MODELLING & SIMULATION OF FLUID FLOW BEHAVIOUR DURING CARBONDIOXIDE SEQUESTRATION IN COAL STRUCTURE USING COMSOL MULTIPHYSICS

A THESIS SUBMITTED IN PARTIAL FULLFILLMENT OF THE

REQUIREMENTS FOR THE DEGREE OF

BACHELOR OF TECHNOLOGY
IN
MINING ENGINEERING

BY

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Under The Guidance of

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CERTIFICATE

This is certify that the thesis entitled "**Modelling & Simulation Of Fluid Flow Behaviour During Carbondioxide Sequestration In Coal Structure Using Comsol Multiphysics**" submitted by **Sri Bimal Prasad Panda (RollNo-111MN0599)** and **Sri Aakash Deep Singhal (RollNo-111MN0436)** in partial fulfillment of the requirements for the award of Bachelor of Technology Degree in Mining Engineering at National Institute of Technology, Rourkela is an authentic work carried out by them under my supervision and guidance.

To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other university/ Institute for award of any Degree.

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ABSTRACT

In the present world, Global Warming has been one of the biggest problems regarding environmental aspect and CO_2 is held responsible for that. It is an inevitable necessity to mitigate the concentration of CO_2 in the atmosphere. CO_2 sequestration is one of the best methods to reduce its concentration by trapping it beneath the earth in different geological conditions. The unmined coal seams and thin bands of coal provide a potential storage for CO_2 with suitable geological environment. These days it has become necessary to study the relationship between coal structure and flow of fluids inside.

In this project, an effort has been made to study the behaviour of fluids i.e. carbondioxide and methane inside of coal and the analysis has been carried out to study their velocity and pressure variations using COMSOL Multiphysics.

Coal contains both cleat and porous structure. Cleats are the natural fractures in coal and pores are the important factors for migration of fluid inside coal. Two separate models are developed to understand the fluid flow behaviour in both cleat and porous structure of coal.

A study on 3D model has also been carried out by developing a uniform coal block to analyze pressure and velocity variations inside it.

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CHAPTER - 1

INTRODUCTION

1.1 Origin and Formation of Coal

The origin, formation, and structure of coal have been studied widely and an enormous amount of literature is available. Coal is an extremely heterogeneous material consisting of organic matter, mineral matter, moisture, and a complex pore network. It is generally accepted that the organic portion of coal was formed from concentrated deposits of swampy organic matter originally derived from terrestrial plants. Plant structures (leaf, stem) were converted into coal through complex biological, chemical, and geochemical processes driven initially by selective microbial action and later by the temperature and pressure generated by overlaying sediments over several hundred millions of years.

1.2 Cleat Structure of coal

Cleats are the natural fractures occurring in the coal bed accounting for the permeability in coal bed and they have the significant aspect regarding the success of engineering control for CO_2 sequestration. These cleats occur in nearly all coal beds. They are the reason behind stability and flow of fluid inside coal. These cleats have been investigated since early days of coal mining and provide a basis for simulation of fluid flow behavior inside coal structure.

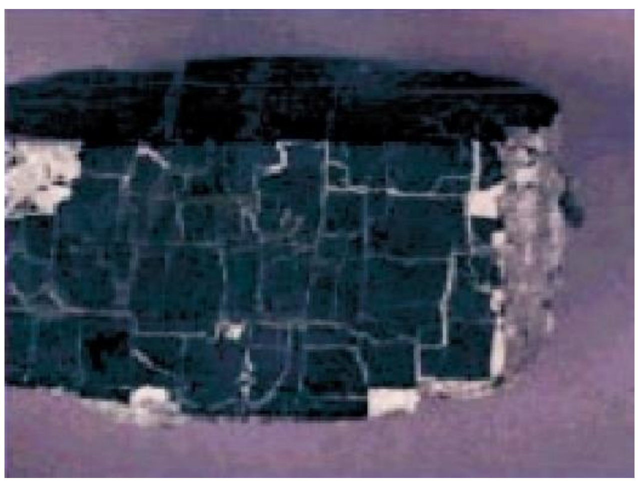

Fig.1 Natural fractures called cleats in coal

These cleats are usually found in two sets which are mutually perpendicular to each other and also perpendicular to bedding. Through-going cleats are formed initially and they are known as face cleats and the cleats which end at the intersection of the face cleats are known as the butt cleats and are formed latter. These fracture and partition inside the bedding planes impart a blocky structure of coal.

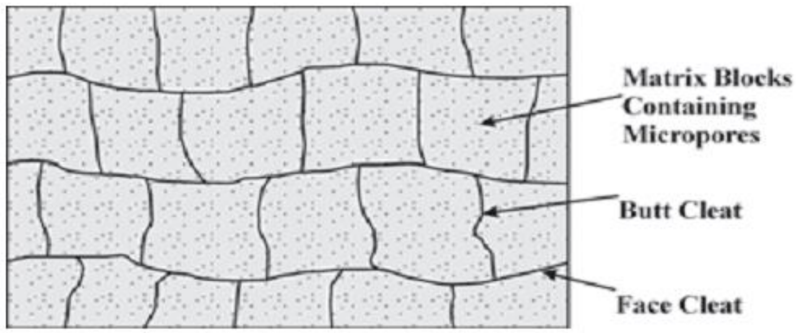

Fig.2 Face cleat and butt cleat in coal

Recent studies and experimentations have estimated that orientation patterns and style of fracturing focuses mostly on the permeability of coal and as per speculation, these cleats are the result of diagenetic and tectonic processes, which are considered to be the vital mechanical processes for the formation of cleats.

