A comparison of CFD Software packages to find the suitable one for numerical modeling of gasification process

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Abstract

The increasing demand for energy, depletion of oil, and gas resources, and threat of global climate change have lead to growing interest in coal gasification throughout the world. Gasification is a process that converts organic or fossil-based carbonaceous materials into carbon monoxide, hydrogen and carbon dioxide. This is achieved by reacting the material at high temperatures (greater than $700\,°C$), without combustion, with a controlled amount of oxygen and/or steam. The resulting gas mixture is called syngas (from synthesis gas or synthetic gas) or producer gas and is itself a fuel. The power derived from gasification and combustion of the resultant gas is considered to be a source of renewable energy if the gasified compounds were obtained from biomass. Fluidized bed combustion and gasification is a multiphase reactive flow phenomenon. It is a multiphase problem between gases and fuel particles and also a reactive flow problem, which involves homogeneous reactions among gases and heterogeneous reactions between fuel particles and gases. Hence, in order to do a comprehensive study and an accurate simulation of such complex flow it is necessary to develop a CFD software. The aim of this project is to make a comparison between CFD software packages in general and choose the a suitable one for modeling of gasification process.

1   Introduction

Fast consumption of fossils fuels, energy security, and environmental concerns are demanding effective use of fossil fuels. Due to this, more and more attention has been focused on clean coal technologies. Among these technologies fluidized bed combustion and gasification devices are crucial technologies to

provide an efficient, economic method for generating power from coal with substantially reduced emission of carbon dioxide and pollutant gases [1]. Fluidized bed combustors and gasifiers are widely used in many chemical and power industries due to their high heat transfer rates, high efficiency, low combustion temperature, and capability of controlling greenhouse emissions. Applications of fluidized bed combustors and gasifiers are developing at a fast pace in the power generating industry because they combine fuel flexibility and high efficiency especially for biomass combustion.

The use of computational fluid dynamics (CFD) as a tool in the design and optimization of combustion systems has greatly increased over the past years due to the availability of ever more powerful and affordable hardware. In pulverized coal combustion and gasification, CFD has successfully been used to study pilot-scale and industrial scale furnaces and gasifiers. The combustion of pulverized coal is a complex interaction of several processes: turbulent gas motion and particle dispersion, particle heat up and mass transfer to the gas phase, turbulent gas phase reactions and heterogeneous particle reactions, and radiative heat transfer [2]. Two-phase flow problem, such as pulverized coal combustion, is characterized by non-linear coupling between the two phases such as gas turbulence influencing the particle motion and particle heat up. In turn, the presence of the particles and their mass and heat transfer modify the gas phase. The accurate prediction of coal combustion requires an accurate description of the continuous gas phase and the coal particle phase [3] and [4]. Therefor, it is crucial to develop a CFD software to do a comprehensive study and an accurate simulation of such complex flow. The purpose of this project is to put together information on the existing CFD packages that

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are already in use in academia or industry, then make a comparison between them, and finally decide which one is appropriate for numerical modeling of the gasification process.

2 Overview of Non-Commercial CFD software

2.1 SU^2

The Stanford University Unstructured (SU^2) suite is an open-source collection of software tools written in C++ for performing Partial Differential Equation (PDE) analysis and solving PDE-constrained optimization problems [5]. The toolset is designed with computational fluid dynamics and aerodynamic shape optimization in mind, but it is extensible (and has been extended) to treat arbitrary sets of governing equations such as electrodynamics, chemically reacting flows, and many others. The software structure has been designed for maximum flexibility, leveraging the class-inheritance features native to the C++ programming language. This makes SU^2 an ideal vehicle for performing multi-physics simulations, including multi-species thermochemical nonequilibrium flow analysis, combustion modeling, two-phase flow simulations, magnetohydrodynamics simulations, etc. Additionally, the decomposition of the flow solver allows for the rapid implementation of new spatial discretization methods and time-integration schemes. However, it seems that SU^2 is in its infancy and has a long way to be mature and bug-free.

2.2 OVERFLOW

The OVERset grid FLOW solver is a software package for simulating fluid flow around solid bodies using computational fluid dynamics [6]. It is a compressible 3-D flow solver that solves the time-dependent, Reynolds-averaged, Navier-Stokes equations using multiple overset structured grids. This software has been widely used to better understand the aerodynamic forces on a vehicle by evaluating the flow field surrounding the vehicle.

