Literature Study Report
Combustion Modelling in OpenFOAM

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Contents

1 Introduction

The purpose of the present work is to gauge the capabilities of the open-source toolbox for CFD applications OpenFOAM(Open Field Operations and Manipulation) in Combustion Modelling. The gas combustion models available in OpenFOAM are transient models and significant calculation time is needed to obtain the steady state. The objective here is to compare the already available solvers for Combustion Modelling in OpenFOAM with its commercial counterparts and to create a new steady state solver for modelling gas combustion using the Eddy Break-Up Model.

The cold-flow and reacting-flow results are obtained for a BFR(Burner Flow Reactor) Geometry. OpenFOAM is evaluated against results obtained from the commerical CFD package Fluent.

After the comparison is made and the results if found satisfactory we aim to proceed further with combustion modelling in OpenFOAM for the much complex Almatis Kiln [8].

2 Problem Definition

To compare the existing combustion capabilities of OpenFOAM with Ansys Fluent we consider the Burner Flow Reactor (BFR) [12] Geometry in 2D(axi-symmetric) .

2.1 Geometry of the Furnace

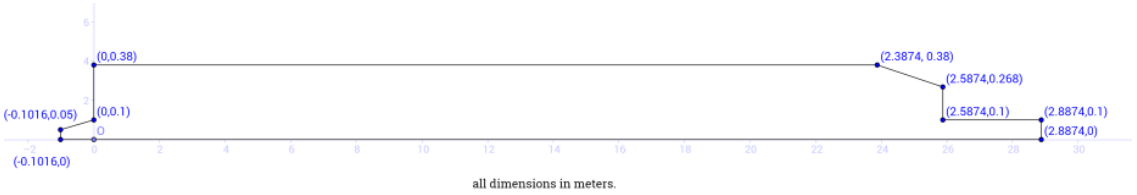

Figure 1: Burner Flow Reactor

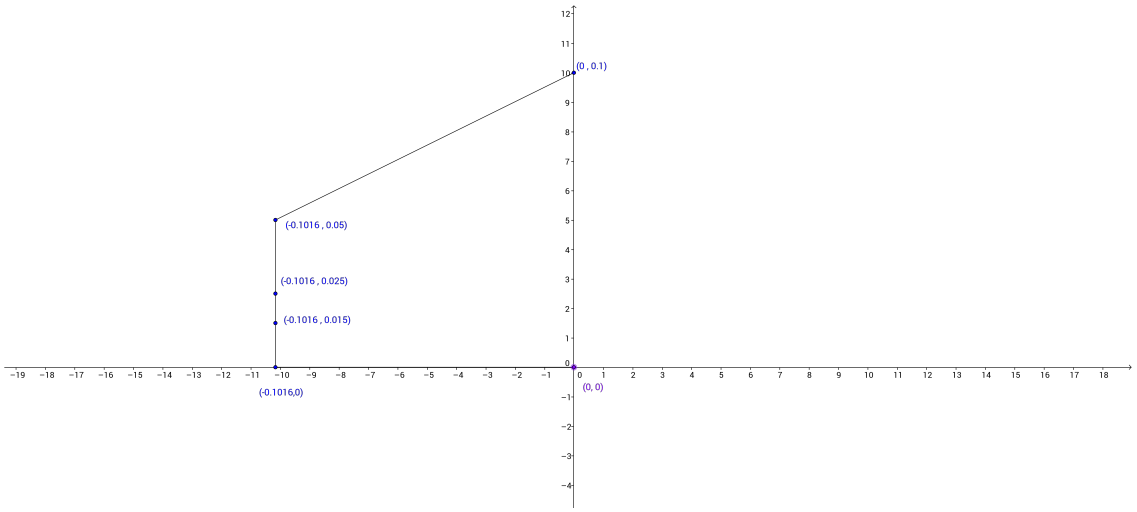

Figure 2: Center, Middle and Secondary Inlet dimensions in meters

2.2 Computational Mesh

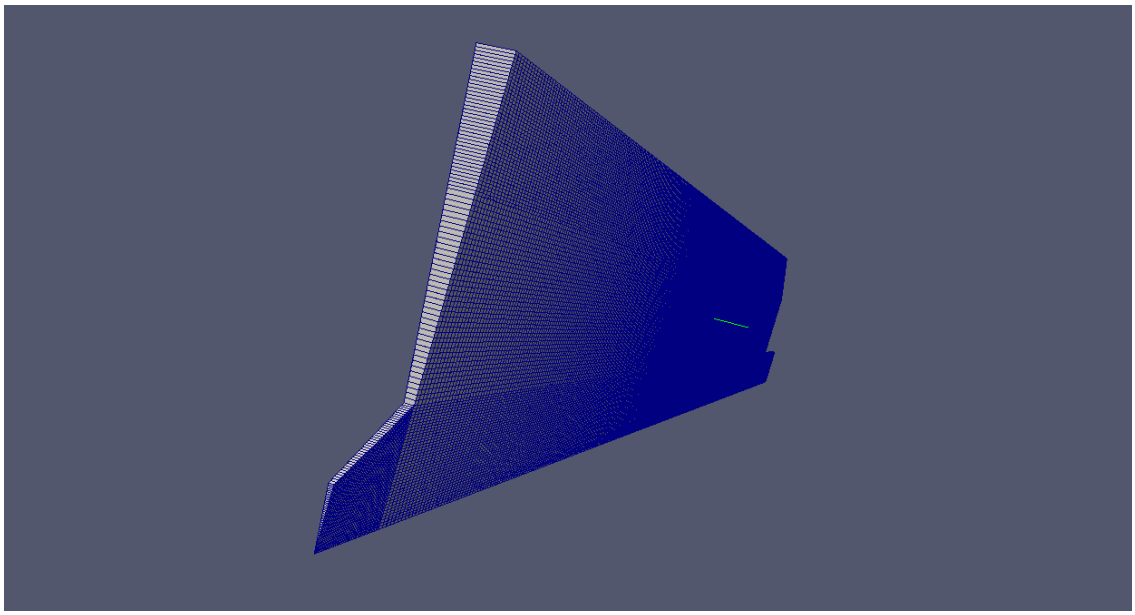

Figure 3: Axisymmetric Mesh with Wedge Angle(Angle of Cone) = 5°.

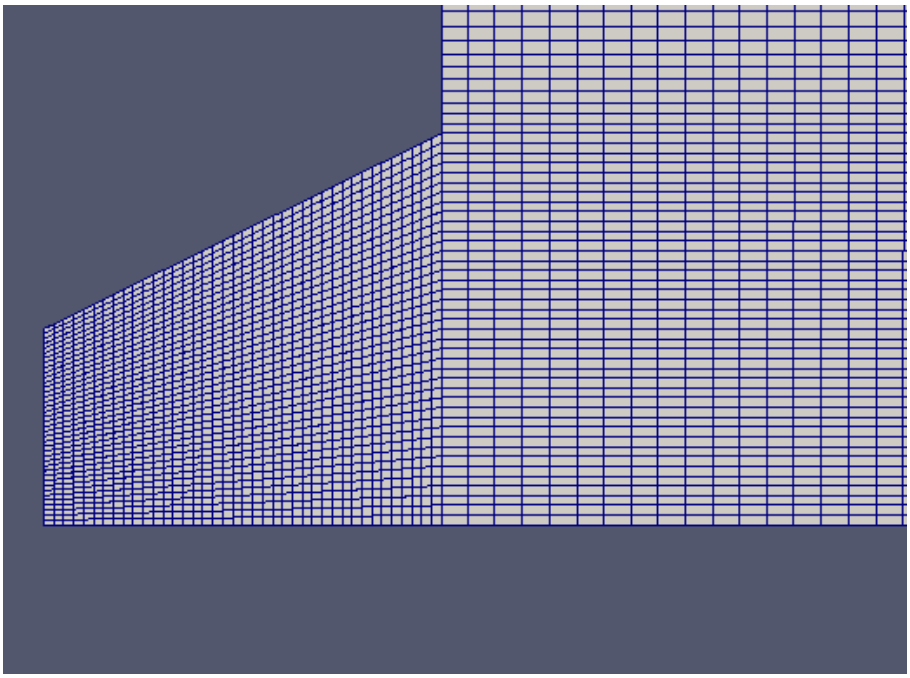

Figure 4: Surface Mesh(Total Number of Cells = 26600.) near Inlet