Cleats generally occur without any observable shear offset and thus, known as opening -mode factures. So far CO_2 sequestration and coal bed methane extraction processes are concerned, the cleat structure and the natural structures play an important role for planning and development of the above processes. The local and regional flow of water and hydro-carbon inside coal cleats is to be considered for study of fluid flow behavior.

1.3 Porous Structure of coal

Porous medium in coal is also an important factor regarding the migration of fluid inside coal structure depending upon the size of the pores and their position. The fluid inside the coal flows with respect to the release of confining pressure, and the gas tends to migrate from a high pressure to low pressure zone via the pores considered as a medium of flow.

The pore structure of coal is of worth consideration regarding the extraction of methane from seams, sequestration of CO_2 and water purification using by activated carbon as well. The pore distribution and size of pores is independent of the rank of coal but it varies usually with the content of vitrinite. It is actually found that the pore available inside the vitrinite rich coal are smaller in size then those of vitrinite – poor coals. Experimental studies have shown that the low volatile bituminous possesses the largest specific internal surface area which indicates that they have the highest gas storage capacity. And the channel-like pores and the interconnected pores are available both in high and low volatile bituminous coal.

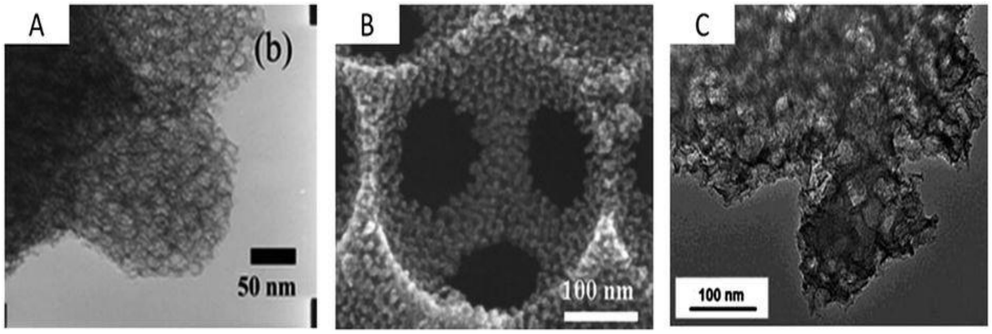

Fig 3. (A) Mesocellular carbon foam (dp = 20 nm)

(B) Macroporous carbon with mesoporous pore walls (dp = 317 nm, 10 nm)

(C) Micro/mesoporous Carbon (dp = 18 nm, 1 nm)

Generally, coal structure possesses dull porosity one is micro pores and other one is macro pores. Pores with width less than or equal to 2nm are called micropores. The pores of width lying between 2 to 50 nm are classified as mesopores and the pores with width exceeding about 50 nm are called macropores. The micropores and mesopores are reservoirs for gas storage and macropores provide the flow path waves. Various methodologies are developed for estimation and characterization of pore size distribution and porosity of the medium.

Experimentation have been carried out to study the fluid flow behavior inside the porous medium of coal to analyze CO_2 sequestration and methane recovery. Simulations have been carried out regarding the fluid flow depending upon the variation of temperature and pressure.

1.4 Effect of Carbon dioxide on Earth

CO_2 comprises nearly 0.04% or 400 ppm of the atmosphere. It has exceeded its concentration of past 80000 years. It is a potent greenhouse gas which is responsible for global warming through radiative forcing. This gas is an integral part for the existence of life on earth and it is a vital part of carbon cycle and biogeochemical cycle in which exchange of carbon takes place between the earth's oceans, soil and biosphere. Plants extract carbon from the atmosphere in the form of CO_2 in photosynthesis process and use it as a source of carbon compound for their growth. So, this plays an important role in the biosphere of earth.

It is one of the major factors for global warming and its concentration has increased markedly from 280ppm to 400ppm as of 2015. Deforestation and burning of fossil fuels are the major anthropogenic sources behind this. The rising rate is 2ppm per year currently and it's getting accelerated.

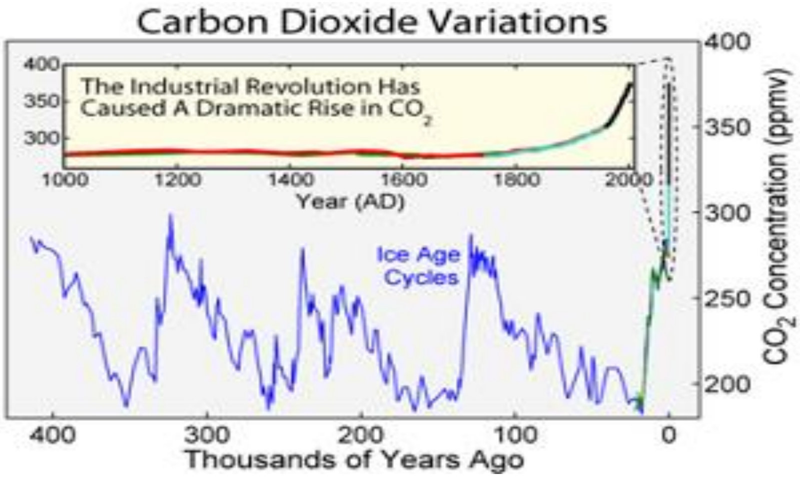

Fig 4. CO_2 concentrations over the last 400,000 years

Atmospheric carbon dioxide and greenhouse effect

In greenhouse effect, the thermal radiations of sunlight get absorbed by atmospheric gases which increases their temperature. The heated gases again emit radiations in all directions towards the surface, thereby heating the surface also.

