CFD Modelling of Underground Coal Gasification using ANSYS Fluent Simulator

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ABSTRACT
Underground Coal Gasification is a non-traditional, in-situ combustion process for converting coal into product gases. In this process coal is combusted and the produced syngas which basically contains CO_2, H_2, CO and CH_4 is extracted to the surface with the help of drilled wells. In this study, with reference to a lab-scaled UCG experiment **[1]** and taking the experimental data as the basis for the research a two dimensional CFD reactor model was created and further studies were done to establish the activity at the different locations of the reactor. The Mass Imbalance, Discrete Phase Variables, Velocity, Turbulent Kinetic Energy, Strain Rate, Mesh contour diagrams along with the Scaled residual plot were obtained to give the reader an extensive knowledge about the process and simulation. The CFD model results obtained in our study were compared with the experimental data from the above citing in order to validate our obtained model and it's results.

Keywords: CFD, Underground Coal Gasification (UCG), Ansys Fluent, Mathematical Modelling, Simulation, Syngas, In-situ Combustion.

1. INTRODUCTION

Underground coal gasification is one of the best and most promising option for the processing of un-used coal in the future. As the world is moving towards unconventional sources of energy, this process enhances this change towards the unconventional by allowing coal to be gasified in situ within the coal bed with the help of a series of interconnected wells. The coal is ignited with specialised techniques and air is flown in to sustain the fire being ignited which is essentially required to reach the coal and produce a combustible synthetic gas further useful for industrial processes such as manufacturing of hydrogen or diesel fuel or gas or most importantly power generation.

Field tests based on Underground Coal Gasification have been in practice since the 1930s. These tests have seen both success and failures and hence since then the number of tests has seen an increase but the plants in functioning are very few due to the varying degrees of success and the fluctuating prices of oil and gas **[2][3]**; based on this experience (especially in the USSR and United States), field designs which are applicable to a varied classification of geological conditions and coal properties has been developed and brought to use. In the past, countries that have a significant amount of low-rank coal reserves increased their attention on the UCG process and related research activities**[4], [5], [6], [7]**.

Appropriate field and laboratory results as well as pre-designed mathematical models of an in-situ gasifier are observed and tested as part of the analysis. A number of UCG tests were conducted on-site and in labs whether in-situ or ex-situ and they showed somewhat similar results. UCG tests in China proved facts showing that when steam is flowed into coal bed, syngas can be obtained containing more than 50% hydrogen concentration **[8]**.

These tests incorporated two-step gasification process wherein, the first step was to supply O_2 rich air into the field to maintain combustion and the second step was to replace the O_2 rich air with steam to start the water gasification reaction in order to produce hydrogen**[9]**. Yang et al. increased the hydrogen production rate of the two-step gasification process by providing the gasification agents through multiple locations which was eventually a form of multilateral formation**[9]**. Apart from these ex-situ and in-situ processes, there are a number of studies that incorporate mathematical modeling which also employ Computational Fluid Dynamics (CFD). Perkins and Sahajwalla created a 2D Geometry to simulate and calculate the mass transfer and heat transfer operations inside the seam during the process of UCG **[10]**. Turbulence models were

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used to investigate and model the effects of turbulent flow due to natural convection and had a low value of K – Epsilon. Sarraf Shirazi et al. created a 3D model in CFD that consisted of a coal seam and a gasification chamber **[11].** Using the ANSYS FLUENT simulator, numerical results were obtained.

Żogała and Janoszek have also performed some notable work in the field of UCG with the help of a 3D model in CFD which had a design similar to a Gas reactor **[12]**. Using ANSYS Fluent solver **[13]**, Authors calculated the effects of flow of steam on the temperature levels inside the reactor and the produced syngas composition.

PROCESS	REACTION	ΔH(kJ/mol)
Drying	Coal → Coal(dry) + H2O	+40
Pyrolysis	Coal(dry) → Volatile Matter + Char	0
CO combustion	$CO + ½ O_2 \rightarrow CO_2$	-111
H_2 combustion	$H_2 + ½ O_2 \rightarrow H_2O$	-242
Water-gas shift reaction	$CO + H_2O \rightleftarrows CO_2 + H_2$	-41
Combustion	$C + O_2 \rightarrow CO_2$	-393
CO_2 gasification	$C + CO_2 \rightarrow 2CO$	+172
H_2O gasification	$C + H_2O \rightarrow CO + H_2$	+131

TABLE 1

In this study, a 2D mathematical model which was dynamic in order and based on kinetic reaction rates was created and investigated in ANSYS FLUENT to evaluate numerical results. The mathematical model prepared in the GeometryModeler of the ANSYS Workbench consists of the inlet and outlet streams and a coal reactor part where the reactions take place. There is a total of 6 species involved in this work mentioned as O2, CO2, CO, H2O, H2 and N2. For these six chemical species there are six chemical reactions involved (Reactions **(3) – (8)**) apart from the reactions of pyrolysis and drying (Reaction **(1)** and **(2)**). Table 1 shows the various enthalpies for the listed reactions.

$$Coal \rightarrow Coal(dry) + H_2O \quad (1)$$

$$Coal(dry) \rightarrow Volatile\ Matter + Char \quad (2)$$

$$CO + ½ O_2 \rightarrow CO_2 \quad (3)$$

$$H_2 + ½ O_2 \rightarrow H_2O \quad (4)$$

$$CO + H_2O \rightleftarrows CO_2 + H_2 \quad (5)$$

$$C + O_2 \rightarrow CO_2 \quad (6)$$

$$C + CO_2 \rightarrow 2CO \quad (7)$$

$$C + H_2O \rightarrow CO + H_2 \quad (8)$$

1.1 SYNGAS

Syngas stands for synthetic gas which is a combination of gases such as hydrogen and carbon monoxide prominently however there are traces of carbon dioxide found as well. It is equivalent to almost half the energy density of natural gas but it cannot be used directly as a fuel and hence is used to establish fuel sources. Syngas is a primitive part in chemical industry, which relates to almost 2% of the total primary energy usage. Syngas obtained is not completely free of impurities and contains some traces which are further eliminated via processing. Syngas can be derived as a product of gasification from a number of sources such as biomass, coal and natural gas, by reaction with steam thermally breaking down the biomass into a combustible gas in a closed reactor is known as thermal gasification and it produces byproducts such as volatiles, char and ash as well.

