

# Numerical simulation of methane jet using OpenFOAM

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## Abstract

The objective of the present study is to numerically simulate methane jets in open source CFD package OpenFOAM. This report will help reader to understand the step-by-step procedure involved in simulating methane jets and also explain the details regarding initial and boundary conditions, solver settings etc. Geometry and mesh has been generated using 'blockMesh' utility available in OpenFoam and flow has been simulated using 'reactingFoam' solver. Two different conditions have been considered here viz. subsonic and supersonic jets. Numerical method has been validated against the benchmark experiments by Birch et al. (1984).

## 1 Introduction

Methane is a highly flammable gas and its unintentional release can leads to explosions, fires, posing risks to human health and property. Computational Fluid Dynamics has been widely used to understand the flammable gas dispersion in open as well as closed spaces. OpenFOAM is an open-source CFD package widely used in research fraternity. In this study OpenFoam has been used to simulate methane jets. Numerical methodology given in Fiates & Vianna (2016) has been used in the present study. The obtained results are validated against the benchmark experimental results available in the literature. The remainder of the report consists of three major sections. Section 2 will discuss the methodology used to solve the problem. The problem statement, governing equations, details of the solver and mesh setup have been explained thoroughly. Section 3 goes over the cases that are simulated. The initial boundary conditions are discussed for each of the cases. The fourth section focuses on the results and the relevant interpretation, contours, graphs, grid independence studies and lastly validation against a classical experiment. The final section provides a conclusion to the study.

## 2 Governing Equations and Models

The primary objective of this study is to validate the axial concentration and velocity decay of a methane jet obtained from OpenFOAM simulation with experimental results. The study analyses the jet characteristics at subsonic and supersonic velocities. The numerical model is developed on the basis of Fiates & Vianna (2016) and is then validated against the classical experiments done by Birch et al. (1984). In the present study, three-dimensional continuity and momentum equations are considered along with the scalar transport equations (due to the involvement of species transfer in the same phase). Governing equations considered in the present study are as follows,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \quad (1)$$

$$\frac{\partial(\rho v)}{\partial t} + \nabla \cdot (\rho v v) - \nabla \cdot \bar{\bar{\tau}} = -\nabla p \quad (2)$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho v h) = -\nabla \cdot q + \frac{\partial p}{\partial t} + v \cdot \nabla p + \bar{\bar{\tau}} : \nabla v \quad (3)$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i v) + \nabla \cdot (\rho Y_i V_i) = w_i \quad (4)$$

where  $t$  is time,  $\rho$  is mixture density,  $v$  is velocity,  $p$  is pressure,  $Y_i$  is the mass fraction of species,  $V_i$  is the diffusion velocity of species  $i$ ,  $w_i$  is the mass reaction rate of species,  $h$  is specific total enthalpy of the mixture, and  $\bar{\bar{\tau}}$  is the stress tensor Yang et al. (2019). The turbulence model used in this simulation is  $k - \epsilon$ . Following equations have been used to compute  $k$  and  $\epsilon$ .

$$k = \frac{3}{2}(UI)^2 \quad (5)$$

$$\epsilon = C_\mu \frac{k^{\frac{3}{2}}}{l} \quad (6)$$

where  $U$  is the flow velocity and the  $I$  is the turbulence intensity. The turbulence intensity chosen for this problem is taken as 5%.  $C_\mu$  is the turbulence model constant and the value is 0.09. The values were computed for this simulation was done using *Wolf dynamics turbulence calculator* (n.d.).

## 3 Simulation Procedure

This section gives a step-by-step process of the simulation procedure. The particulars are either explained or referred to a source for better comprehension.

### 3.1 Geometry and Mesh

The geometry considered to replicate the problem in CFD is given in Fig. 1, which is taken from Fiates & Vianna (2016).