Major contributing gases to the greenhouse effect are:

- Water vapor, 36-70%
- Carbon dioxide, 9-26%
- Methane, 4-9%
- Ozone, 3-7%

1.5 Carbon dioxide sequestration

Carbon dioxide sequestration is a process of minimizing CO_2 from the atmosphere or from large scale stationary sources like industries and power plants and putting them into long term storage. This process is significantly used for the mitigation of the level of concentration of carbon occurring in the atmosphere in the form of CO_2 and for reducing the release of the gas to atmosphere from various sources. There are various methods which have been scientifically developed for long term storage of CO_2. The methods being:

- Storage in oil reserves and gas reserves
- Storage in deep saline aquifers
- Storage in deep ocean
- Mineral carbonation

- Storage as clathrates
- Artificial fertilization of ocean
- storage in unmined coal seams
- Storage in salt caverns

1.5.1 Storage in depleted oil and gas reserves

The exhausted field of oil and gas reservoirs are considered to be the places for storing CO_2 beneath the earth. The advantages of CO_2 storage in such areas is that the hydrogeological conditions which allow the hydrocarbons to accumulate in the first place, also permit the accumulation and trapping of CO_2 in the space i.e. vacated by the produced hydrocarbon. The cap rock of oil and gas reservoirs retains the sequestered CO_2 for thousands of years. Scientific studies have been suggested to retain the sequestered CO_2 in the cap rock without over pressuring during the injection by the presence of unsealed and abandoned wells, tectonic plate movements or pH change. More than 80% of the world's hydrocarbon reserves are at intense depths which is more than 800m, thus fulfilling the required criterion of high temperature and pressure for efficiently storing CO_2 as a super critical fluid. The infrastructure geological construction properties and construction of cap rock of depleted oil reserves seem to be a suitable option for CO_2 sequestration. Under pressured, abandoned, closed and depleted gas reservoirs are also considered to be excellent geological trapes for CO_2 storage. For this to happen, firstly, the original gas present in the reservoir is removed up to 95% creating a large storage potential for CO_2. Secondly, the injected CO_2 is trapped to the original pressure of the gas reservoir thus preventing the collapse of original pressure. Hardly, mechanisms have been conducted to ensure that CO_2 does not reach the surface.

1.5.2 CO_2 storage in deep saline aquifers

Deep saline aquifers are considered to be better storage places for CO_2 as compared to hydrocarbon reservoirs. These aquifers are found in the sedimentary basins around the world and they contain high salinity connate water which is not useful for human use or agricultural purpose. These aquifers are the best places for injection of hazardous and non-hazardous liquid wastes hence providing a viable option for CO_2 sequestration. Scientific studies have been carried out and it is found that approximately 2% of the total effective volume in deep aquifers can be made available for CO_2 storage. Suitable aquifers should be kept by a regional aquitard like shale without any fracture or fragmentation. The top of the aquifers should be at least at a minimum depth of 800 meters for storing CO_2 in a super critical state. The aquifer should have high local permeability for injection but regional scale permeability should be low for long term disposal of CO_2. When CO_2 is injected in the aquifer, it rises up due to buoyancy effects, spreads out and forms a layer of CO_2 under the cap rock. In the primary stages of geochemical reactions the CO_2 dissolution in to formation of water is expected to be the predominant process and the surface area of CO_2 in contact with the formation water controls the rate of dissolution. The undissolved portion of injected CO_2 segregates and forms a plume at the top of the aquifer due to the difference in density. Plume will be driven by the result of its buoyancy force and hydrodynamic force. If the density and viscosity difference within the CO_2 and formation fluid is greater, the process of separation of undissolved CO_2 and flowing upwards in the aquifer will be more. So CO_2 should be injected with high pressure to ensure high density of the gas and the high solubility rate in the formation of water.

1.5.3 Storage in Deep Ocean

Ocean is considered to be a best option for CO_2 storage. It is considered to be the best sink available for disposal of CO_2 with a residence time of four to five hundred years. The stratified thermocline located between the surface layer and the ocean is a suitable place for CO_2 storage. Ocean and atmosphere are in contact over 70 % of the total globe and there is a continuous exchange of inorganic carbon between them. Oceans are removing CO_2 at a rate of six gigatonnes per year from the atmosphere.

Anthropogenic CO_2 can be disposed in liquid form below the thermocline at depth greater than 1500m and the sequestration is carried out either by dissolution in water column or by formation of CO_2 hydrates.