1.2 IN SITU GASIFICATION

In situ combustion can be defined as a method of recovery of fuel in which fire is generated inside the reservoir by injecting air containing oxygen. In situ combustion is also known as the process of fire flooding and is one of the oldest and most used methods of recovering oil using tertiary methods, from the reservoir. Specialised heaters in the well are accommodated to ignite the oil in the reservoir and start a fire.
A continuous flow of air is essential to keep the fire ignited and hence air or oxygen-rich air is made to flow through the well **[14].** This flow of air or the entire process of **fire flooding** is dependent on the direction of the flow or propagation and is further classified as **Forward** or **Reverse** combustion. The high temperatures in the well leads to **hydrocarbon cracking and vaporisation** of light hydrocarbons. The process of breaking long chain hydrocarbons into lesser complex products has been an essential and widely used process in the petroleum industry. As discussed in this section, in-situ gasification or combustion is obtained by injecting gases to the well that is done with the application of multilateral completion:

1.2.1 MULTILATERAL COMPLETION

In order to develop an image of a multilateral well, it may be defined as a well with a horizontal as well as a vertical lateral drilled from a main well. As far as the drilling is concerned, multilateral completions are required in the process of underground coal gasification as this system facilitates to re-enter an existing well and enter another lateral to it. This leads to a single well-being capable of producing from a number of reservoirs. Multilateral completions are often employed or used in terrains of field designs such as layered, compartmental, fractured or structural designs. Also, on the basis of the design complexity of the completions, they can be classified into 6 levels of **Technology Advancement Multi Laterals**. All of these 6 levels have their own descriptions, advantages and disadvantages.

2. THE ANALYTICAL STUDY

A two-dimensional mathematical model along with its solution geometry having the dimensions of an UCG reactor was developed using the ANSYS WORKBENCH and ANSYS FLUENT software environment. Developing a mathematical model in two dimensions and working on it for its solution geometry is less complex and sufficient to analyse the effects of gasification parameters.

A 2D model is first created using the ANSYS Workbench and then a grid is created using ANSYS Meshing. The Computational Fluid Dynamics model created using the software environment is used to investigate the thermal and chemical heat and mass transfer interactions between the source and parameters.

2.1 EQUATIONS INVOLVED IN THE STUDY [15]

• continuity equation:

$$\frac{\partial \rho}{\partial t} + div(\rho\, \vec{u}) = s_m$$

• momentum equation:

$$\frac{\partial(\rho\vec{u})}{\partial t} + div\left(\rho\, \overrightarrow{u\vec{u}}\right) = div(\mu\, \mathrm{grad}\vec{u}) + s_u$$

• energy equation:

$$\frac{\partial(\rho e)}{\partial t} + div(\rho\, e\vec{u}) = div(\lambda\ \mathrm{grad}T - P\vec{u}) + s_e$$

• species transport equation:

$$\frac{\partial(\rho C_\alpha)}{\partial t} + div(\rho\, C_\alpha\vec{u}) = div(\rho D_\alpha\ \mathrm{grad}C_\alpha) + s_\alpha$$

where:
ϱ – density of fluid, kg/m3 ;
P – pressure, Pa;
$\vec{u}$ – velocity vector of fluid element, m/s;
μ – viscosity of fluid, Pa·s;
e – total energy related to unit mass of fluid, kJ/kg;
λ – thermal conductivity, W/mK;
D_α – diffusion coefficient, m2 /s;
T – temperature, K;
C_α – concentration of species α in mixture, kmol/m3.

S_m, S_u, S_h and S_α are the source terms in the above equations, which is associated with mass, momentum, energy and transport of species.

- Mass Source term is considered in the continuity equation.
- Momentum Source term is considered in the momentum equation.
- Energy Source term is considered in the energy equation.
- Species Source term is considered in the species transport equation.

2.2 MATHEMATICAL ANALYSIS METHODS [16]

All the above equations are Partial Differential Equations which are usually referred to as PDE's and the solution or analysis of PDE in using mathematical analysis can be done using two approaches which are:
1. **Deterministic** and
2. **Stochastic (probabilistic)**
A deterministic approach is one in which the output is completely dependent on the input parameters whereas the stochastic method is the one in which the results are based on principle of statistics and the output values may not be the same for each input value. The three main methods to determine the results over numerical analysis are:

2.2.1. FINITE DIFFERENCE METHOD:

This method involves the PDE to be satisfied at a given set of interconnected points in the geometry obtained. These points are called as nodes and the overall figure obtained by these interconnected points is called as a mesh. Both, the governing PDE and boundary layer equation, are satisfied at the nodes at either the surface or the boundary layer.

2.2.2. FINITE VOLUME METHOD:

As the name suggests, this method involves the PDE to be satisfied over a set of ***controlled volumes*** between the interconnected points rather than satisfying at the nodes. These controlled volumes are referred to as ***cells.***

2.2.3. FINITE ELEMENT METHOD:

The third or the final method which involves the use of test functions and the definite integration of the integration for boundary limits that define the whole domain. The method used in our study for numerical analysis of the 2D model is Finite Element Analysis.

2.3 TWO-DIMENSIONAL GEOMETRY

A 2D solution geometry was prepared using the ANSYS Workbench software and the geometry included three different sections viz. inlet, outlet and the reactor. The dimensions of all the sections were predefined in the 'Dimension' section of the modelling part of the Workbench. These dimensions are in correspondence with the experimental study have been specified in the figure attached with the paper which shows the ex-situ reactor for 2D CFD study. [Fig. 1]

2.4 MESHING

The next step after the successful formation of the two-dimensional geometry on the ANSYS DesignModeler is Meshing. As discussed above in

the various methods of numerical analysis, the calculations are made at the interconnected points known as nodes and the overall geometry obtained along with these nodes is called a mesh. The number of nodes and elements in a specific geometry can be set which is visible in the ***Statistics*** section of the ***Details*** window. The number of nodes can be changed by changing the sizing values in accordance with the actual dimensions of the two-dimensional geometry.
The different sections of the geometry need to be assigned with a particular name in order to define the calculations. The named sections in our study are as follows:
1. Inlet
2. Walls
3. Base
4. Outlet

Generating Mesh is the next step and this completes the first half of our study. The overall mesh with the specified number of nodes can be seen as attached with this paper as picture [Fig. 2].