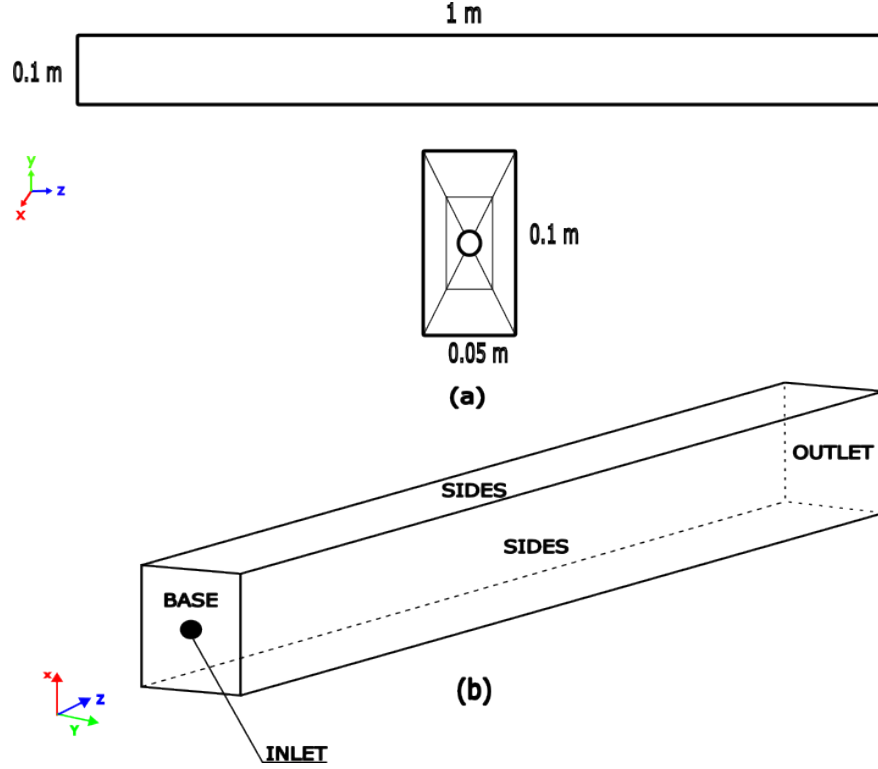


Figure 1: (a) Dimensions of the domain considered in the present study, and (b) isometric view of the domain with patch names

Base	Modelled as an Inlet/Outlet
Sides	Modelled as an Inlet/Outlet
Inlet	Modelled as a pure Inlet
Outlet	Modelled as a far field patch

Table 1: Boundary conditions

Geometry as well as meshing has been done using 'blockMesh' utility available in OpenFOAM. Structured non-uniform mesh has been generated. Different patch names and corresponding boundary conditions have been listed in Table 1. The domain is broken into 9 major blocks where the orifice has 5 other blocks as it is made using O-grids as shown in Fig 2 (b). Three different mesh grids have been considered for the purpose of grid independence study. The grid sizes are given in the Table 2.