1.5.4 Mineral carbonation

In this process, CO_2 is combined with Mg or Ca silicate minerals chemically and this process is exothermic in nature which produces huge amount of heat in this process. CO_2 is stored in the form of carbonates or any other byproducts. The magnesium carbonates and the calcium carbonates are very stable in the geological condition and they are potentially storing CO_2 for millions of years. Magnesium silicates are more preferable as compared to calcium silicates as they are more wide spread. They form larger bodies and contain more reactive materials per ton of rock. Enstatite, asbestos tailing, fly ash and other tailings and industrial residues are considered to be potential starting materials for industrial carbonation process. Recent studies have emphasized that olivine [(Mg, Fe) Sio4] and serpentine [$Mg_3Si_2O_5$] are the most appropriate substances for mineral carbonation. The following reactions illustrate the CO_2 carbonation principle using olivine and serpentine as shown below:

Equation: Mg_2SiO_4 [olivine] +2CO_2=>2$MgCO_3$ [magnesite] +SiO_2 (1)

$Mg_3SiO_3\,(OH)_4$[serpentine] +3CO_2=>3$MgCO_3$ [magnesite] +2SiO_2 + H_2O (2)

As a natural phenomenon, carbonation process involving silicates are very slow in process. So industrial sequestration process should be accelerated rapidly by adopting certain process. Some typical processes are increasing surface area of magnesium silicate, agitating the slurry, adding catalyst (Nacl, $NaHCo_3$, Hcl) to the solution or slurry prior to the carbonation process. Carbonation process can be optimized by adopting suitable temperature control and partial pressure control. Olivine can be subjected to super critical conditions to increase its rate of dissolution. In Case of serpentine, an energy intensive heat treatment is sometimes required such that activation- destabilization of the crystal structure takes place at temperature above 600 degree Celsius. This pretreatment removes the chemically bound water and increases overall porosity.

1.5.5 Storage as clathrates

It is a type of ocean deposition of CO_2 at a depth of more than 3000 meters. At such greater depth, the pressure is very high and the temperature is very low in value. So CO_2 can be stored in form of clathrates, which is nothing but an ice like combination of water and CO_2. Pure CO_2 hydrate is denser than sea water and it generates sinking plume settling in the bottom of the ocean. The sequestration process in this way forms submarine pools in hollows or trenches in deep sea. In this process, the dissolution of CO_2 is decreased significantly due to formation of hydrates of CO_2. Direct disposal of CO_2 at greater depth is not currently possible technically but it is technically possible to send cold CO_2 or dry ice from mid depth to ocean floor. The density of dry ice is greater than water and hence the dry ice will sink to ocean bottom and will be effectively stored.

CO_2 sequestration is also carried out by clathrates blocks. Experimental analysis has been carried out to confirm that the stream lined blocks have higher terminal velocity and thus they can reach the sea bed faster than equidimensional blocks. These blocks can be penetrated in to the sea where the CO_2 in solid form would react physically and chemically with sediments before reacting with ocean water. So retention time would be significantly increased as compared to the gaseous or liquid CO_2 disposal methods.

1.5.6 Artificial fertilization of ocean

The artificial fertilization of ocean is carried out using additional nutrients like nitrites and phosphates or iron to increase the draw-down of CO_2 from the atmosphere. The nutrients increase the biological material there by drawing down additional CO_2 from atmosphere by the process of photosynthesis of phytoplankton. The additional benefit of this process being, this will increase the fish population and causes atmospheric CO_2 sequestration as a secondary benefit.

1.5.7 Storage in unmined coal seams

Coal beds are one of the most appropriate places for storage of carbon dioxide. There are a lot of coal beds which are either unmineable due to greater depth or because of very small thickness. At greater depth, conventional mining is not possible in coal seams so they are implemented as the potential storage places for storage of CO_2.

CO_2 can be adsorbed in the coal surface or it may be trapped inside the pore structure of the coal seam and locked up permanently. There is an alternative to CO_2- only storage in injection of flue gas, a mixture of CO_2 and nitrogen in to coal beds.

There is a possibility of huge cash flow by CO_2 sequestration in coal beds by carrying out enhanced coal bed methane process. In this process, CO_2 is injected in methane rich coal beds. The disposal of CO_2 in these methane rich coal beds increases the drive pressure and the coal bed methane recovery rate. So the gas injection process enables more methane extraction at the same time sequestering CO_2.

Number of companies are carrying out CBM recovery in Western Canada. Primary coal bed methane recovery process nearly recovers 20 to 60% of gas in the coal seam. Some of the remaining gas can be recovered by CO_2 enhanced coal bed recovery method.

It can be achieved by drilling wells at suitable places into the coal deposits and the wells are made usually in the five point pattern such that the central well is considered to be the injection well and the wells in the four corners are made for recovery purpose.

After discharging formation waters from the coal bed, CO_2 is injected in to the coal seam. The affinity of CO_2 with coal is more than methane and about double the times as compared to methane just below the critical point.

The carbon dioxide molecules displace the adsorbed methane molecules that disrobe from coal matrix in to the cleats and flow to the production wells.

Flue gas injection is also carried out for enhanced methane production to a greater degree than CO_2 alone. But nitrogen has a lower affinity in the coal structure as compared to carbon dioxide or methane. So when flue gas or carbon dioxide enriched flue gas is injected, the nitrogen breaks out of the production wells. So nitrogen will be re injected in to the coal seam.

Recent studies have been carried out regarding the injection of CO_2 in the coal bed. The continuous injection of carbon dioxide in the coal bed has resulted a decreased permeability of cleat system which surrounds the injection well area. In general, the desorption of methane causes shrinking of coal matrix that results the opening of the cleats and hence increases the CO_2 injection rate in to the system and the recovery rate of methane. Simultaneously, the replacement of CO_2 by the methane gas causes matrix to swell. The swelling will partially block the passage in the cleat system and provide a negative impact on the whole system.