2.6 SOLUTION MODEL:
One of the main steps in the numerical analysis of the two-dimensional geometry representing Underground Coal Combustion is ***Initialization*** & ***Calculations.*** These calculations in our study were done on ANSYS FLUENT ***(Fluid Flow (FLUENT) Parallel Fluent***) and the models used in the setup are as follows:
1. Energy model
2. Viscous model (k-epsilon)
3. Radiation model
4. Species Transport model
5. Discrete Phase model

The materials used in this study were the common combustion materials including coal and volatile air. The boundary conditions and the overall setup has been specified in the next section. The boundary layer conditions and the cell zone conditions have also been specified in Table 2**.**

	Boundary Conditions		Initial Conditions
Inlet	Ignition	1000 K, 10 m3/h, Air	Temperature 400 K
Oxygen	Oxygen-Gasification	300 K, 3 m3/h, Pure	Initial Porosity 0.04 (% 4)
	Steam-Gasification	400 K, 5 m3/h, Steam	Initial Permeability (1 mD)
			Coal moisture scalar 0.10011
Outlet	1 atm (Absolute Pressure)		Coal volatile scalar 0.347
			Coal fixed carbon scalar 0.3801

TABLE 2

The Species Transport model contains a coal calculator as well which gives the results for the Ultimate and Proximate analysis. The ultimate analysis takes place in accordance with the Dry-ash-free basis (DAF). The coal properties have been tabulated below in Table 3 and the overall results have been attached with the paper as the image [Fig. 3].

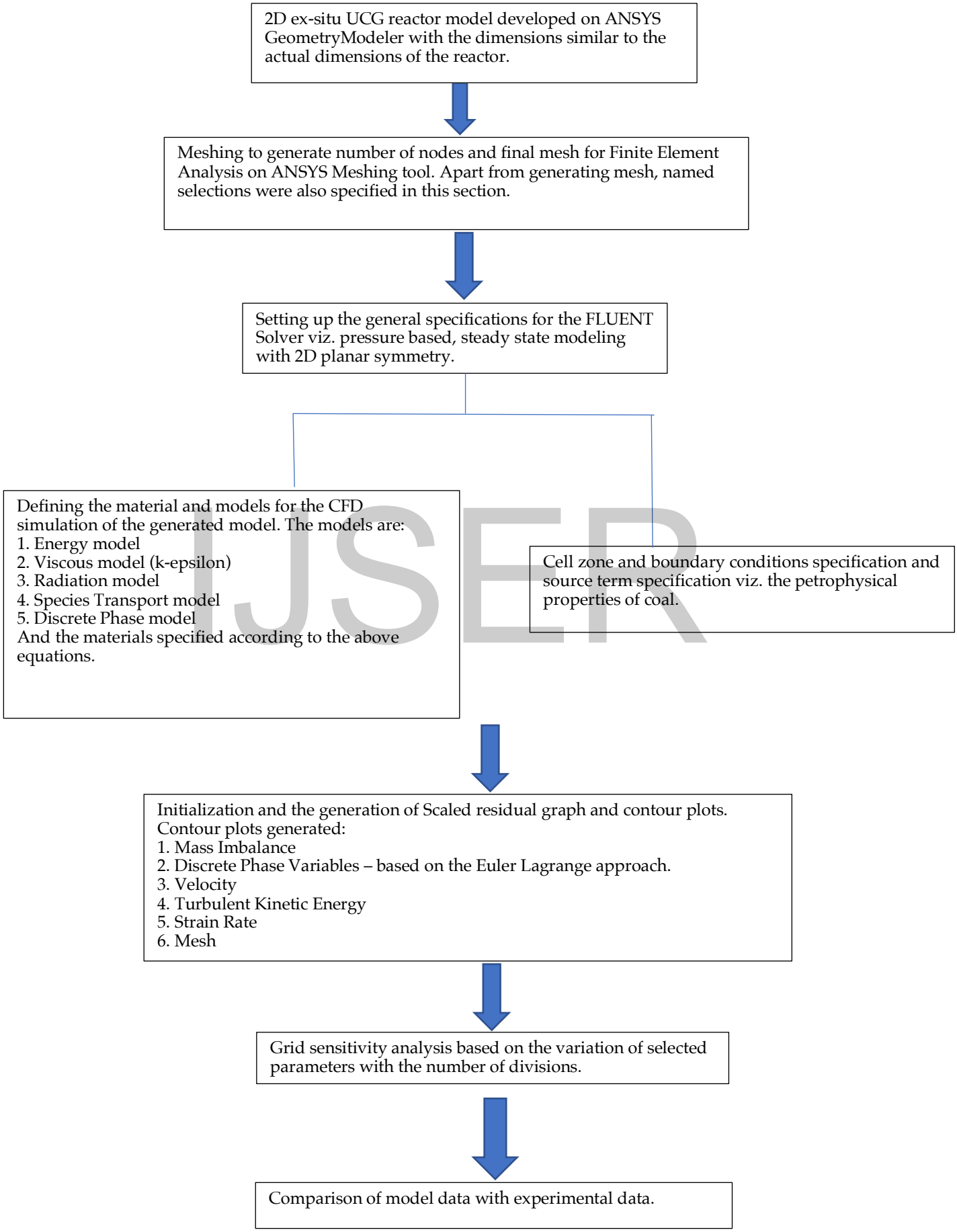
Coal Properties			
Proximate Analysis		Ultimate Analysis (DAF)	
Volatile	0.5	Carbon	0.85
Fixed Carbon	0.3	Hydrogen	0.1
Ash	0.1	Oxygen	0.04
Moisture	0.1	Nitrogen	0.01

TABLE 3

2.5 OVERALL MODEL SETUP [Fig. 4]
The process of meshing involves a number of conditions to be specified during the process. These include the boundary and initial conditions which are used for the numerical analysis during meshing. The main aim behind this is to specify the Flow Rates of the gasification agents in the process of UCG experiment that are implemented in the mathematical modeling. The total number of iterations performed during the simulation were 300 and the final graph and contour figure can be obtained as the images attached to the paper.