Grid	Grid size (cells)
Grid 1	48000
Grid 2	75000
Grid 3	95000

Table 2: Grid sizes

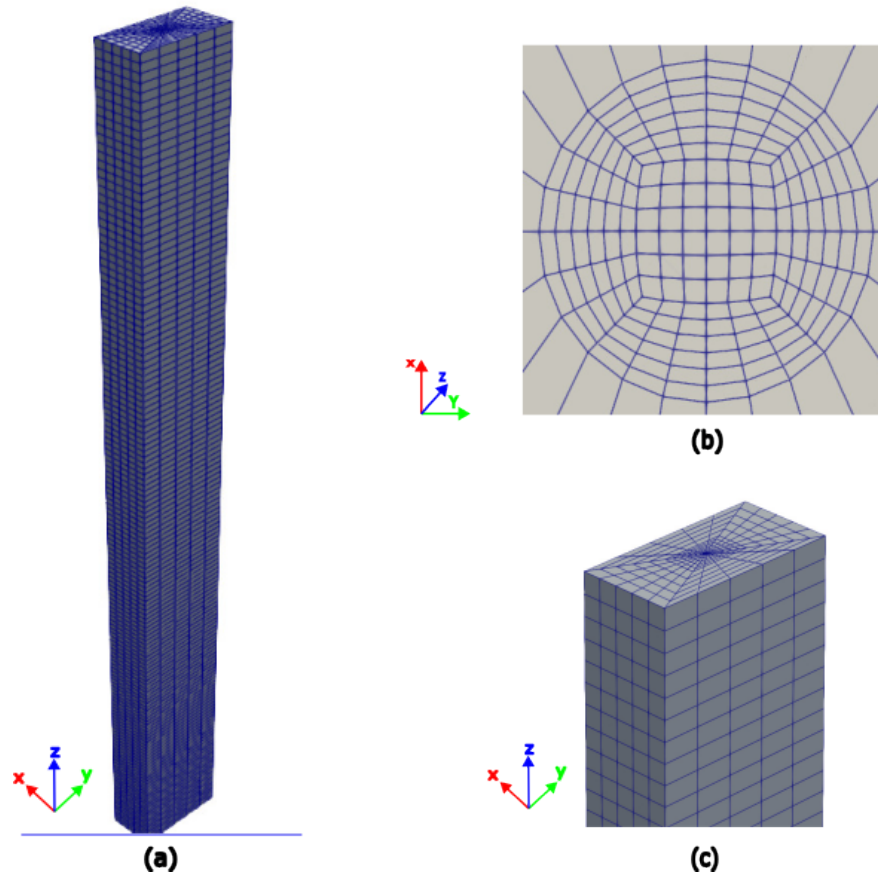


Figure 2: (a) Meshed domain (b) O-Grid for the orifice (c) Close up of the O-Grid with the domain

### 3.2 Initial and Boundary Conditions

Two different cases were simulated in OpenFOAM. The boundary conditions considered for various boundaries are given below.

Patch name	Velocity	Pressure	Temperature
Inlet	fixedValue	zeroGradient	fixedValue
Outlet	zeroGradient	fixedValue	fixedValue
Base	pressureInletOutletVelocity	fixedValue	fixedValue
Side	pressureInletOutletVelocity	fixedValue	fixedValue

Table 3: Boundary conditions for flow properties

Patch name	$CH_4$	$N_2$	$O_2$
Inlet	fixedValue	calculated	fixedValue
Outlet	inletOutlet	calculated	zeroGradient
Base	zeroGradient	calculated	zeroGradient
Side	inletOutlet	calculated	zeroGradient

Table 4: Boundary conditions for individual species

The patch types used in this case are explained below whose explanation and understanding are taken from the the reference Greenshields & Weller (2022).

- *pressureInletOutletVelocity* - It sets the outflow condition as a zero-gradient condition and the inflow velocity calculated by from the flux averaged over the patch. The initial value for the patch must be given which is usually (0 0 0).
- *zeroGradient* - It the boundary condition that basically states that the value normal to the patch remains constant. That is the value is constant with respect to space.
- *fixedValue* - It is the boundary condition that gives fixed value properties to each of the patches. In this boundary condition the value remains constant with respect to time.
- *inletOutlet* - It combines the behavior of an inlet and an outlet. When fluid is flowing into the domain, it behaves like a fixed value boundary condition; when fluid is flowing out, it acts like a zero gradient boundary condition.
- *calculated* - It is a boundary condition where the value is decided by the solver by calculating the patch values from the adjacent cells. It is used in places where the value is not mentioned.

As discussed in the section before the two cases simulated that is subsonic and supersonic and the initial conditions for both the cases are given below in Tables 5 and 6.

Patch name	Velocity (m/s)	Pressure (Pa)	Temperature (K)
internalField	uniform (0 0 0)	uniform 200000	uniform 300
Inlet	347.2	-	300
Outlet	-	200000	300
Base	value (0 0 0)	200000	300
Side	value (0 0 0)	200000	300

Table 5: Initial conditions for Case 1.

Patch name	Velocity (m/s)	Pressure (Pa)	Temperature (K)
internalField	uniform (0 0 0)	uniform 200000	uniform 300
Inlet	440.95	-	300
Outlet	-	350000	300
Base	value (0 0 0)	350000	300
Side	value (0 0 0)	350000	300

Table 6: Initial conditions for Case 2.

The initial conditions for the individual species is given below. They are the same for both the subsonic and the supersonic case.

Patch name	$CH_4$	$N_2$	$O_2$
internalField	uniform 0	uniform 0.79	uniform 0.21
Inlet	uniform 1.0	\$internalField	uniform 0
Outlet	\$internalField	\$internalField	-
Base	-	\$internalField	-
Side	\$internalField	\$internalField	-

Table 7: Initial conditions for Individual Species

### 3.3 Solver

The solver used in the problem is 'reactingFoam'. Solver 'reactingFoam' is a pressure-based solver designed for transient simulations of compressible, reacting flows. It handles laminar and turbulent, multispecies flows with temperature and density variations (it solves the energy equation). This solver is well-suited for the simulation of combustion processes and chemical reactions within fluids, accommodating a variety of reaction kinetics and species transport mechanisms. The tutorial file used for this setup is the 'membrane' tutorial available in OpenFoam 10.