2.3 OpenFOAM

This code is really a library of C++ routines that facilitates the numerical solution of partial differential equations. Using this library, many different solvers (included with the software) have been built to address many classes of problems in fluid dynamics (and other fields as well). Applications range from laminar incompressible flow to fully turbulent reacting compressible flow. OpenFOAM is freely available under the GNU Public License [7]. It solves partial differential equations on an unstructured meshes and for post-processing, the distribution comes with a version of ParaView. Because OpenFOAM is a library of routines for solving partial differential equations, various people have contributed applications which address all sorts of physics. And, if you can not find a pre-built solver to meet your needs, you have the source code and all the required tools for building your own, customized application. Compared to writing your own code from scratch, the OpenFOAM library functions make it remarkably simple to create a solver.

The spatial discretization of equations is based on Finite Volume Method

(FVM). The time integral can be discretised in three ways:

Euler implicit uses implicit discretisation of the spatial terms, thereby taking current values ϕ^n.

$$\int_t^{t+\triangle t} \Lambda^* \phi \, d\mathbf{t} = \Lambda^* \phi^n \triangle t \tag{1}$$

It is first order accurate in time, guarantees boundedness and is unconditionally stable.

Explicit uses explicit discretisation of the spatial terms, thereby taking old values ϕ^0.

$$\int_t^{t+\triangle t} \Lambda^* \phi \, d\mathbf{t} = \Lambda^* \phi^0 \triangle t \tag{2}$$

It is first order accurate in time.

Crank Nicholson uses the trapezoid rule to discretise the spatial terms, thereby taking a mean of current values ϕ^n and old values ϕ^0.

$$\int_t^{t+\triangle t} \Lambda^* \phi \, d\mathbf{t} = \Lambda^* \left(\frac{\phi^n + \phi^0}{2} \right) \triangle t \tag{3}$$

It is second order accurate in time, is unconditionally stable but does not guarantee boundedness.

2.4 Mfix

Mfix is an open-source multiphase flow solver. Mfix is written in FORTRAN and uses The spatial discretization of equations is based on Finite Volume Method (FVM). The time integral is discretised using Implicit Euler or Crank-

Nicholson scheme [8].

2.5   Nek5000

Nek5000 which is written in F77 and C and uses MPI for message passing can be used for simulation of unsteady incompressible fluid flows with thermal and passive scalar transport. It is a time-stepping based code and does not currently support steady-state solvers, other than steady Stokes and steady heat conduction. It can handle general two- and three-dimensional domains described by isoparametric quad or hex elements. In addition, it can be used to compute axisymmetric flows [9].

For time discretization a kth-order backward- difference/ extrapolation (BDFk/ EXTk) scheme is used. Here the time-derivative of any scalar (such as velocity components, temperature and ...) is approximated to order k, using a one-sided backward differentiation, and the convection and diffusion terms are evaluated at time t^n. To avoid implicit treatment of the nonsymmetric convection term, we approximate it at tn by extrapolation of order k (EXT k), using values from t^{n-q}, q= 1,...,k. For example consider the convection-diffusion equation,

$$\frac{\partial u}{\partial t} + c \cdot \nabla u = \nu \nabla^2 u \tag{4}$$

Discretisation in space yields:

$$B\frac{\partial \underline{u}}{\partial t} + C\underline{u} = -\nu A\underline{u} \tag{5}$$

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which is equivalent to :

$$B\frac{\partial \underline{u}^n}{\partial t} + C\underline{u}^n = -\nu A\underline{u}^n \tag{6}$$

By evaluating each term at t^n ;

$$B\frac{\partial \underline{u}^n}{\partial t} = B\frac{3\underline{u} - 4\underline{u}^{n-1} + \underline{u}^{n-2}}{2\triangle t} + O(\triangle t^2) \tag{7}$$

$$Cu^n = 2Cu^{n-1} - Cu^{n-2} + O(\triangle t^2) \tag{8}$$

$$\nu A u^n = \nu A u^n \tag{9}$$

Rearranging the above equations, we get to :

$$Hu^n = \frac{1}{2\triangle t}\left(4Bu^{n-1} - Bu^{n-2}\right) + 2Cu^{n-1} - Cu^{n-2} + O(\triangle t^2) \tag{10}$$

With $H = \frac{3}{2\triangle t}B + \nu A$. H is well-conditioned and symmetric positive definite.

The spatial discretisation of equations is based on the spectral element method (SEM), which is a high-order weighted residual technique similar to the finite element method. In the SEM, the solution and data are represented in terms of Nth-order tensor-product polynomials within each of E deformable hexa-hedral (brick) elements. Typical discretisations involve E=10010,000 elements of order N=816 (corresponding to 5124096 points per element). The SEM exhibits very little numerical dispersion and dissipation, which can be

important, for example, in stability calculations, for long time integrations, and for high Reynolds number flows [9].