2.7 GRID SENSITIVITY ANALYSIS
Any CFD results obtained from a simulation can never be trusted unless it is tested for the dependence on the grid. As discussed in the above section of meshing, the relevance center needs to be assigned between coarse, medium and fine. And the results obtained for a coarser mesh and finer mesh can never be the same. Therefore, the mesh needs to be varied so that an acceptable level of tolerance can be obtained and hence the **Grid Independence Test** comes into picture. The terms grid sensitivity analysis and grid independence test are often interchangeable.
This can be done by varying a set parameter related to the mesh size along with some output parameters. In our study, the 'Element Size – Number of Divisions' was compared with the output surface velocity and the output pressure. The data was plotted in a CSV [Fig. 5] file and the point where the variation becomes negligible was taken as the optimum number of divisions.

2.8 SIMULATION ALGORITHM



3. RESULTS [FIG. 6]

The graph shows the simulation of the UCG 2D model for a set of 300 iterations. The number of iterations can be varied as and when a stability in the results is visible which in this graph can be seen. The main approach behind this study is to satisfy a set of Partial Differential Equations which are mainly the:
1. Energy equation
2. Momentum equation
3. Continuity equation
4. Species Transport equation.

All the above equations are based on and find applications in Computational Fluid Dynamics.
Apart from the **Scaled Residual Graph** that shows the variation of all the residuals with the iterations, a set of **Contour graphics** can also be obtained with the simulation.
The different contour plots are:

1. Mass Imbalance
2. Discrete Phase Variables – based on the Euler Lagrange approach.
3. Velocity
4. Turbulent Kinetic Energy
5. Strain Rate
6. Mesh

The graphics of all these contours are attached with the paper. **[FIG. 7 – FIG. 12]**
As shown by the contour figures, the experiment was initiated by supplying oxygen from the inlet in order to start and support the combustion. The supply of oxygen was characterized by parameters such as the flow rate, temperature at the inlet and pressure. All the parameters have been pre-defined in **Table 2.** The flow rate was a varied value of 3 m^3/hr to 5 m^3/hr. The temperature was fixed to 400 k. The main aim behind performing these CFD simulations was to define the trends in CO_2 and H_2O which totally shows the dependence of Water-Gas shift **[REACTION 5].**

4. APPLICATIONS

The estimated reserves of crude oil and natural gas in India as on 31.03.2018 stood at 594.49 million metric tonnes (MMT) and 1339.57 billion cubic meters (BCM), respectively. As on 31.03.18 the estimated reserves of coal were around 319.04 billion tones, an addition of 3.88 billion over the last year. Coal deposits are mainly confined to eastern and south-central parts of the country.

There has been an increase of 1.23% in the estimated coal reserves during the year 2017-18 with Odisha accounting for the maximum increase of 2.6% whereas there was decrease of 1.59% in the estimated reserve of crude oil for the country as a whole during 2017-18 as compared to the position a year ago.

Hence, UCG is the only economically profitable method to harness the inaccessible reserves. There are a few organizations looking to set up UCG projects in Gujarat and Rajasthan. A pilot project of UCG was conducted by ONGC in collaboration with Gujarat Industries Power Company Ltd in Surat, Gujarat. Now, as the process of UCG has established its importance in the field of unconventional sources, the organization has taken over the Vastan mines in Surat and in collaboration with Messrs. National Mining Research Center-Skochinsky Institute of Mining (NMRC-SIM), Russia is progressing towards their goal to complete this project.

4. CHALLENGES OF UCG

In situ gasification of coal, exposes the groundwater to a potential environmental hazard which is mainly a result of local hydrogeological conditions but is somewhat affected by the process of UCG. Further analysis of the samples brings out the effects of UCG on the groundwater. The process of underground coal gasification is a complex procedure with a series of techniques involved in it. These techniques often lead to the production of unwanted traces of pollutants that can be transmitted to the surrounding strata by the processes of diffusion or direct injection. Most commonly found pollutants in the groundwater strata maybe divided into categories as minor, organic and inorganic. Mathematical is often useful to attribute the flow of groundwater once the process of underground coal gasification takes place and this can prove the effects of contaminants. Some of the organic contaminants are phenols, benzenes, naphthalene, toluene, xylene. Some of the inorganic contaminants are ammonium, boron, calcium, iron, lead, magnesium, manganese, zinc, mercury, sulphate.

6. CONCLUSIONS AND FUTURE PERSPECTIVES

The shift from a conventional process to an unconventional can never be achieved with ease. However, once in use, it can be an alternative to the orthodox methods. Underground Coal Gasification is one such example and the aim of this study was to apprise readers with the process and its underlying dynamics. Theoretically defined, UCG is an industrial process that aims towards the in-situ combustion of a coalseam leading to the production of product gases that can be extracted for various purposes. An application of UCG is Carbon dioxide capture and sequestration industrially also known as (CCS) can be referred to as a set of technologies or processes that can help in reducing the carbon dioxide emissions. These emissions are mainly from the new or existing power plants and large industrial sources which use coal or gas as the main source is fuel or energy for the process to take place in.
CCS takes place mainly in three-steps:
1. Initially the carbon dioxide produced from power plants or industrial processes needs to be captured.
2. Once the CO2 is captured, it needs to be compressed and transported through pipelines.
3. Once transported, it is stored in the geologic formations several kilometres below the surface and is known as Geologic sequestration.

Apart from the theoretical knowledge about the UCG process, this study also shed light on the numerical analysis of an experimental model and emphasized on the technical aspects. The basic parameters such as the calorific values or the velocities of different species and their other properties used in the hydrogen oriented underground coal gasification experiment and properties of the sample were brought in use for the 2D simulation of a UCG reactor. Initial parameters such temperature was set to 400 K, porosity 0.04 (% 4), permeability (1 mD), Coal moisture, volatile and fixed carbon content as 0.10011%, 0.347% and 0.3801 respectively. The Fluent simulation gave various contour plots viz. Mass Imbalance, Discrete Phase Variables, Velocity, Turbulent Kinetic Energy, Strain Rate, Mesh. The contour diagrams show the variation of the above-mentioned parameters or the species used in the simulation over the reactor.