Note: We do not consider the full 3D geometry for combustion since the gas combustion model available in OpenFOAM is a transient model and significant calculation time is needed to obtain the steady state.

2.3 Physics Incorporated

- Turbulent Incompressible Flow.
- Gas Combustion of Methane - one step Irreversible Arrhenius Reaction
  $CH4 + 2O2 \longrightarrow CO2 + 2H2O$.

2.4 Boundary Conditions

Inlet	Velocity-Inlet (Swirling Flow Profile) Fixed Temperature Profile. Methane injected through the center and middle inlet. Air injected through the secondary inlet.
Outlet	Pressure-Outlet
Wall	No slip condition. Fixed Temperature (550K)
Internal Field	Initial Temperature (2000K) Initially Air is present.

3 Introduction to OpenFOAM

The OpenFOAM (Open Field Operation and Manipulation) CFD Toolbox is a free, open source CFD toolbox [1] capable of solving anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics. It includes tools for meshing, notably snappyHexMesh, a parallelised mesher for complex CAD geometries, and for pre- and post-processing. Almost everything (including meshing, and pre- and post-processing) runs in parallel as standard, enabling users to take full advantage of computer hardware at their disposal.

By being open, OpenFOAM offers users complete freedom to customise and extend its existing functionality, either by themselves or by others. It follows a highly modular code design in which collections of functionality (e.g. numerical methods, meshing, physical models, ...) are each compiled into their own shared library. Executable applications are then created that are simply linked to the library functionality.