Both the processes of fracturing of coal and swelling have opposite impacts on the system. The best solution for appropriate rate of CO_2 injection is to maintain the near well-gas pressure in the cleat system which will exceed the hydraulic fracturing pressure. But if there is a necessity of repeated hydraulic fracturing for maintaining connectivity between the well bore and the permeable areas of the coal seam, this may result in over or under burden connectivity between the well bore and the permeable areas of coal seam CO_2 leakage.

1.5.8 Storage in salt caverns

Generally salt is found as an evaporate bed or domal or ridge type intrusive deposits and in such places, salt from the major underlying sources are forced up to create the overlying formations. In the process of solution mining, large cavities are created in the salt bed and water is injected in to these beds or dome and the brine solution is pumped out. The volume can be extended up to

5*10^5m^3. As salt is highly impermeable in nature, these cavities provide an appropriate option for storage of CO_2. So the technological studies are currently in progress for salt mining. Dry ice or solid CO_2 can also be stored in these places which is surrounded by thermal insulation to minimize heat transfer and leakage of carbon dioxide. Salt and rock caverns usually provide a large storage capacity for carbon dioxide. But the cost associated with this process is very high and the advanced and eco- friendly aspects regarding this concept are yet to be developed. The environmental aspects regarding large amount of mined rock and brine disposal are significantly high which are to be taken care of.

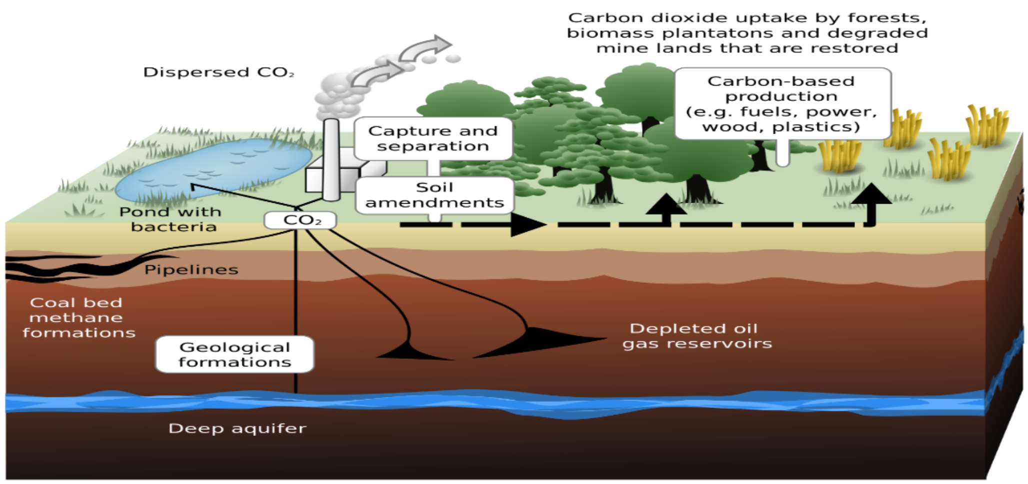

Fig 5. Different methods for carbon dioxide sequestration

1.6 Objective of the Project

In order to ensure the behaviour of fluid flow inside the coal structure, many detailed simulations of gas-coal interaction need to be performed. Such simulations should take into account geological properties such as density, Porosity, permeability and Poisson's ratio etc.

The main objective of this modelling is:

- To investigate the fluid flow behaviour in coal structure with cleats.
- To investigate the fluid flow behaviour in coal having porous structure.
- To investigate the fluid flow behaviour in a 3D structure of coal.
- To correlate between all the above mentioned models.

CHAPTER - 2

LITERATURE REVIEW

2.1 Introduction

An extensive literature review has been carried out to find out different approaches those have been made by various researchers in the field of simulation of carbon dioxide sequestration using COMSOL Multiphysics. In our thesis these various approaches have been reviewed widely.

Guoxiang andSmirnov (2007) proposed a model for computer simulation and conducted the modelling with a purpose to predict the transportation of carbondioxide in two phases, multilayer environment of an unminable coal bed basin based on variable saturation model.

Marin (2006) proposed a method for solidification of a free surface liquid phase and solved with COMSOL Multiphysics.

Danae A. Voormeij and George J. Simandl (2004), provided a technical review regarding geological mineral and oceanic CO_2 sequestration methods.

Lai Zhou, Qiyan Feng, Zhongwei Chen and Jishan Liu (2011), proposed a modelling and up scalling of binary gas coal interactions in CO_2 enhanced coal bed methane recovery. As per their simulations the net change in the permeability of coal is accompanied by binary gas dispersion.

Dr. R. W. Zimmerman (2002-2003), provided a review regarding diffusion equation for fluid flow in porous rocks.

M. Gharasoo, C. Deusner, N. Biglke and M. Haeckel conducted a model for simulation of methane hydrate dissociation by injection of super-heated carbondioxide using COMSOL Multiphysics. They performed the experiment in different temperatures and pressures and examined the dissociation rate of methane hydrate. They also compared the results of their simulation with the experimental results.

Song Li, Dazhen Tang, Hao Xu, Zi Yang (2012) established a model for pore structure system properties of coal bed methane reservoirs in china, Guizhou and Panguan Syncline the result shows that the medium rank coals in Panguan syncline are the best prospective targets for the exploration and production of coal bed methane.

Curtis M. Oldenburg, Steven L. Bryant, Jean Philippe Nicot (2009) provided a framework on effective trapping for geologic carbon sequestration.

Nilay J. Prajapati and Patrick L. Mills (2009) proposed a numerical study for flux models of CO_2. They concluded that binary diffusion and absorption play the key roles for the flow of fluid in shale nanopores.