3   Overview of Commercial CFD software

3.1   COMSOL

COMSOL Multiphysics is a finite element solver and Simulation software package for various physics and engineering applications, especially coupled phenomena, or multiphysics. COMSOL Multiphysics also offers an extensive interface to MATLAB and its toolboxes for a large variety of programming, preprocessing and postprocessing possibilities. The packages are cross-platform (Windows, Mac, Linux). In addition to conventional physics-based user interfaces, COMSOL Multiphysics also allows for entering coupled systems of partial differential equations (PDEs) [10].

3.2   Aerosoft

Most of the applications of this software have been in the area of rocket combustion, but that does not mean it can't be used for other things. In its areas of strength this package has had great success. Aerosoft also makes the GUST unstructured (mesh) CFD solver, which comes with grid generation software [11].

3.3   ANSYS

Both of Fluent and CFX solvers come as integrated packages with grid generation and post-processing. CFX is now integrated into the ANSYS Workbench,

which allows user to take advantage of its vast structural analysis capability as well [12]. By reputation, CFX has traditionally been focused on turbomachinery applications, whereas Fluent is seen as a more general code. Fluent is an extremely versatile code that has probably been applied with success to more classes of flow than any other. Fluent's great strength is that they provide reasonably powerful tools in a tightly integrated package. Unlike CFX, Fluent has a great speed of calculations.

3.4   BARRACUDA VR

Barracuda Virtual Reactor enables users to accurately simulate industrial fluidized systems with complex particulate-solids chemical reactions, including catalysts or reacting solids, the effects of particle collisions, and dense-phase heat transfer. Specifically, this software is designed to focused on chemically reactive particle/gas flows. The graphical user interface provides customizable features with a logical workflow for efficient and rapid project setups, plus easy mesh generation and powerful post-processing are built in to the package [13].

4   Calculation

Being able to make a real comparison between different CFD packages and having a better idea of the possibilities they can offer, first, we choose three of them i.e. Nek5000, OpenFOAM and Mfix, Each of which has its own distinctive characteristics. Second, we run the same problem with them to compare the results.

4.1 Problem Specification

We decide to simulate a fluid flow over a cylinder which is a fundamental fluid mechanics problem of practical importance. The flow field over the cylinder is symmetric at low values of Reynolds number. As the Reynolds number increases, flow begins to separate behind the cylinder causing vortex shedding which is an unsteady phenomenon. Different patterns that a fluid might experience as it passes over a circular cylinder have been represented in Figure 1.
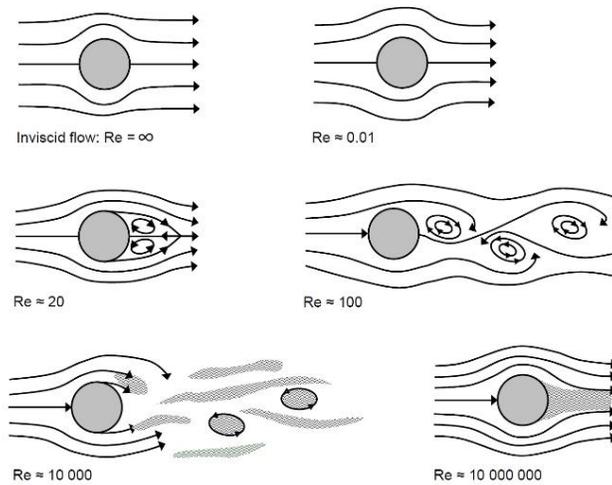

Figure 1: Flow patterns at various Reynolds Numbers [14]

The fluid viscosity slows down the fluid very close to the body. As a result, a thin slow-moving fluid layer called a boundary layer will be formed. The flow velocity is zero at the surface to satisfy the no-slip boundary condition. Now, suppose a fluid particle flows within the boundary layer around the circular cylinder. It is obvious that the pressure is a maximum at the stagnation

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point in front of the cylinder and gradually decreases along the front half of the cylinder. The flow stays attached in this region as expected. However, the pressure starts to increase in the rear half of the cylinder and the particle now experiences an adverse pressure gradient. Consequently, the flow separates from the surface and creates a highly turbulent region behind the cylinder called the wake. The boundary layer separating from the surface will eventually roll into a discrete vortex and detach from the surface (a phenomenon called vortex shedding).

The von Karman vortex shedding is observed at Reynolds number around 50. It is well known that up to Re= 100 the flow regime remains laminar, though it is unsteady and asymmetric. For Reynolds number greater than 300 the wake will be completely turbulent.

In this project, we choose three different Reynolds number to run the simulation i.e 20, 100 and 600 which correspond to laminar flow without vortex shedding, laminar flow with vortex shedding and turbulent flow, respectively.