The OpenFOAM source code comprises of four main components:

- src: the core OpenFOAM source code
- applications: collections of library functionality wrapped up into applications, such as solvers and utilities.
- tutorials: a suite of test cases that highlight a broad cross-section of OpenFOAM's capabilities
- doc: supporting documentation

3.1 OpenFOAM structure

One distinguishing feature of OpenFOAM is the way it represents the physics of the problem at hand. Its syntax for tensor operations and partial differential equations closely resembles the equations being solved. For example the equation For example the equation

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot \phi \mathbf{U} - \nabla \cdot \mu \nabla \mathbf{U} = -\nabla p \tag{1}$$

is represented by the code

```
solve
(
      fvm::ddt(rho,U)
    + fvm::div(phi,U)
    - fvm::laplacian(mu,U)
      ==
    - fvc::grad(p)
);
```

3.2 OpenFOAM versus Commercial Package

OpenFOAM is a C++ library, used primarily to create executables, known as applications and unlike its commerical counterparts it is not a GUI-based, mouse-driven "package".

4 Turbulence Modelling

- There are many approaches to turbulence modelling available in OpenFOAM [4]. For our case the primary factors affecting the choice of turbulence model are
  - The model should be reasonably accurate in modelling the physics encompassed in the flow.
  - The amount of time available for the simulation should be practically realizable considering the much complex turbulence-chemistry interaction that follows.
- The Reynolds Stress Model may take more iterations to converge than the k- ϵ model due to the strong coupling between the Reynolds stresses and the mean flow. Since for most practical engineering applications the Boussinesq hypothesis perform very well citefluent, the additional computational expense of the Reynolds stress model is not justified. Therefore we consider only Reynolds-averaged Navier-Stokes(RANS) models.
- There are many variants of RANS models available in OpenFOAM. The most suitable for our case are the standard and realizable k- ϵ models. Both the models have similar forms, with transport equations for k and ϵ. The major differences in the models are as follows:
  - the method of calculating turbulent viscosity
  - the turbulent Prandtl numbers governing the turbulent diffusion of k and ϵ
  - the generation and destruction terms in the ϵ equation
- Because of the following reasons we prefer the realizable k- ϵ model over the standard k- ϵ model
  - The standard k- ϵ model is valid only for fully turbulent flows.
  - The prediction of the spreading rate for axisymmetric jets is unexpectedly poor by the modeled dissipation equation in the standard k- ϵ model. Whereas the realizable k- ϵ model better predicts the spreading rate of both planar and round jets and also provides superior performance for flows involving rotation and recirculation due to complex secondary flow features.
  - The realizable k- ϵ model requires only slightly more computational effort than the standard k- ϵ model.

5 Combustion Modelling

The last section was dedicated to making a suitable choice for the turbulence model that would predict sufficiently accurate results for our case, at a moderate computational cost. This section is dedicated to making a similar choice for the chemistry model and turbulence-chemistry interaction.

There are many types of combustion processes and here we are only concerned with Gaseous Combustion(i.e. fuel and the oxidant both are in gas phase.). In particular we are concerned with turbulent non-premixed (diffusion flames) combustion in a furnace.

Combustion is a complex phenomenon involving many complicated physical and chemical processes, among which the following are the indispensable components.

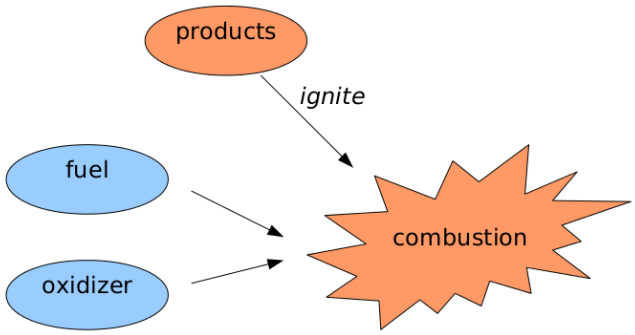

Figure 5: Combustion = Fuel + Oxygen

- turbulent fluid flow
- heat transfer
- chemical reactions
- radiative heat transfer

that would be needed to predict the flow, temperatures, resulting species concentrations and emissions from various combustion systems for the design and improvement of combustion equipment.

To be able to obtain reasonably accurate results in real time one has to make an intelligent choice of the models to be considered for each component. A fully detailed physical model would certainly give the best prediction but is not feasible considering the computational cost.

5.1 Chemistry Model

Combustion of a fuel does not occur in a single reaction, but may involve a number of different steps. [5]

Chemical kinetics determines how long it takes for a system to reach its final equilibrium state. Detailed reaction mechanism would best predict the concentration of the species and the associated thermodynamics, but at the cost of computational time. Therefore the decision is a trade-off between accuracy and cost.

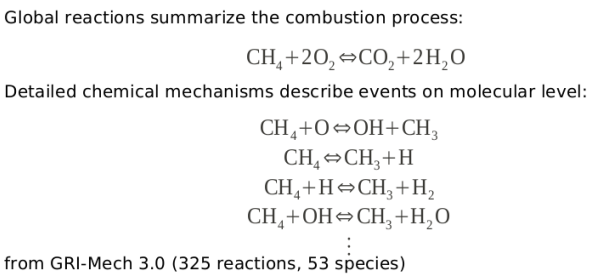

Figure 6: Combustion of Methane

5.2 Turbulence Chemistry Interaction

In combustion modelling it is required to determine rates of reactant consumption and product formation. These are used as source terms in transport equations for each of the species. There are many models available in literature that have been implemented in practice [7] and are found to be accurate to different degrees based upon there complexity and the physics they represent.