The available tutorial has been modified with geometry, mesh, flow conditions, and boundary conditions, which are specific to methane jets. Other solver conditions and algorithms are taken as it is from 'membrane' tutorial. As mentioned above the 'membrane' tutorial is used, the modifications made to the *constant/physicalProperties* file is given below in Table 8. These modifications are necessary so that the solver can be made to fit the problem that is being simulated. The heP-siThermo model uses compressibility as a major parameter to calculate the temperature of the gas. The const transport model uses viscosity and Prandlt number to compute the transport characteristics of the species. Since enthalpy is computed for compressible flows the hConst thermodynamic model is used instead of the eConst which is preferred for incompressible flows.

Turbulence model used	$k-\epsilon$
Thermodynamic model used	hePsiThermo
Mixture	multiComponentMixture
Transport	const
Thermodynamic property	hConst
energy equation used	sensibleEnthalpy
Equation of State	PerfectGas
Specie	Multi-specie
Combustion models	Off

Table 8: Solver settings

### 3.4 Probe Function

The probe function acts as non-intrusive method to monitor a certain quantity at any point in the domain. Following code snippet has been added to *controlDict* file in order to monitor velocity at a point (0.25, 0.5, 0.05) in the domain.

```
functions
{
    probes
    {
        type    probes;
        libs    ("libsmapping.so");
        writeControl timeStep;
        writeInterval 1;

        fields
        (
            U
        );

        probeLocations
        (
            (0.25 0.5 0.05)
        )
    }
}
```

In this present study, probe function has been used to monitor velocity at a particular point in the domain to understand flow characteristics during simulation. For every time step, the data is read at the prescribed point, and it is appended to a file called probe in the *postprocessing* folder. This subroutine can be synced with the time step or can be independent of it .ie. a separate write interval can be set for the subroutine. The results of the probe function is given below. The probe location

is set at a distance of 0.05 m from the inlet axially. As we can interpret, the flow at that point stabilizes at 0.01 seconds, yet it is run for a longer time such that the flow stabilizes downstream as well.

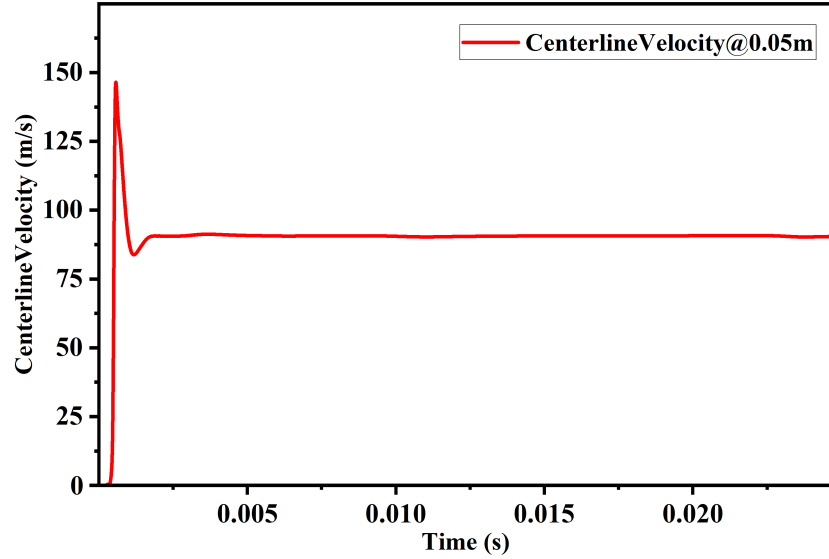


Figure 3: Variation of center line velocity monitored at a location in domain with time.

## 4 Results and Discussion

Comparison of numerical results with experimental results and different contours are presented here in this section. Three different mesh sizes were simulated for each of the two cases and the plots are displayed for the same. Keeping this as the basis, the validation of axial concentration decay is done against the classical experiments conducted by Birch et al. (1984).

### 4.1 Case 1: Subsonic case

The study was conducted for three different grid sizes and the mean concentration in the x axis and the axial displacement in the y axis is plotted. Refer to Table 2 for the number of cells in each grid. Fig. 4(a) shows the three grids and the solution of the 3 grids. The maximum error between coarse and the fine grid is 12.536%. Figure 4 (b) shows the variation of mean concentration against axial displacement corresponds to grid 2 against the experimental data. The maximum percentage error difference in the experimental to the numerical data is found to be 7%. This is within the acceptable error range for a CFD simulation against experimental data.