A. F. Gulbransen and V. L. Hauge (2008) proposed a multiscale mixed finite element method for naturally fractured vuggy reservoirs. Their results indicate that this multi scale method can resolve the interaction of free flow and porous region, fine scale capture details and long range correlation.

Zhaoqin Huang (2010) modeled two phase flow in porous media that is strongly heterogeneous. This modelling has been implemented with COMSOL Multiphysics 3.5 (a) and pressure saturation model was used. He coupled pressure saturation and discrete-fracture model for simulation in fractured media. His results conclude that fractures are the dominating flow path and the prime factor for intensifying anisotropy and heterogeneity. The discrete vugg network model provides a way of modelling fluid flow through vuggy and fractured porous structure.

M. A. Diaz Viera (2008) presented a model for multiphase fluid flow in porous media using COMSOL Multiphysics. They used a finite element approach, an oil phase pressure and total velocity formation and also used capillary pressure to implement the modelling.

CHAPTER - 3

METHODOLOGY

3.1 Introduction

The drastic increase in the concentration of CO_2 in the atmosphere along with other greenhouse gases such as CH_4, NO_2. NO, etc. is due to the massive increase in anthropogenic activities and increase in industries. The concentration of CO_2 has risen from the pre- industrial levels of 280 ppm to present levels of 365 ppm which indicates, there is an yearly accumulation of 1.5 ppm of CO_2 on an average.

The main sources of emission of CO_2 are combustion of fuels used for electricity generation and various industrial processes such as cement production, oil, cement and steel industries emitting several million tons of CO_2 annually. The enormous emission of CO_2 results in global warming such that the global surface temperature increases by 30 ± 0.6 degree Celsius on an average. These increase in CO_2 concentration has a great impact on the environmental aspects which is of worth consideration so studies are going on long term storage of CO_2 in coal bed to control the further pollution of the environment.

The injection of CO_2 into gassy coal beds is a suitable solution to control over the increase in concentration of CO_2 in the atmosphere. This process includes various concepts like gas adsorption on the surface of coal, replacement of coal-bed methane by CO_2 and advanced methane recovery, etc. A lot of researches have been carried out to study the fluid flow through porous media as well as cleat structure for carrying out sequestration of CO_2. Experimental and numerical modellings help to provide good understandings regarding the fluid flow behavior in coal structure.

3.2 Background problem

Coal is a porous medium but the pore structure is very complex and very difficult to study. Cleats are natural creations and the fractures present in the cleats are very difficult to analyze regarding the permeability of coal which is a big factor of consideration for fluid flow behavior in coal. The coal matrix fracture and coal permeability in in-situ conditions are still unclear in experimental field. The success of CO_2 sequestration depends on our understanding of gas–coal interactions and how they affect the properties of CO_2 transport in coal seams. Comsol multiphysics is a software which provides a path for the study and analysis of the fluid flow behavior inside coal structure.

3.3 Two-phase Darcy law

The concept that provides the theory behind fluid flow in the subsurface is called Darcy's law. Darcy’s law comprises various equations those define the ability of a fluid to flow through a porous media such as rock. This law states that the amount of fluid flow between two points is directly related to the difference in pressure between the points, the distance between the points, and the interconnectivity of flow pathways in the rock between the points. This interconnectivity within the flow pathway is called permeability.

Here pressure indicates the excess of local pressure over the normal hydrostatic fluid pressure which increases with depth like in a standing column of water due to gravity. The flow impedance ted during fluid flow is referred to as permeability. Darcy's law gives a simple proportional relationship between the instantaneous discharge rate through a porous medium and the pressure drop over a given distance.

The two-phase flow of Darcy law is often referred to as fractional flow formulation. The background for the two-phase flow equations are the general mass balance equations. This approach treats the two-phase flow problem as a total fluid flow of a single mixed fluid, and then describes the individual phases as fractions of the total flow.

The governing equations in two phase Darcy law are:

$$\frac{\partial \epsilon_p \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0, \quad \mathbf{u} = -\frac{\mathbf{\kappa}}{\mu} \cdot \nabla p$$

$$\rho = s_1 \rho_1 + s_2 \rho_2, \quad \frac{1}{\mu} = s_1 \frac{\kappa_{r1}}{\mu_1} + s_2 \frac{\kappa_{r2}}{\mu_2}, \quad s_1 + s_2 = 1$$

$$\frac{\partial \epsilon_p c_1}{\partial t} + \nabla \cdot c_1 \mathbf{u} = \nabla \cdot D_c \nabla c_1, \quad c_1 = s_1 \rho_1$$

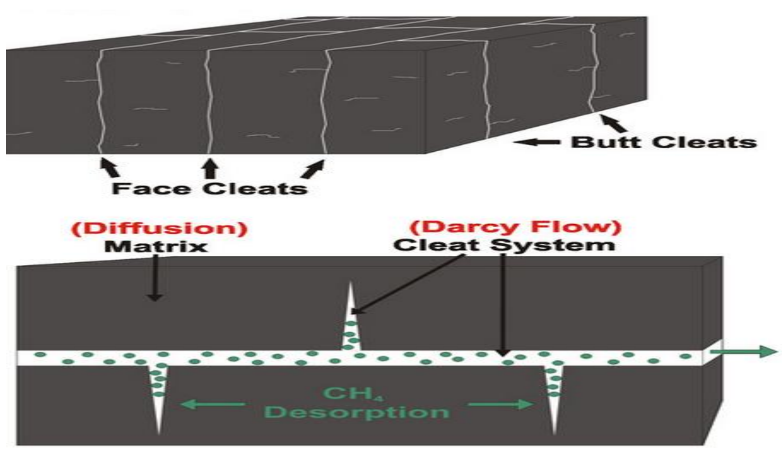

Fig 6. Darcy flow of fluid inside coal cleat and porous structure

Table 1: Input properties of coal

Property	Value	Unit
Porosity(ε_p)	.069	1
Permeability(k)	5*(10^-15)	m^2
Density(ρ)	1360	Kg/m^3
Poisson's ratio(u)	0.35	1