These results were then compared with the previously conducted hydrogen oriented UCG experiment and there was not much variation in the results and presented a good agreement. According to the Scaled Residual Graph, the values of various parameters for the successive iterations showed a resemblance with the experimentally obtained values, which was the primary objective of our study.

7. FIGURES:

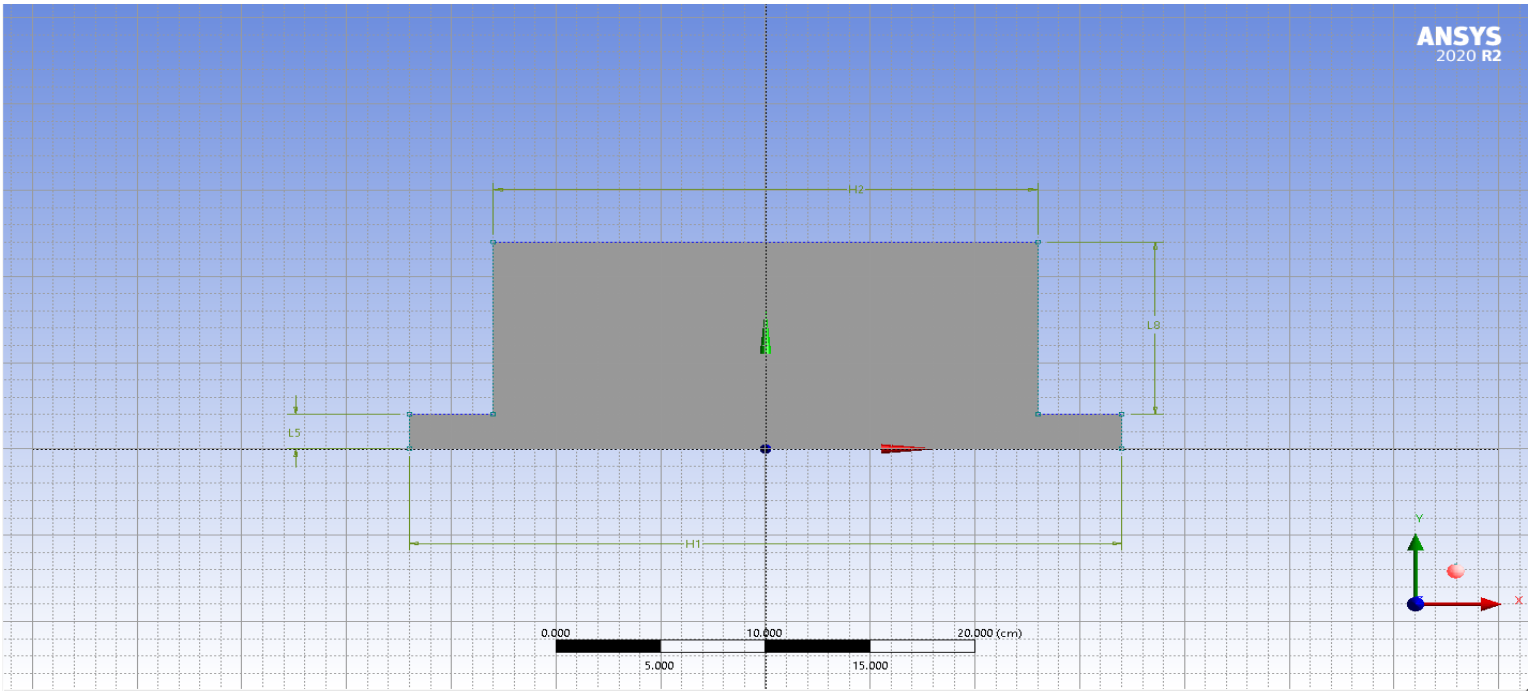


FIG. 1

Fig.1 shows the 2D model with the dimensions similar to the in-situ reactor used in the experiment for the hydrogen oriented underground coal gasification. The 2D model has named selections as the 'outlet', 'inlet', 'outlet' and the 'wall'. These named selections were done during the meshing part of the simulation study.

Fig. 2 shows the mesh generated. The mesh has a total of 8024 nodes and 7808 elements which were further iterated for the grid independence analysis.