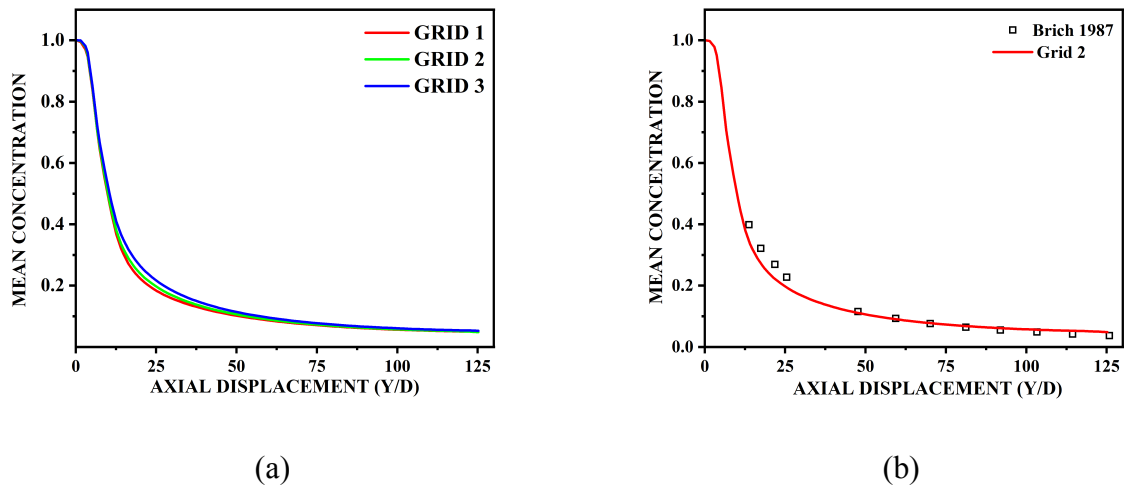


Figure 4: (a) Mesh independence study, and (b) Plots the solution against the experimental data.

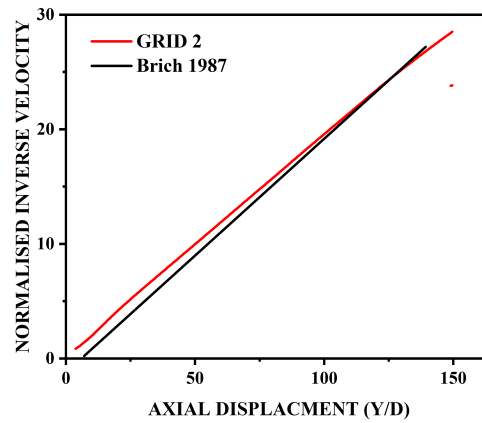


Figure 5: Velocity validation of against experimental data

The contours for the concentration of the plume are shown in Fig. 6. As expected, the concentration of CH<sub>4</sub> near the orifice is the maximum, and the concentration decreases axially. Fig 5 plots the normalised inverse velocity against the axial displacement. The maximum error observed is 11.07% which is acceptable.