4.2 Geometry

A computational domain is created surrounding the cylinder. The upstream length is 3 times the diameter of the cylinder, and the downstream length is 12 times the diameter of the cylinder. To facilitate meshing, a square with a side length of 6 times the diameter of the cylinder is created around the cylinder as shown in Figure 2.
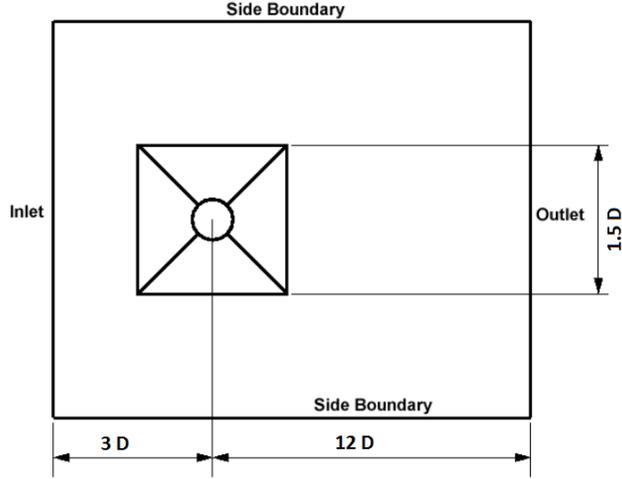
Figure 2: Geometry of the Problem

4.3 Laminar Flow

We model a laminar flow (Re=20 and 100) over a circular cylinder using Nek5000 and OpenFOAM.

Assuming the fluid is incompressible, single-phase and Newtonian with constant properties, the governing equations are continuity and Navier-Stokes equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0 \tag{11}$$

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + (V \cdot \nabla)V \right] = -\nabla p + \rho g + \mu \nabla^2 V \tag{12}$$

In which, ρ and $\mu=$ are density and viscosity of the fluid and V and p are the velocity and pressure fields, respectively.

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4.4   Boundary Conditions

A uniform velocity is given at the inlet (left side). The pressure at the outlet (right side) is set to zero as the boundary condition assuming that the fluid is going out to the atmospheric pressure (zero relative). Zero gradient boundary conditions have been applied on side walls.

5   Results (Laminar Flow)

5.1   Nek5000

Figure 3 shows the velocity-magnitude field for Re=20 at final time. As we expect, the result confirms that there is no vortex shedding at this Reynolds number. However, two symmetric circulating region have been formed just behind the cylinder.

In Figure 4 the velocity-magnitude field for Re=100 at final time has been represented. The Von Karman vortex street is clearly observable.

5.2   OpenFOAM

Figure 5 depicts the velocity-magnitude field obtained by icoFoam solver in OpenFOAM for Re=100 at the final time.

6   Validation

In analyzing a fluid flow over a cylinder, predicting the angle at which the boundary layer separates from the solid boundary is important. Here, we choose this criterion to see how accurate the predicted results are.
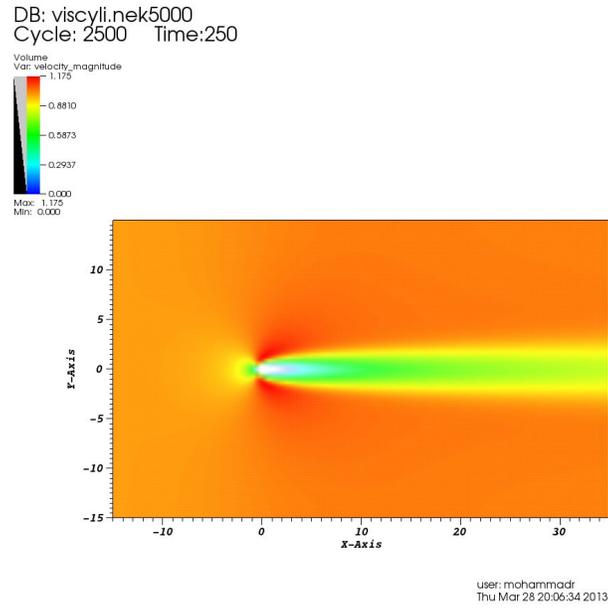
DB: viscyli.nek5000
Cycle: 2500   Time:250

Volume
Var: velocity_magnitude
— 1.175
— 0.8810
— 0.5873
— 0.2937
— 0.000
Max: 1.175
Min: 0.000

user: mohammadr
Thu Mar 28 20:06:34 2013

Figure 3: Velocity-magnitude field at Re=20, Nek5000

DB: vis.nek5000
Cycle: 2500   Time:250

Volume
Var: velocity_magnitude
— 1.343
— 1.007
— 0.6715
— 0.3357
— 0.000
Max: 1.343
Min: 0.000