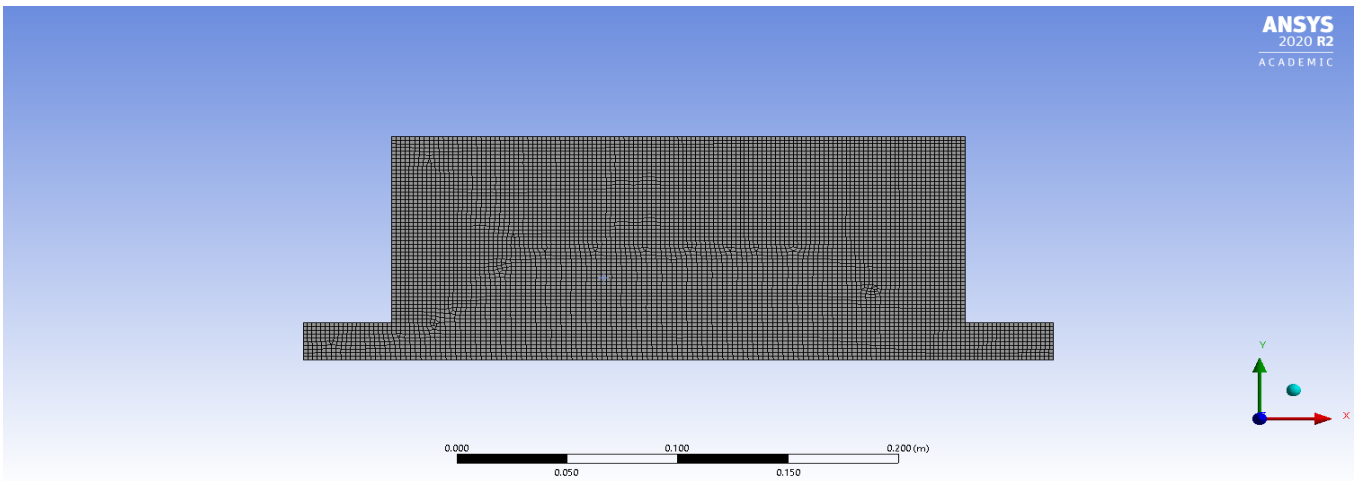


FIG.2

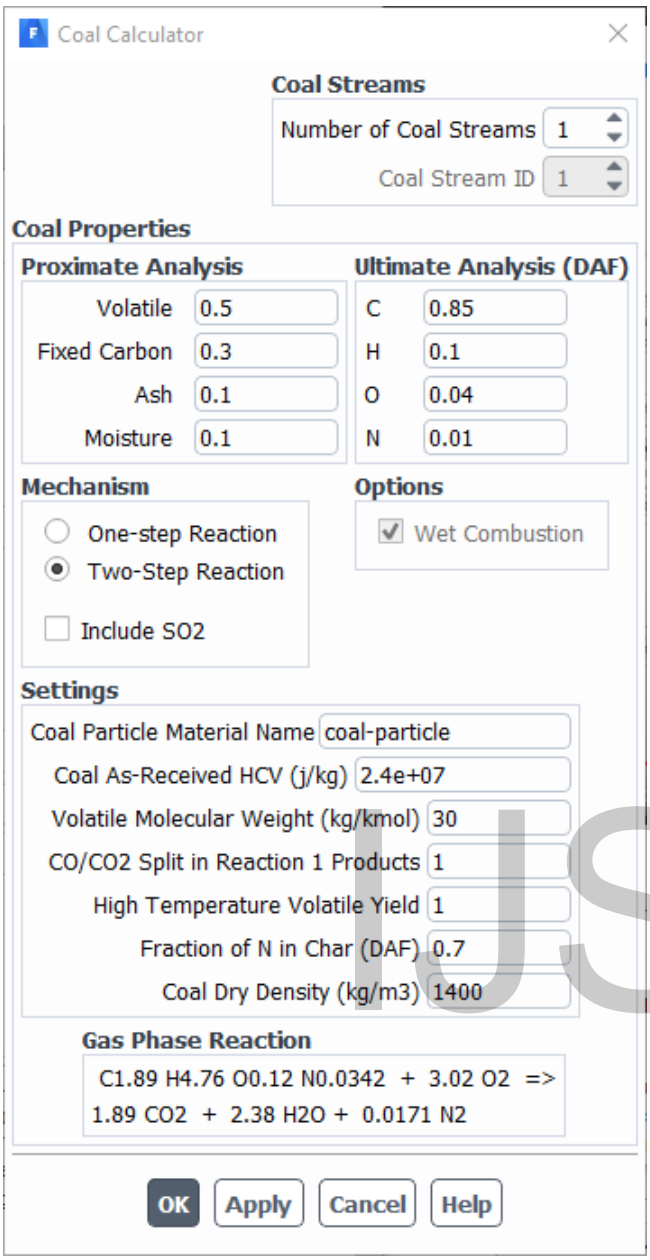


FIG. 3

FIG. 3 illustrates the coal calculator. The coal properties during the simulation study are mentioned in this which include the volatile content, fixed carbon, ash and moisture content during the proximate and ultimate analysis along with the mechanism of the reaction.

FIG. 4 represents the overall model setup as obtained in FLUENT for the numerical analysis. The coal calculator is also found in the FLUENT module where the species and models are set for the calculations.

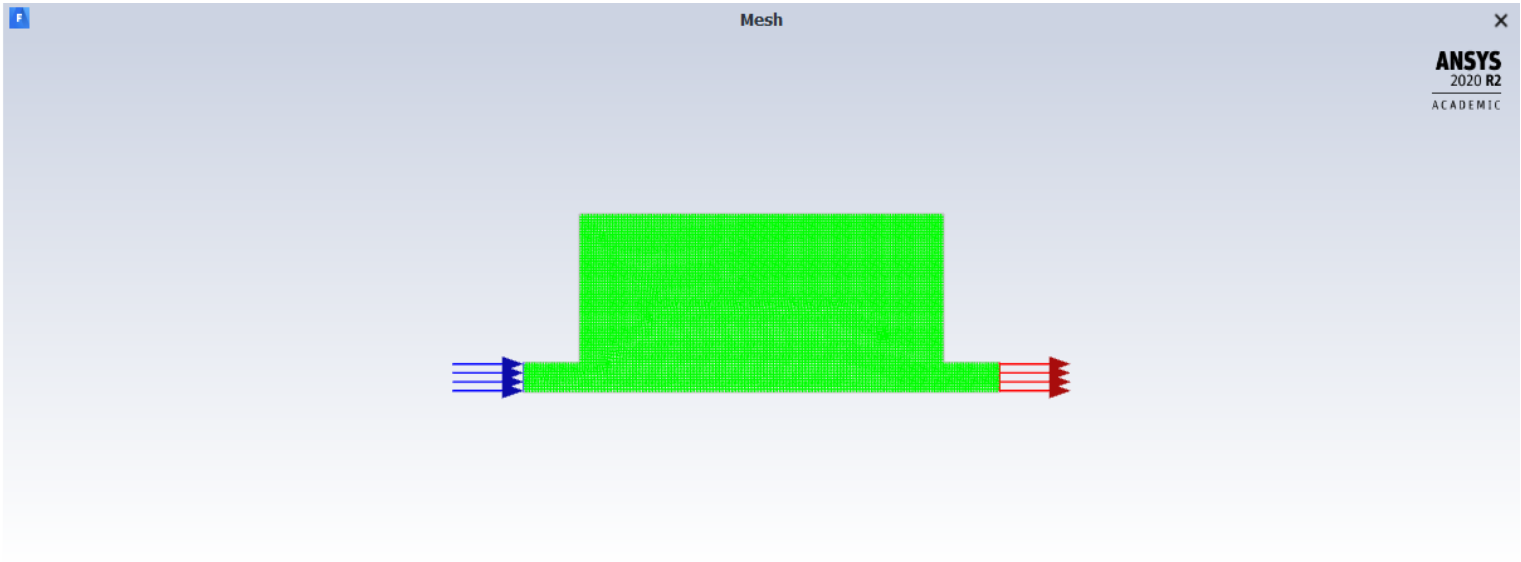


FIG. 4

FIG. 5 represents the Grid Sensitivity Analysis or the Grid Independence Test. Different parameters were chosen for the test such as:

- Number of divisions
- Surface velocity
- Inlet Pressure
- Outlet max. velocity
- Mesh nodes
- Mesh elements

And the number of divisions was varied for the selected parameter to obtain a scatter chart that would show the convergence defining the independence at that point.