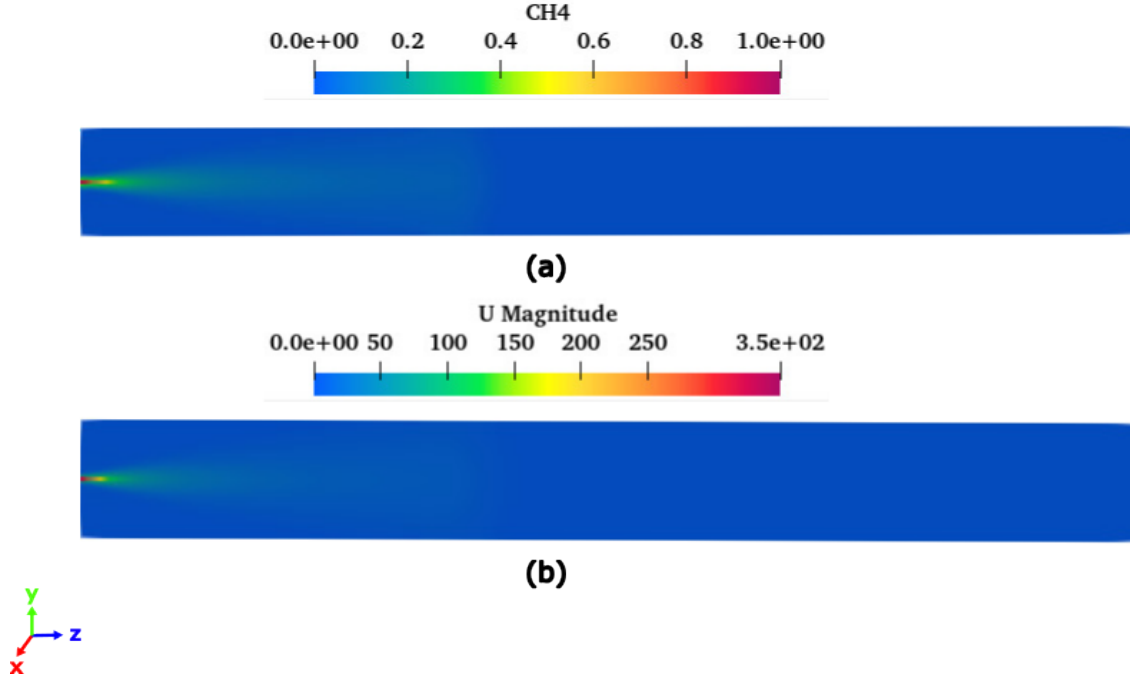


Figure 6: (a) Mean concentration contours, and (b) Velocity contours.

## 4.2 Case 2: Supersonic case

Figure 7 (a) shows the variation of mean concentration of CH<sub>4</sub> with axial displacement for three grids considered in the present study. The maximum error between coarse and the fine grid is found to be 10.865%. Figure 7 (b) shows the variation of obtained numerical mean concentration of CH<sub>4</sub> with axial displacement of grid 2 against the experimental data. The maximum percentage error difference between the experimental to the numerical data is found to be 8%. This is within the acceptable error range for a CFD simulation and experimental data.

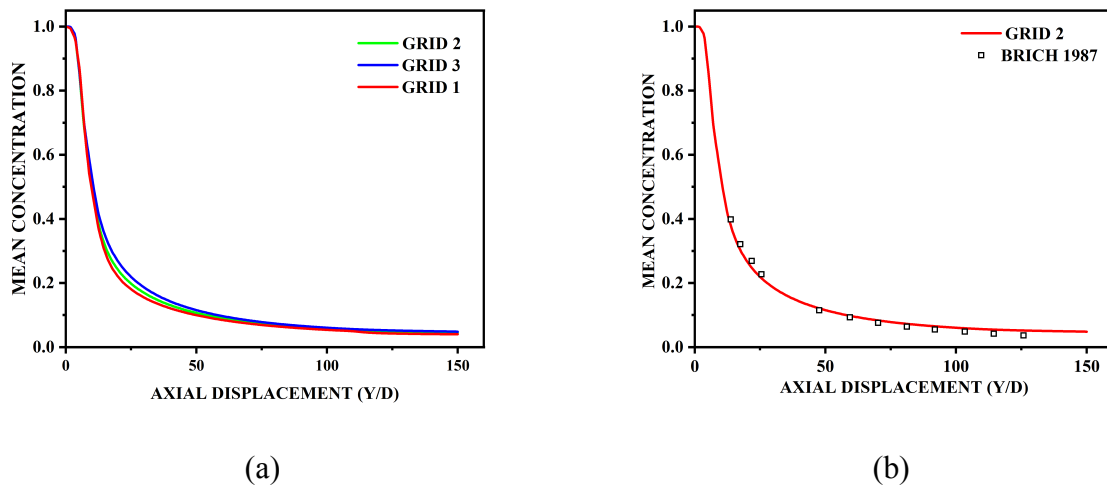


Figure 7: (a) Mesh independence study, and (b) Plots the solution against the experimental data.