Table 2: Input properties of Fluid 1 (CO_2)

Property	Value	Unit
Density(ρ_1)	1.98	Kg/m^3
Relative permeability(k_{r1})	1	1
Dynamic Viscosity(μ_1)	14*(10^-6)	Pa.s

Table 3: Input properties of Fluid 2 (CH_4)

Property	Value	Unit
Density(ρ_2)	0.66	Kg/m^3
Relative permeability(k_{r2})	1	1
Dynamic Viscosity(μ_2)	10^-5	Pa.s

3.4 COMSOL Multiphysics and its operation

Comsol multiphysics is a software which works on finite element analysis. Finite element analysis is a numerical technique which is used for finding approximate solutions in boundary value problems and partial differential equations. This analysis subdivides the whole domain into simpler and discrete parts which is called finite elements and uses integration over the whole set to get the results or to model over the whole domain. It uses the idea of connecting many tiny straight lines to approximate a larger circle, and this method encompasses methods for connecting many simple element equations over many small subdomains, named finite elements, to approximate a more complex equation over a larger domain.

COMSOL is called a Multiphysics software because it carries out simulations that involve multiple simultaneous physical phenomena. For example, combining two fields like chemical kinetics and fluid mechanics or combining fields of finite elements with molecular dynamics.

Multiphysics also involves the processes of solving coupled systems that comprises partial differential equations.

Many physical simulations involve coupled systems, like electric and magnetic fields for electromagnetism applications, pressure and velocity for sound applications, or the real and the imaginary part of the quantum mechanical wave function.

This software provides an extensive idea regarding physics and engineering applications. It provides a conventional physics-based user interface. Differential equations have huge application in comsol. Comsol allows the coupled system of Partial differential equations for the applications of various physics used in this software.

It also provides an interface for application programming interfaces. Comsol also provides a nice extension to Matlab. We can extend the modelling using comsol to the use of Matlab. Complicated object oriented code is used by comsol for use of soft wares.

Comsol provides various applications in mechanical, electrical, chemical, fluid, and multipurpose and interface background. In mechanical it has various modules like heat transfer module, structural mechanics module, fatigue module etc., in electrical field, it provides the modules like AC/DC module, RF module, wave optics module etc. In the field of fluid it has huge applications regarding the modules like CFD module, micro fluid module, mixer flow module. For multipurpose applications, it uses optimization module and particle tracing module. In interface applications, it uses live link module, CAD import module, and file import for CATIA etc.

In our modelling, we have used porous media and subsurface flow module in the field of fluid. We have used two-phase Darcy law for our modelling in which we have modelled the fluid flow behavior in carbon dioxide sequestration.

3.4.1 Modeling in COMSOL Multiphysics

Comsol provides an intuitive and smooth operation during the modelling in any module under any field.

This uses the concept of Multiphysics during our Modeling, and it has the application in the field of simulating scientific and engineering applications. It finally gives the summary how we can model multiphysics applications with COMSOL Multiphysics software.

3.4.2 Creation of geometries

The first step in modelling is to create either the geometrical model with proper dimensions of our component or the dimensional space attribute that clearly describes our concept of modelling.

In particular, the demonstration summarizes:

- Creating and manipulating geometries using the built-in CAD tools
- Importing geometries from a CAD tool
- De featuring geometries to reduce mesh size
- The live interaction with SolidWorks

3.4.3 User-defined and interactive meshing

After the generation of model and insertion of properties, we do the meshing, in which, we need to discretize or mesh it before solving. COMSOL Multiphysics provides an automatic meshing feature, with a large number of tools for manipulating subsequent meshes.

Various meshing processes used by COMSOL

- The structured and unstructured meshing capabilities
- Swept meshing
- Interactive meshing
- Importing mesh and creating geometries from a mesh
- Adaptive meshing

3.4.4 Using and fine-tuning the solvers

COMSOL Multiphysics provides the solvers for the following types of analysis:

- Stationary problems
- Eigenvalue analyses
- Parametric analyses
- Time-dependent problems

3.4.5 Post processing of Results

After the model is solved, post processing of results is needed which help for best communication of our simulations to the wider community. Visually or mathematically, post processing is easily handled in COMSOL Multiphysics. It basically contributes to:

- Manipulate the visualization parameters to best see the results
- Integrate and treat results mathematically
- Present work as a report

