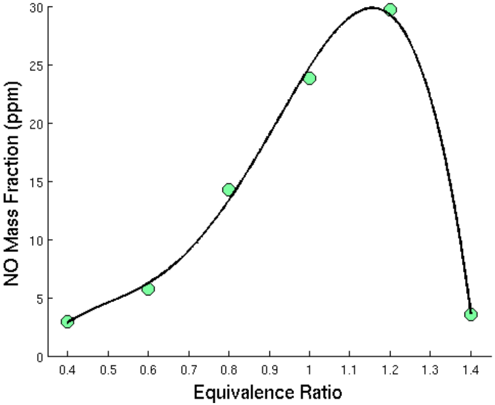

Figure: Variation of NO mass fraction with equivalence ratio $\phi = \frac{(A/F)_{st}}{(A/F)_{ac}}$.

Overview

Conclusions

- Validated furnaceFoam with Sandia Flame D experimental data.
- Validated NOxFoam with ANSYS Fluent using BFR test case.
- Demonstrated the effectiveness of NOx reduction mechanisms using BFR test case.
- OpenFOAM is found to be a promising alternative to costly commercial packages.

- The transient solver furnaceFoam is found to be 10 times slower then the steady state combustion solver in ANSYS Fluent.
- OpenFOAM is sensitive to mesh Non-orthogonality.

Recommendations

- Implementation of Conjugate Heat Transfer into furnaceFoam.
- Implementation of computationally less expensive equilibrium chemistry models.
- Implementation of steady state combustion solver to reduce the runtime.
- Prediction of other sources of NO i.e Prompt NO and NO from intermediate N2O.
- Linking PETSc with OpenFOAM for the solution of large sparse linear systems.

Thank you for your Attention !!