Turbulence Chemistry Interaction models are broadly divided into two categories viz Equilibrium Chemistry and Detailed Chemistry [3].

Equilibrium Chemistry Models			
Model	Summary	Suitable For	Cost
Eddy-Break Up (EBU)	computes only the mixing rate	turbulent flows, single step, global infinitely fast stoichiometric irreversible chemical reaction	less
Eddy-Dissipation (EDM)	modified EBU with product mass fraction replaced by the mean mass fraction of the deficient species in turbulent reaction rate expression	same as EBU	less

Detailed Chemistry Models			
Model	Summary	Suitable For	Cost
Laminar Finite-Rate Model	computes only the Arrhenius rate and neglects turbulence-chemistry interaction	relatively slow chemistry and small turbulent fluctuations	costly
Eddy-Dissipation-Concept (EDC)	extension of the EDM (EDC + infinite fast chemistry assumption = EDM), models turbulence-chemistry interaction with detailed chemical mechanisms, reaction rate depends on turbulent flow properties and chemical kinetics approach	turbulent flows where assumption of fast chemistry fails	costly

- **Laminar Finite-Rate Model:** The effect of turbulent fluctuations are ignored, and reaction rates are determined by Arrhenius expressions.The model is very accurate for relatively slow chemistry and small turbulent fluctuations. Since the chemical kinetic mechanisms are usually highly non-linear and form a set of stiff coupled ordinary differential equations the

cost of computations is very high. There are further possibilities of considering dissociation(backward reactions) along with the forward reactions. OpenFOAM and most commercial softwares allow detailed reaction mechanisms to be imported in CHEMKIN file format.

- **Eddy-Dissipation (EDM) Model:** Most fuels are fast burning and therefore reaction rates are assumed to be controlled by the turbulence, so expensive Arrhenius chemical kinetic calculations can be avoided. In non-premixed flames, turbulence slowly convects/mixes fuel and oxidizer into the reaction zones where they burn quickly. The combustion is said to be mixing-controlled, and the complex, and often unknown, chemical kinetic rates can be safely neglected.

  The chemical reaction rate is governed by the large-eddy mixing time scale, k/ϵ, (as in the eddy-breakup model). Combustion proceeds whenever turbulence is present ($k/\epsilon > 0$), and an ignition source is not required to initiate combustion. This is usually acceptable for non-premixed flames, but in premixed flames, the reactants will burn as soon as they enter the computational domain, upstream of the flame stabilizer. To remedy this both the Arrhenius, and eddy-dissipation reaction rates are calculated. The net reaction rate is taken as the minimum of these two rates. In practice, the Arrhenius rate acts as a kinetic switch, preventing reaction before the flame holder. Once the flame is ignited, the eddy-dissipation rate is generally smaller than the Arrhenius rate, and reactions are mixing-controlled.

  The model is computationally cheap, but, for realistic results, only one or two step heat-release mechanisms can be used. To incorporate multi-step chemical kinetic mechanisms in turbulent flows, the EDC model described below can be used.

- **Eddy-Dissipation-Concept (EDC):** The eddy-dissipation-concept (EDC) model is an extension of the eddy-dissipation model to include detailed chemical mechanisms in turbulent flows. Typical reaction mechanisms are invariably stiff and their numerical integration is computationally costly. Hence, the model should be used only when the assumption of fast chemistry is invalid.

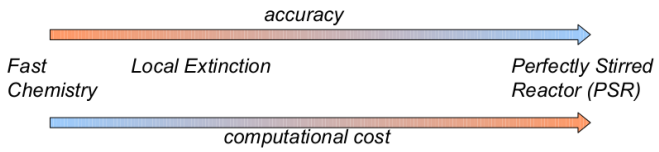

Figure 7: Different Approaches to EDC

  - **Fast Chemistry Model** approach assumes infinitely fast reactions.
  - **Perfectly Stirred Reactor Model(PSR)** (detailed chemistry) approach determines the steady state of a perfectly stirred reactor.
  - **Local Extinction Model** approach employs data fraom a priori PSR calculations.
  - **Partially Stirred Reactor Model(PaSR)** is a variant of **EDC-PSR**. The assumption in PSR that the entire cell is a perfectly stirred reactor is a severe overestimation and thus each cell is divided into a reacting part and a non-reacting part [9]. The reacting part is treated like a perfectly stirred reactor(PSR), in which all present species are homogeneously mixed and reacted. After reaction has taken place, the species are assumed to be mixed due to turbulence for the mixing time τ_{mix}, and the resulting concentration gives the final concentration in the entire, partially stirred, cell.

5.3 Choice of the Turbulence-Chemistry Interaction Model

Since combustion of turbulent diffusion flames in furnaces are physically controlled, i.e. the rate of combustion depends on flow, turbulence and diffusion processes, hence turbulence dominate mixing and subsequent combustion rather than chemical kinetics. This motivates the choice of **Equilibrium Chemistry Models** because of there simplicity and less computational cost.