# ,,,,,,							
# 06/19/2021 13:38:18,,,,,,							
# The parameters defined in the project are:,,,,,,							
#	P4 - Edge Sizing Number of Divisions	P1 - Surface [m s^-1]	P2 - in [pa]	P3 - base [m s^-1]	P5 - Mesh Nodes	P6 - Mesh Elements	
# ,,,,,,							
# The following header line defines the name of the columns by reference to the parameters.,,,,,,							
Name	P4	P1	P2	P3	P5	P6	
DP 0	10	0.00858405	-0.0347159	0.10197586	8024	7808	
DP 1	15	0.05188396	-0.0780158	0.13111182	16381	15072	
DP 2	20	0.09518386	-0.1213157	0.16024778	22184	20094	
DP 3	25	0.13848377	-0.1646156	0.18938375	34436	31134	
DP 4	30	0.17132449	-0.2079155	0.21851971	43456	42174	
DP 5	35	0.19132449	-0.2512154	0.24765567	67630	64254	
DP 6	40	0.28178367	-0.2945153	0.27679163	104256	102894	
DP 7	50	0.36076157	-0.3378152	0.30592759	152320	147054	
DP 8	60	0.36076157	-0.3811151	0.33506355	197632	180174	
DP 9	70	0.36791394	-0.424415	0.36419951	281088	263294	
DP 10	80	0.37913935	-0.4677149	0.39333547	342925	342925	