user: mohammadr
Thu Mar 28 19:13:43 2013
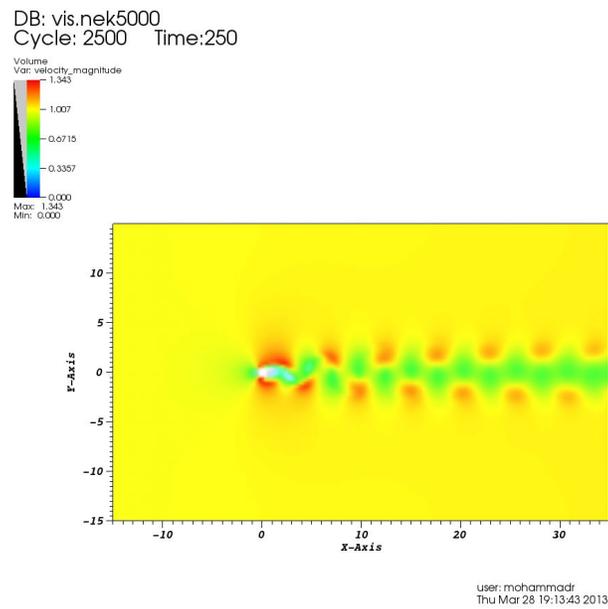
Figure 4: Velocity-magnitude field at Re=100, Nek5000

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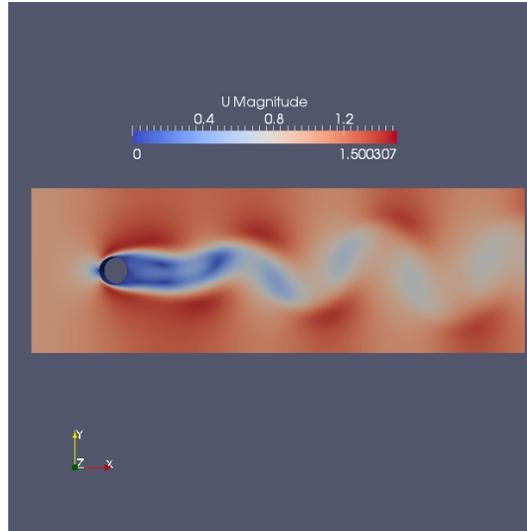
Figure 5: Velocity-magnitude field at Re=100, OpenFOAM

The boundary layer separation occurs at the position on the cylinder wall where the shear stress is zero. Hence, at the separation point the normal gradient of velocity at the wall is zero i.e. If we draw the velocity profile near the wall, the point at which the velocity is tangent to normal axis is the separation point After which there is a rivers flow, as depicted in the Figure 6. Figures 7, 8 and 9 show the velocity profile, obtained by OpenFOAM, of
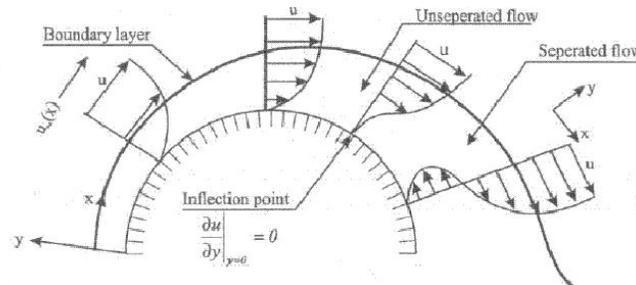
Figure 6: Separation of the Boundary layer on the solid surface [15]

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the fluid near the cylinder wall at 90, 119 and 135 degree, respectively. From the figures we can conclude that the separation occurs at about 119 degree. After that point the velocity near the wall will become negative and hence the fluid flows reversely.
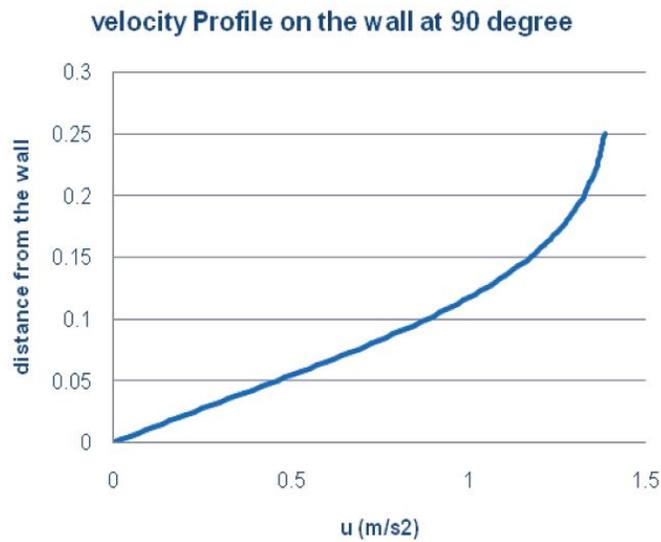

Figure 7: Velocity profile on the cylinder at $90\,^{\circ}$

We plot the velocity profiles obtained by Nek5000 which predict the separation angle to approximately 118 degree.