However there are certain drawbacks of the Equilibrium Chemistry Models:

- Concerning Combustion, many things are not in equilibrium.
- chemical kinetics can play an important role under certain conditions, e.g. when the pressure is low or the supply of oxygen is restricted.
- Infinite rate assumption is a special case and works only with irreversible reactions.
- Strong turbulence can suppress combustion $\longrightarrow$ **Local Extinction** [6]

Since our final objective is to have a realistic model of the much complex Almatis Kiln(3D), apart from turbulence and combustion we would need to incorporate other important physical processes viz Radiation Modelling, Conjugate Heat Transfer etc. This would render the overall computational cost very high. Therefore considering the computational cost as the bottleneck, at this stage we restrict ourselves to the Equilibrium Chemistry Models i.e. Eddy-Break Up and Eddy Dissipation Models.

6 Cold Flow Computation

6.1 OpenFOAM Implementation

6.1.1 Boundary Conditions

BC	p	U	k	ε
Center Inlet	zG	(2.053,0,0)	0.0375	0.15
Middle Inlet	zG	(4.827,0,0)	0.0375	0.15
Secondary Inlet	zG	(10,4.5,12)	0.0375	0.15
Internal Field	0	(0,0,0)	0.0375	0.15
Walls	zG	(0,0,0)	0.0375	0.15
Outlet	0	zG	zG	zG

.
zG - zeroGradient.
(axial , radial , tangential).
wall functions used for k and ε
quantities in SI units.

Table 1: Boundary conditions for simpleFoam

For cold Flow Computation the constant kinematic viscosity of 1e-05 was used.

6.1.2 Solver Setup

- solver: simpleFoam
  Description: Steady-state solver for incompressible, turbulent flow.
- Turbulence Model: standard kEpsilon
  OpenFOAM is distributed with a large library of RAS(Reynolds-Averaged Simulation) turbulence models (ex. kEpsilon, realizableKE, etc). The open architecture of OpenFOAM allows developers to add turbulence models that can be selected at run time by the user.
- Equations Solved:
  The following equations are discretized using finite volume method and solved for obtaining the 6 unknowns p $\overline{u_1}$ $\overline{u_2}$ $\overline{u_3}$ k ϵ.

$$\frac{\partial \overline{u_j}}{\partial x_j} = 0$$

$$\overline{u_j}\frac{\partial \overline{u_i}}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu_{eff}(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i})\right], \quad i = 1,2,3$$

$$\frac{\partial k}{\partial t} + \overline{u_j}\frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\nu_{eff}\frac{\partial k}{\partial x_j}\right] + \nu_T\frac{\partial \overline{u_i}}{\partial x_j}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) - \epsilon$$

$$\frac{\partial \epsilon}{\partial t} + \overline{u_j}\frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left[(\nu + \frac{\nu_T}{\sigma_\epsilon})\frac{\partial \epsilon}{\partial x_j}\right] + C_{1\epsilon}\frac{\epsilon}{k}\nu_T\frac{\partial \overline{u_i}}{\partial x_j}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) - C_{2\epsilon}\frac{\epsilon^2}{k}$$

$$\nu_{eff} = \nu + \nu_T$$

$$\nu_T = C_\mu\frac{k^2}{\epsilon + \epsilon_s}$$

$$\sigma_k = 1 \quad \sigma_\epsilon = 1.3 \quad C_\mu = 0.09 \quad C_{1\epsilon} = 1.44 \quad C_{2\epsilon} = 1.92$$

Note:

σ_k and σ_ϵ are the turbulent Prandtl numbers for k and ϵ.

ϵ_s is a sufficiently small no added in OpenFOAM to avoid division by zero.

The $\frac{1}{\rho}$ factor infront of the pressure term in the RANS euqations is dropped in OpenFOAM. So if the true mean pressure field is sought for, one has to take this in consideration.

The default value of the model constants $C_{1\epsilon}, C_{2\epsilon}, C_\mu, \sigma_k$, and σ_ϵ have been determined from experiments with air and water for fundamental turbulent shear flows including homogeneous shear flows and decaying isotropic grid turbulence. They have been found to work fairly well for a wide range of wall-bounded and free shear flows. Although the default values of the model constants are the standard ones most widely accepted, one can change them (if needed) in OpenFOAM.

6.1.3 Control Parameters & Numerical Schemes

Control Parameters	
application	simpleFoam
endTime	10000

Numerical Schemes	
gradient	Gauss linear
velocity	bounded Gauss limitedLinearV 1
turbulence	bounded Gauss limitedLinearV 1
laplacian	Gauss linear corrected
interpolation	linear

Linear Solvers	
pressure	solver GAMG
	tolernace 1e-08
	relative tolerance 0.01
velocity	solver smoothSolver
	tolernace 1e-08
	relative tolerance 0.01
turbulence	solver smoothSolver
	tolernace 1e-08
	relative tolerance 0.01
SIMPLE	
nNonOrthogonalCorrectors	3
pressure	1e-08
velocity	1e-08
turbulence	1e-08
relaxation factors	
pressure	0.3
velocity	0.7
turbulence 0.7	