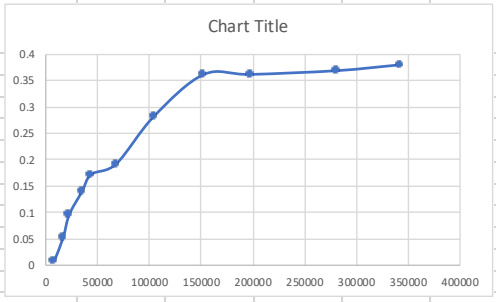


FIG. 5

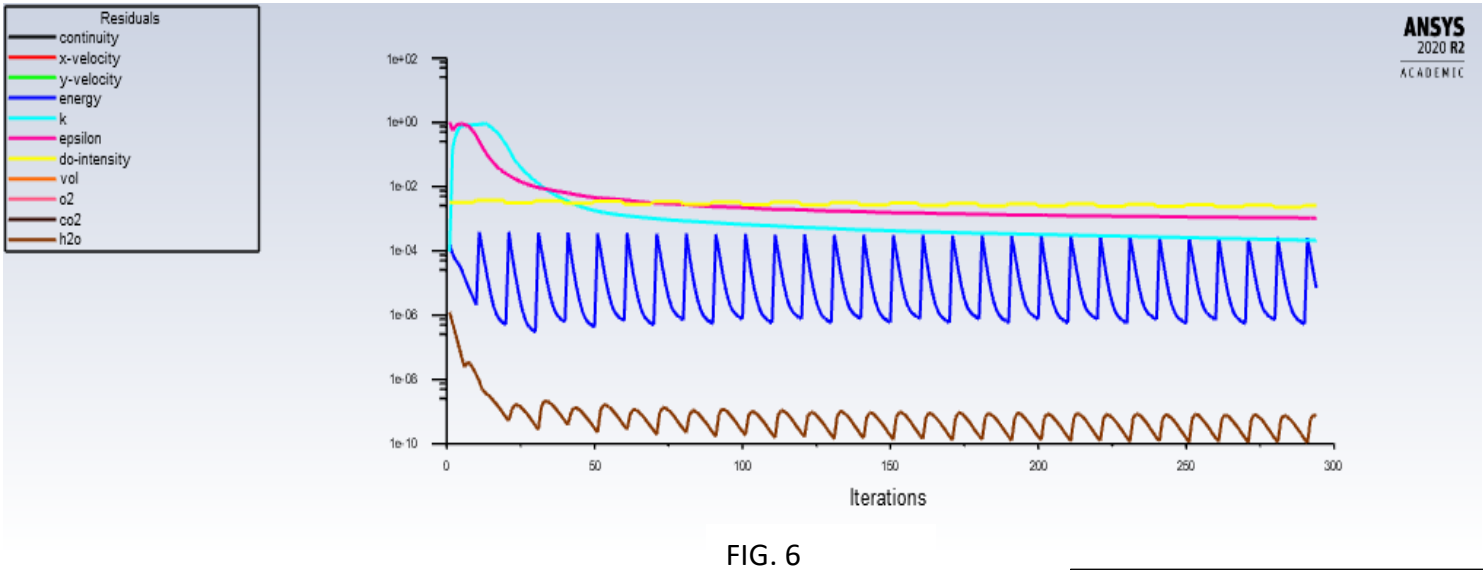


FIG. 6

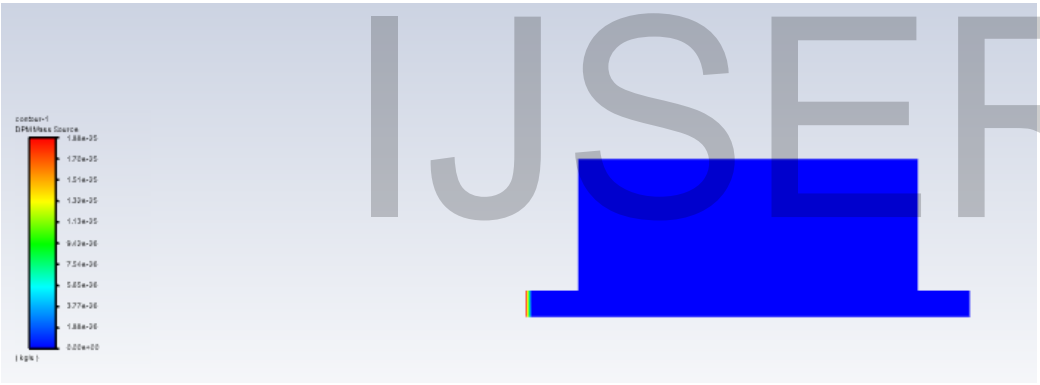


FIG. 7

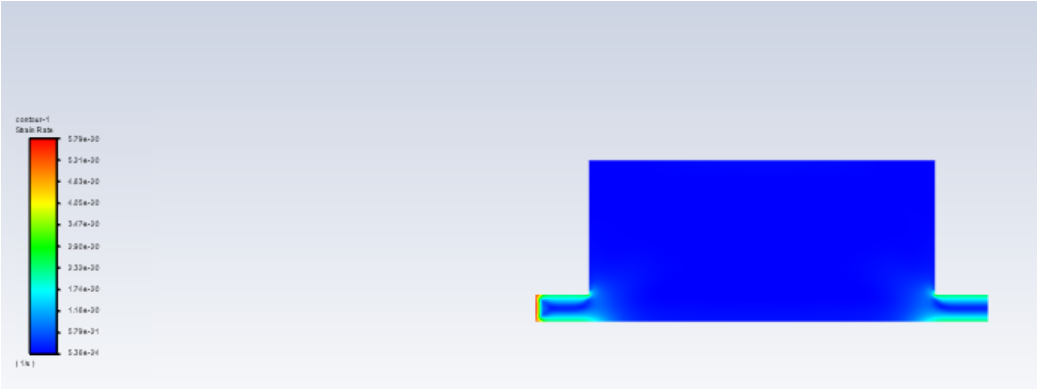


FIG. 8

FIG. 6 is the plot for the overall simulation of the UCG model for a total of 300 iterations. This involves all the species viz. 'x-velocity', 'CO_2', 'energy', 'continuity', etc.

FIG. 7 is the contour diagram for the velocity variation over the reactor.

FIG. 8 shows the contour diagram for the strain rate variation. Strain rate is the rate of deformation over the given model.

FIG. 9 shows the contour diagram for the mesh.

FIG. 10 shows the mass imbalance contour diagram representing the mass flow values at the interface.

FIG. 11 shows the turbulent kinetic energy contour diagram for the 2D UCG model.

FIG. 12 shows the contour diagram for the Discrete Phase Variables which are used for the continuous or the discrete phase flow.

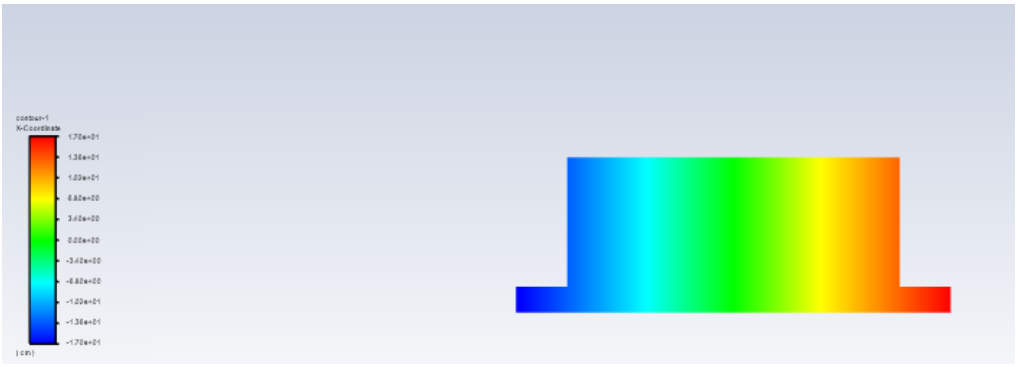


FIG. 9

FIG. 10

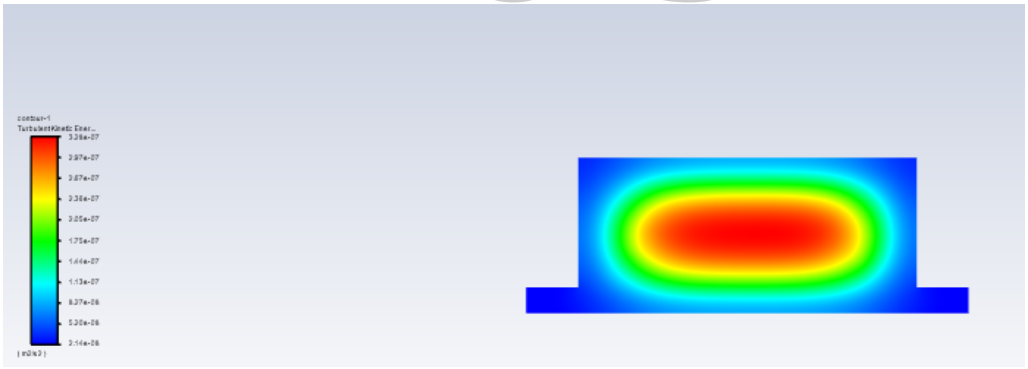


FIG. 11

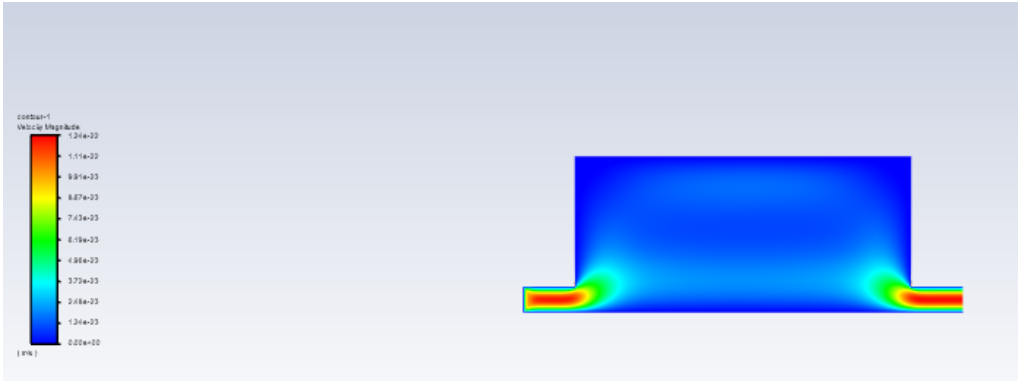


FIG. 12

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