For the problem at hand some researchers measured the separation angle for Re=100, experimentally [16]. They report it around 120 degree.

Because the predicated results by OpenFOAM and Nek5000 are close enough to experimental data we conclude that the procedure chosen for taking the results is correct and accurate enough.
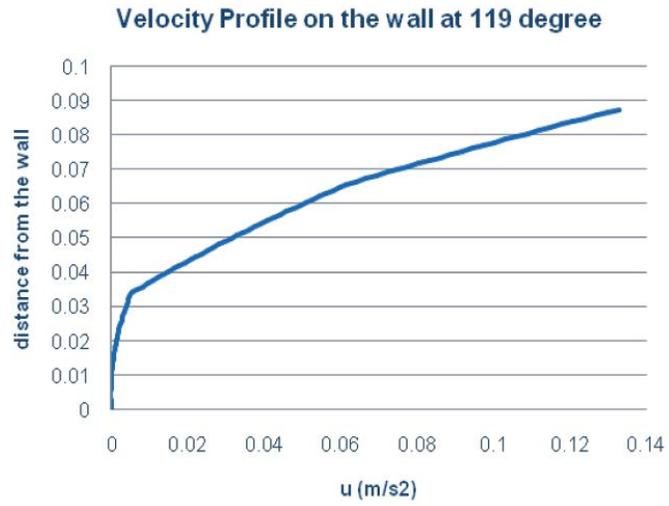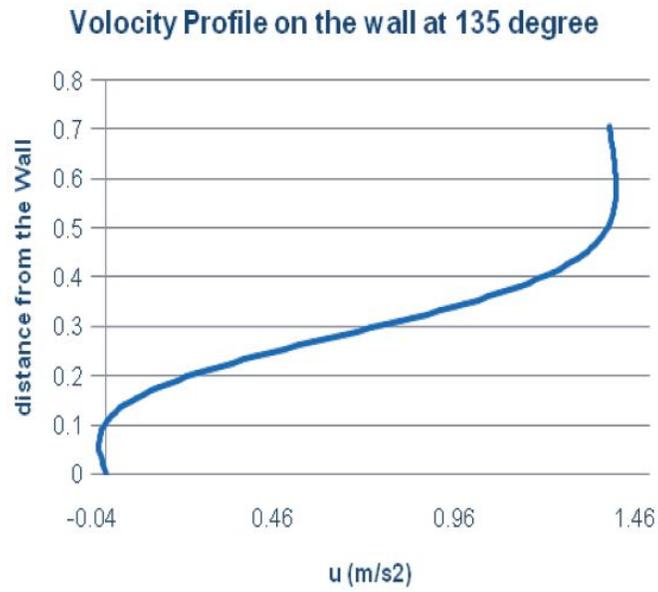
Figure 8: Velocity profile on the cylinder at 119 °

Figure 9: Velocity profile on the cylinder at 135 °

7   Turbulent Flow

We increase the Reynolds number to 600 at which the wakes formed in the flow become turbulent. We solve Reynolds Averaged Navier-Stokes Equations (RANS) using the k-ε modeling.

$$\frac{\partial \mathbf{U}}{\partial x} + \frac{\partial \mathbf{V}}{\partial y} = 0 \tag{13}$$

$$\rho\frac{\partial \mathbf{U}}{\partial t} + \rho U\frac{\partial \mathbf{U}}{\partial x} + \rho V\frac{\partial \mathbf{U}}{\partial y} = -\frac{\partial \mathbf{P}}{\partial x} + \frac{\partial \left[\mu(\frac{\partial \mathbf{U}}{\partial x}) - \rho\left\langle u^2 \right\rangle\right]}{\partial x} + \frac{\partial \left[\mu(\frac{\partial \mathbf{U}}{\partial y}) - \rho\left\langle uv \right\rangle\right]}{\partial y}$$

$$\tag{14}$$

$$\rho\frac{\partial \mathbf{V}}{\partial t} + \rho U\frac{\partial \mathbf{V}}{\partial x} + \rho V\frac{\partial \mathbf{V}}{\partial y} = -\frac{\partial \mathbf{P}}{\partial y} + \frac{\partial \left[\mu(\frac{\partial \mathbf{V}}{\partial x}) - \rho\left\langle uv \right\rangle\right]}{\partial x} + \frac{\partial \left[\mu(\frac{\partial \mathbf{V}}{\partial y}) - \rho\left\langle v^2 \right\rangle\right]}{\partial y}$$

$$\tag{15}$$

It uses an eddy viscosity model (EVM) closure for the Reynolds stress tensor,

$$-\left\langle u_i u_j \right\rangle = \nu_t \left[\frac{\partial \mathbf{U}_i}{\partial x_j} + \frac{\partial \mathbf{U}_j}{\partial x_i}\right] - \frac{2}{3}\delta_{ij}k \tag{16}$$

This closure solves two additional transport equations for the turbulence kinetic energy, k and its dissipation rate, ε, which are then used to calculate the local eddy viscosity

$$\nu_t = C_\mu \frac{k^2}{\varepsilon} \tag{17}$$

In which $C_\mu = 0.09$.