6.2 Comparison of results with Fluent

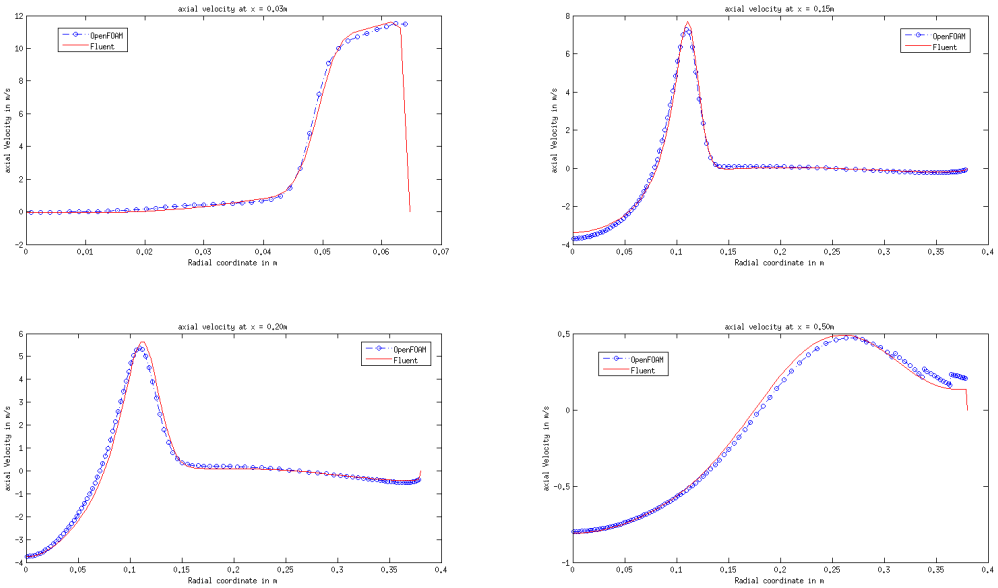

Figure 8: axial velocity profile comparison of OpenFOAM and Fluent

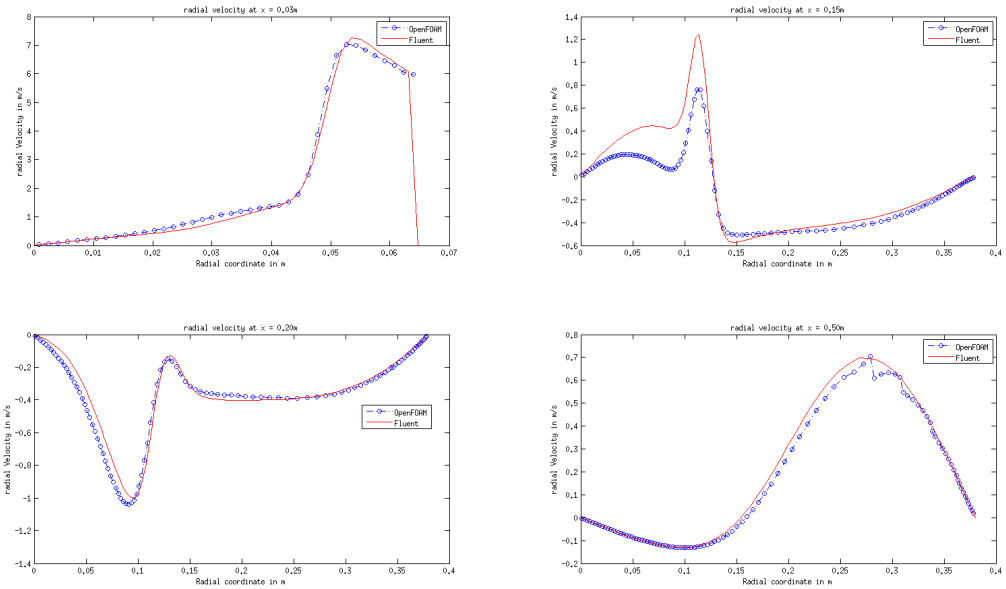

Figure 9: radial velocity profile comparison of OpenFOAM and Fluent

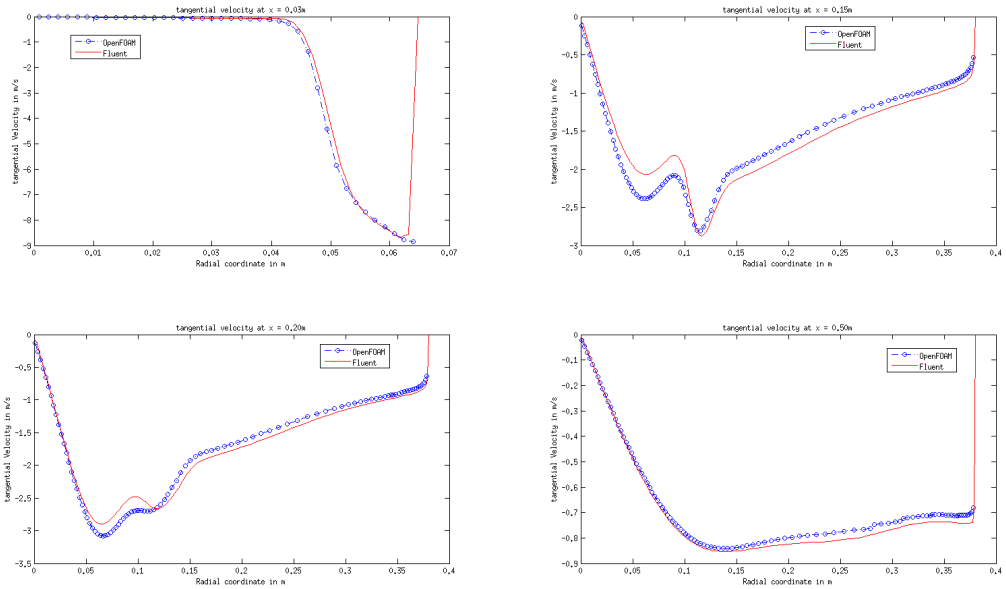

Figure 10: tangential velocity profile comparison of OpenFOAM and Fluent

7 Reacting Flow Computation

7.1 OpenFOAM Implementation

7.1.1 Boundary Conditions

BC	p	U	k	ε	T(K)	CH_4	O_2	N_2
Center Inlet	zG	(2.053,0,0)	0.0375	0.15	300	1.0	0	0
Middle Inlet	zG	(4.827,0,0)	0.0375	0.15	300	1.0	0	0
Secondary Inlet	zG	(10,4.5,12)	0.0375	0.15	411	0	0.234	0.766
Internal Field	1e+5	(0,0,0)	0.0375	0.15	2000	0	0.234	0.766
Walls	zG	(0,0,0)	0.0375	0.15	550	zG	zG	zG
Outlet	1e+5	zG	zG	zG	zG	zG	zG	zG

.
zG - zeroGradient.
(axial , radial , tangential).
wall functions used for k and ε
quantities in SI units.
mass fraction of species used.

Table 2: Boundary Conditions for reactingFoam

7.1.2 Control Parameters & Numerical Schemes

Control Parameters	
application	reactingFoam
endTime	10
deltaT	1e-02
adjustTimeStep	yes
maxCo	0.2

Numerical Schemes	
time integration	Euler
gradient	Gauss linear
pressure	Gauss limitedLinear 1
velocity	Gauss limitedLinearV 1
turbulence	Gauss limitedLinear 1
species	Gauss limiteLinear 1
laplacian	Gauss linear orthogonal
interpolation	linear

Linear Solvers	
density	solver diagonal
pressure	solver PCG
	preconditioner DIC
	tolernace 1e-06
	relative tolerance 0.1
velocity	solver PBiCG
	preconditioner DILU
	tolernace 1e-06
	relative tolerance 0.1
turbulence	solver PBiCG
	preconditioner DILU
	tolernace 1e-06
	relative tolerance 0.1
energy & species	solver PBiCG
	preconditioner DILU
	tolernace 1e-06
	relative tolerance 0.1
PIMPLE	
momentumPredictor	no
nOuterCorrectors	1
nCorrectors	2
nNonOrthogonalCorrectors	0