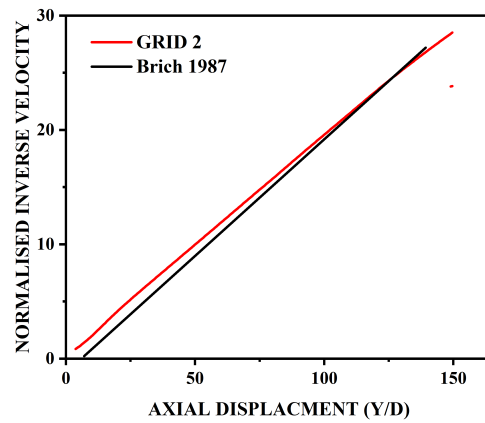


Figure 8: Velocity validation of against experimental data

The contours for the concentration of the plume are shown in Fig. 9. As expected, the concentration of CH<sub>4</sub> near the orifice is the maximum, and the concentration decreases axially. Fig 8 plots the normalised inverse velocity against the axial displacement. The maximum error observed is 13.4% which is acceptable.

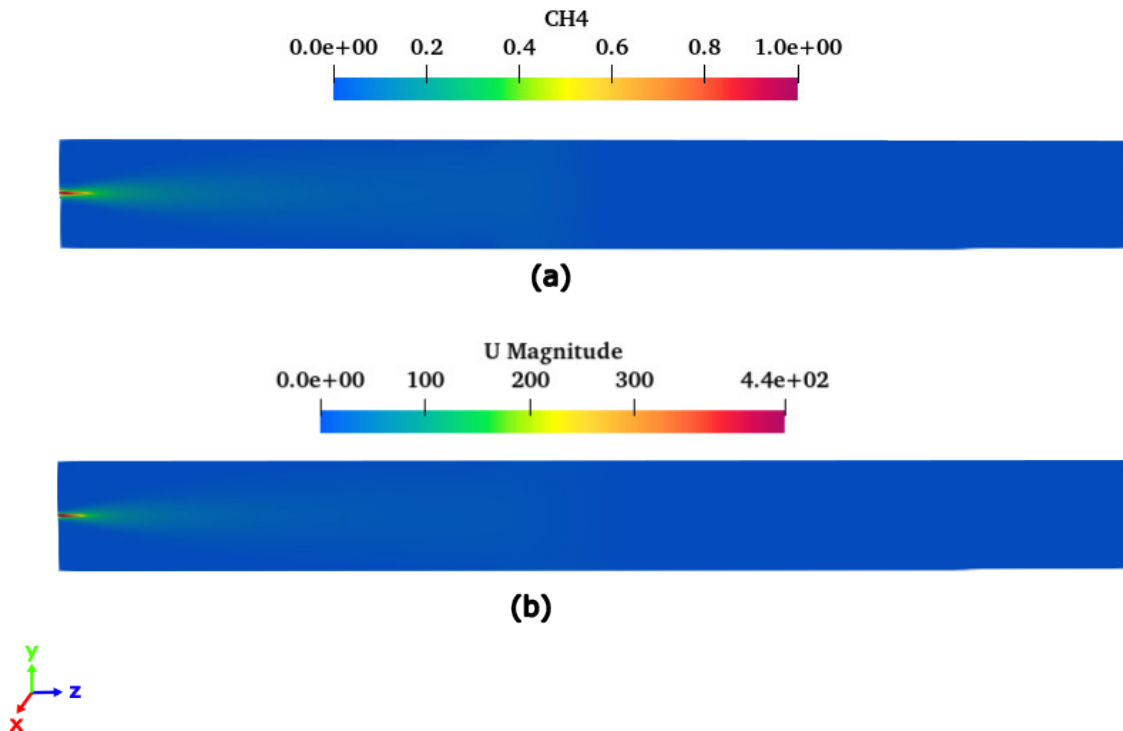


Figure 9: (a)Mean concentration contours, and (b) Velocity contours.

## Conclusion

In the present study, numerical simulations have been carried out using open source CFD package OpenFOAM to simulate methane jet dispersion. OpenFoam solver 'reactingFoam' has been used in simulations. Detailed step-by-step procedure, boundary conditions, initial conditions as well as solver details are explained in the report. The results were then validated against the classical experiments done by Birch et al. (1984). A grid independence study was done, and the mesh size independence was confirmed. The run time for the mesh with the highest grid cells is about 7 hours. The machine used for the study is a Intel i5 8th gen 64 bit processor, 8 Gb RAM, Ubuntu 20.04 LTS on OpenFoam version 11. Maximum percentage error between experimental and numerical results are found to be 8, which is found to be reasonable.

## References

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