The turbulence kinetic energy is solved from a transport equation that is

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very similar to the generic transport equation:

$$\frac{\partial \mathbf{k}}{\partial t} + U_j \frac{\partial \mathbf{k}}{\partial x_j} = \frac{\partial \left[\left(\frac{\nu_t}{\sigma_k} + \nu \right) \frac{\partial \mathbf{k}}{\partial x_j} \right]}{\partial x_j} - \langle u_i u_j \rangle \frac{\partial \mathbf{U}_i}{\partial x_j} - \varepsilon \qquad (18)$$

Where $\sigma_k = 1$

The dissipation is solved from a very similar transport equation:

$$\frac{\partial \varepsilon}{\partial t} + U_j \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial \left[\left(\frac{\nu_t}{\sigma_\varepsilon} + \nu \right) \frac{\partial \mathbf{k}}{\partial x_j} \right]}{\partial x_j} + C_{\varepsilon 1} \frac{\varepsilon}{k} P - C_{\varepsilon 2} \frac{\varepsilon}{k} \varepsilon \qquad (19)$$

Where $\sigma_\varepsilon = 1.3, C_{\varepsilon 1} = 1.44, C_{\varepsilon 2} = 1.92$

This equation is tightly coupled to the k equation through the source terms.

The near-wall treatment procedure, based on a straight extension of the wall functions, is included in solver.

Numerical calculation schemes using turbulence models for the computation of turbulent flows usually adopt wall functions to bridge the viscous sublayer adjacent to a wall. This method of modeling the near-wall region avoids the need to use numerous mesh points to resolve the very steep gradients prevailing in the viscous sublayer.

With the wall-function approach the near-wall mesh point is placed in the fully turbulent fluid, and semi- analytical expressions called wall functions are employed, which connect the wall conditions (e.g., wall shear stress and heat flux, wall temperature) to the dependent variables just outside the viscous sublayer.

8 Results (Turbulent)

8.1 Mfix

Mfix is mostly developed to address the gas-particle flows. Hence, almost all of the equations and turbulent models available in the Mfix is based on the fact that there is a two-phase flow being to be simulated. However, here we want to visualize a single-phase flow over a cylinder. Although, it is hard but we can do so by controlling the numerous parameters available in the software. Figure 10 Shows the velocity-magnitude field for Re=600 at the final time.
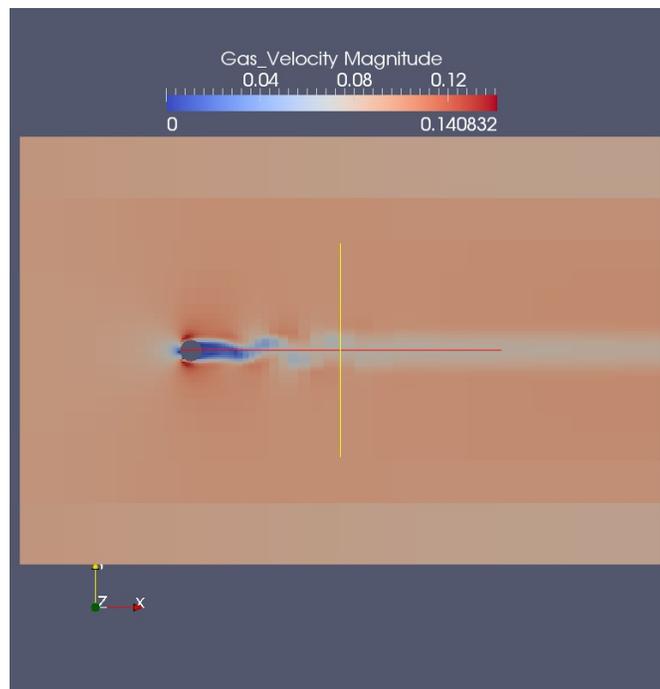

Figure 10: Velocity-magnitude field at Re=600, Mfix

8.2   Nek5000

Currently, Nek5000 does not support any turbulence modeling. In other words, if someone interested in simulation of a turbulent flow they should use Direct Numerical Approach in which the exact Navier-Stokes equations are solved. Figure 11 Shows the velocity-magnitude field for Re=600 at final time. Theoretically, we know that at Re=600 the wakes formed behind the cylinder are turbulent. In fact, when we use k-ε model, it does not represent the fluctuations that exist in the vortexes because it is solving the averaged Navier-Stokes equations. That is why it seems there is no difference between flow pattern at Re=100 and Re=600. However, solving the exact equations governing laminar flows is not correct if we are trying to solve a turbulent flow because, we have to somehow impose the effects of fluctuations which are the most distinctive difference between nature of laminar and turbulent flows. On the other hand, while using a specific kind of turbulence modeling we should pay attention to near-wall treatment. It is worth mentioning that if someone is interested in capturing those fluctuations they should use DNS or LES (large-eddy simulation).