7.2 Comparison of results with Fluent

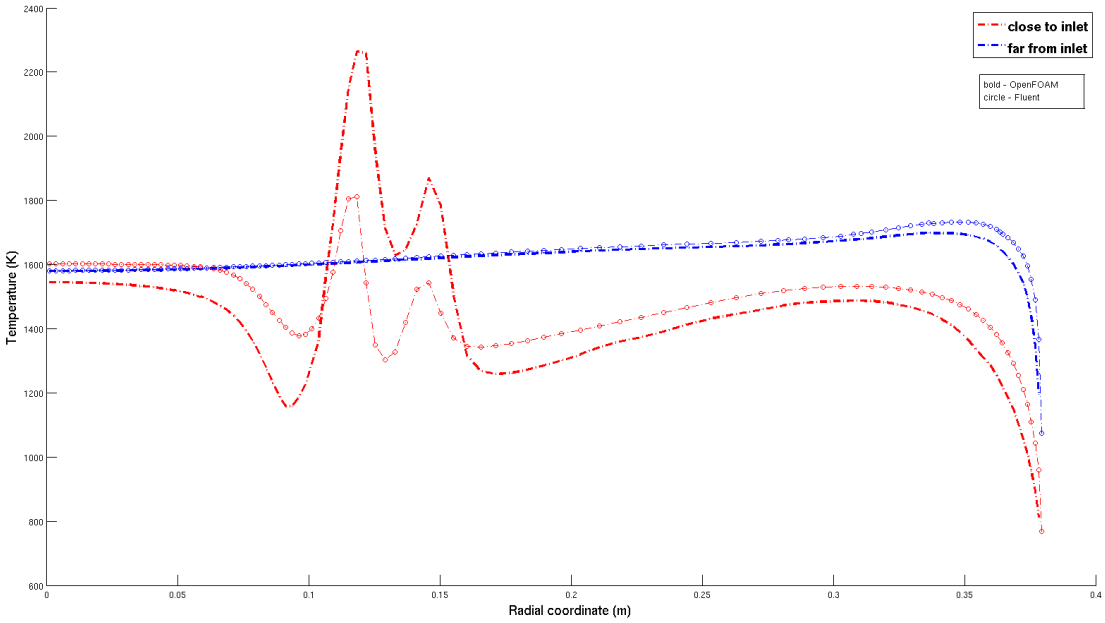

Figure 11: Temperature profile across the furnace

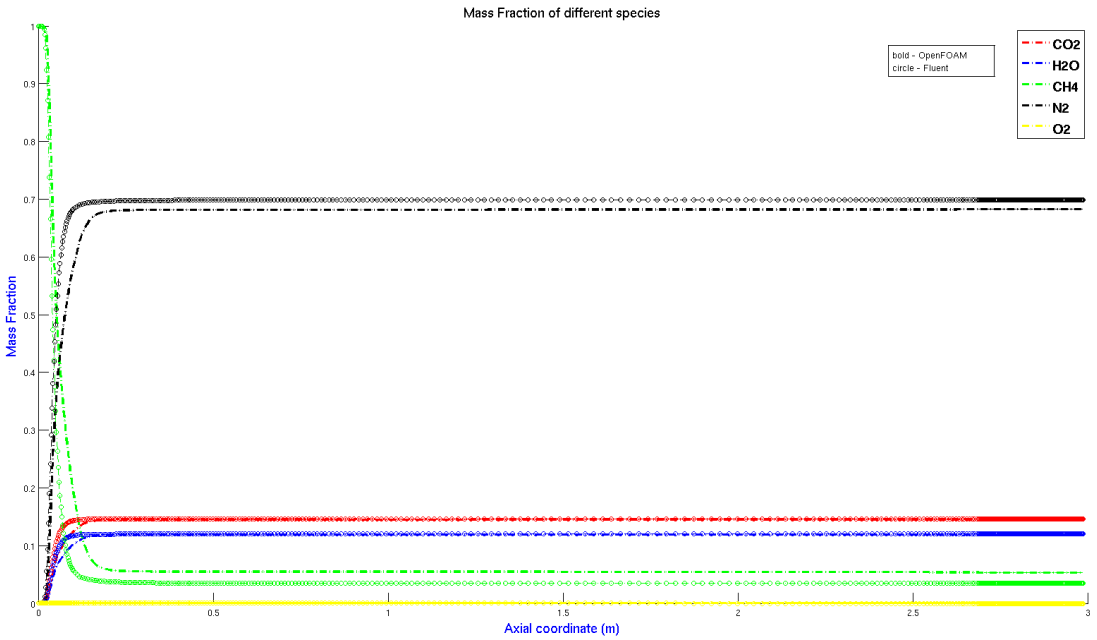

Figure 12: Mass Fraction along the axis

8 Results & Conclusions

8.1 Cold-Flow

The cold flow comparison gave almost identical results for both OpenFOAM and Fluent. The small difference is ascribed due to the interpolation of cell values to point values in post-processing. Considering the quality of the results and the time complexity overall both codes perform equally well.

8.2 Reacting-Flow

The reacting flow results obtained using OpenFOAM showed varying agreement with Fluent. The mass fraction of species showed good agreement with Fluent but the temperature profile showed significant differences. The peak temperature recorded in OpenFOAM is about $\sim$ 2200K whereas that observed from the Fluent results is about $\sim$ 2000K.

Specie	OpenFOAM(EDC-PaSR)	Fluent(EDM)	Fluent(EDC)
CO2	0.1455	0.1467	$\sim$
H2O	0.1191	0.1201	$\sim$
CH4	0.0527	0.0349	$\sim$
N2	0.6827	0.6982	$\sim$
O2	8e-07	1e-20	$\sim$

Table 3: Mass Fraction of Species at the Outlet

However, the current bottleneck considered with OpenFOAM is the very high computational cost of the transient solver reactingFoam as compared to the cost of the steady state solver in Fluent.

Criteria	**reactingFoam(transient)**	**Fluent(steady state)**
Setup Time	$\sim$ 1 hour	$\sim$ 1 hour
Solver Time	$\sim$ 3 days	$\sim$ 1 hour

9 Future Work

9.1 Revisit - What has been done

- Implemented standard $k-\epsilon$ turbulence model for incompressible flows in OpenFOAM using the steady-state solver simpleFOAM and compared the steady-state cold-flow results with the same model in Fluent 6.3.
- Implemented Partially Stirred Reactor(PaSR) combustion model in OpenFOAM for simulating non-premixed gas combustion of Methane. Reaction mechanism for methane considered - one step Irreversible Arrhenius Reaction CH4 + 2O2 $\longrightarrow$ CO2 + 2H2O. Species modelled CH4, O2, H2O, CO2, N2. The comparison is made with a steady state combustion model in Fluent based on the Eddy Dissipation Model.

9.2 Future Work

Since currently OpenFOAM has no steady state gas combustion model, it would be of great interest to develop such a model. Considering the computational cost as the bottleneck of the problem we would emphasis much on developing the equilibrium chemistry models.

A comparison would be made between the results of OpenFOAM and Fluent for the same model. If the results are found satisfactory we would proceed further with combustion modelling in OpenFOAM for the much complex Almatis Kiln. There are two possible directions which needs to be explored further.

- One would be to consider different combustion models for obtaining more accurate results compared to the equilibrium chemistry models. To make a better prediction of the temperature distribution in the furnace Conjugate Heat Transfer and Thermal Radiation needs to be incorporated in the existing model.
- The other direction would be to consider the complete geometry of the Almatis Kiln. This would require exploring better mess generation utilities and the parallel processing capabilities of OpenFOAM.

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