8.3   OpenFOAM

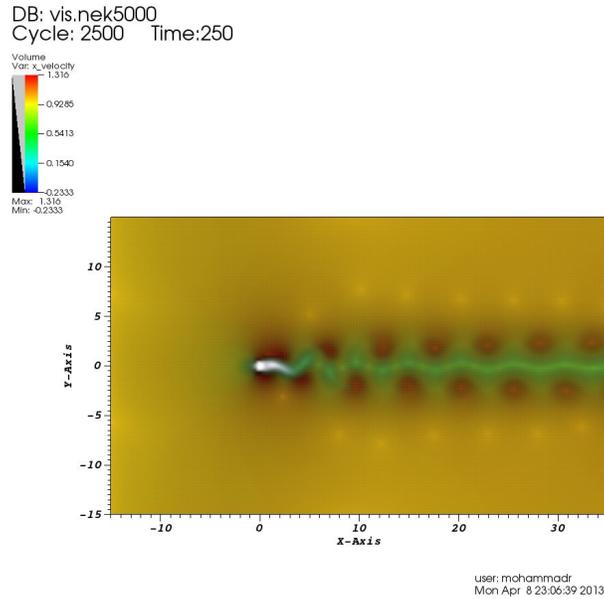Figure 12 depicts the velocity-magnitude field obtained by pisoFoam solver in OpenFOAM for Re=600 at the final time.

Figure 11: Velocity-magnitude field at Re=600, Nek5000

9   Conclusion

Comparison between the Non-commercial (open source) software reveals that: OVERFLOW is suitable for compressible single-phase external flows. Mfix is appropriate for simulating gas-particle flows. Also, OpenFOAM is a general-purpose software and enjoys a variety of schemes to descritise the equations. Moreover, it is more straightforward to work with in comparison with Nek5000 and Mfix. In terms of time to perform the calculations the Nek5000 was amazing. Since, the Nek5000 is the only software among those three packages examined that is based on spectral element method it is not necessary to choose fine grids to get the desired accuracy, which in turn, increases the speed of convergence. for the problem solved by these packages Nek5000
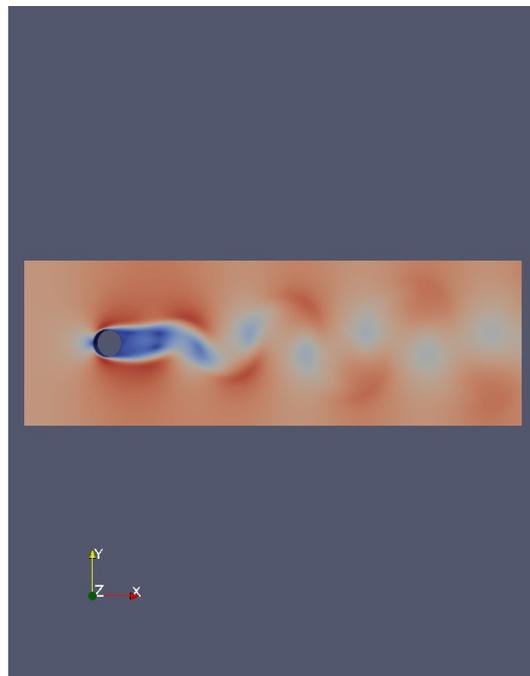
Figure 12: Velocity-magnitude field at Re=600, OpenFOAM

took 30 minutes, OpenFOAM took 6 hours and Mfix took 8 hours to yield the converged solutions. So, depend on the application, desired accuracy and considering the costs of calculations the chosen option might vary. in the case of Nek5000, it must be noticed that despite the fact that it seems more powerful that the other two packages i.e. OpenFOAM and Mfix, it's applications is limited.

It seems that for simulation of gasification, because it is a two-phase turbulent flow, Nek5000 is not applicable. Between, Mfix and OpenFOAM, working with OpenFOAm is more straightforward and you have access to a lot of options that are not available in Mfix. for example, someone can use LES through OpenFOAm, while they do not have access to this amazing approach via Mfix.

Although the SU^2 can be a good software, it is developing at the moment to be bug-free.

On the other hand, it seems that among Commercial software the BARRACUDA VR is just designed to focus on chemically reacting turbulent flows while Ansys CFX and Fluent are general-purpose software packages.

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