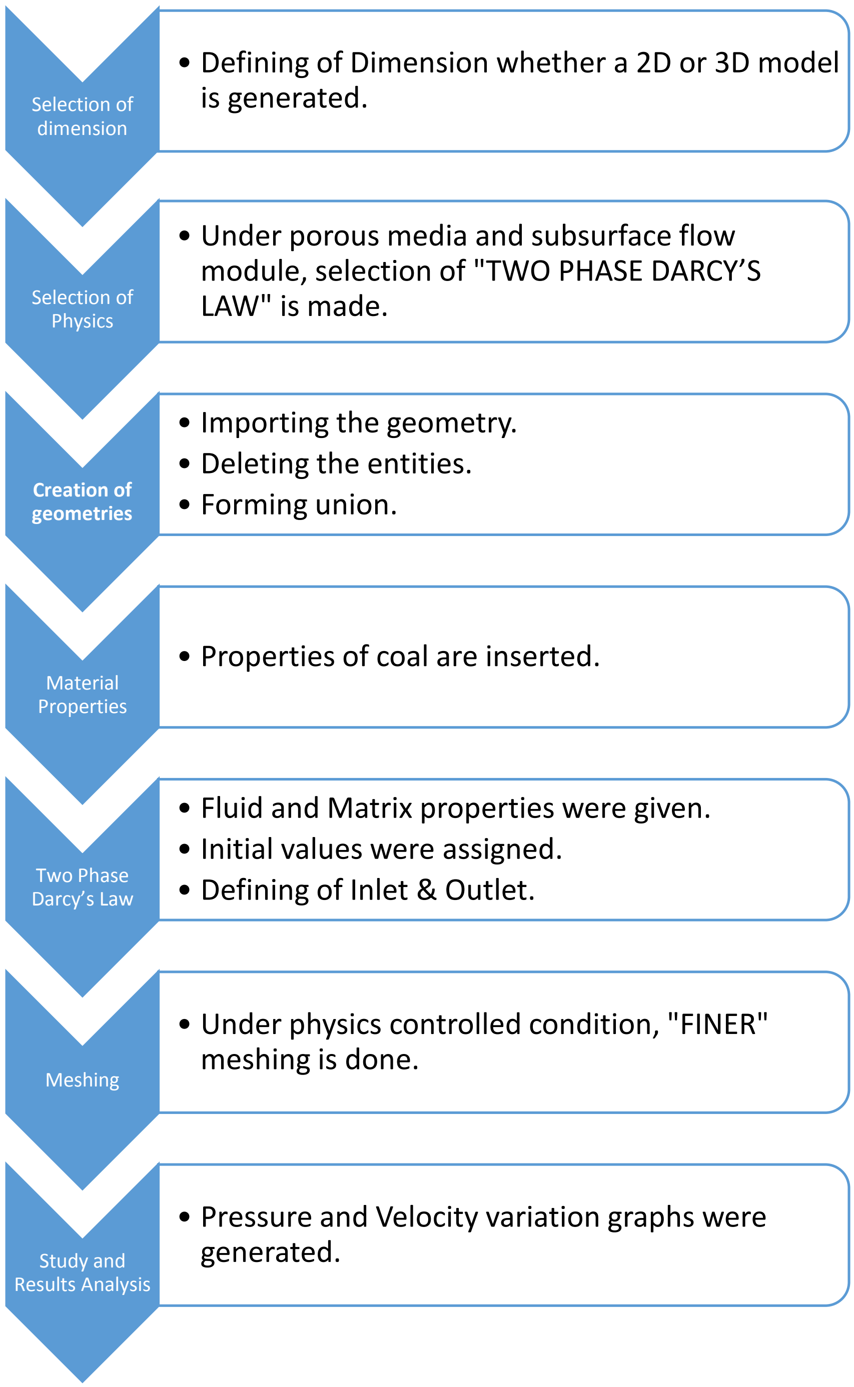

Fig 7. Flow diagram of methodology of simulation in COMSOL Multiphysics

CHAPTER - 4

MODELLING & SIMULATION with RESULT ANALYSIS

4.1 Fluid Flow behavior in cleat structure of coal

1. **Geometry:** This is a rectangular 2-Dimensional layer representing a cleat system of dimension 400 μm * 400 μm. The primary zone of interest is the rectangular region with lower left corner at (0, 0) μm and lower right coordinate at (400, 0) μm. The cleat structure of above specification has been developed in AUTOCAD and imported as a dxf file to COMSOL Multiphysics. The properties of coal are taken as input according to Table-1.

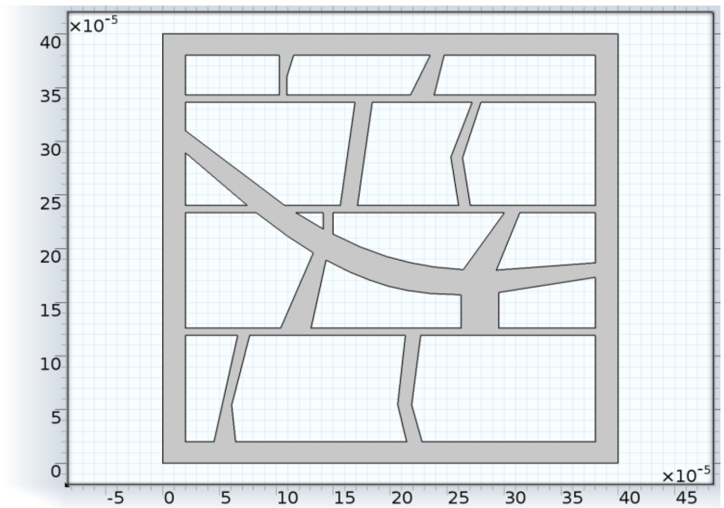

Fig 8. Geometry of cleat structure

2. **Inlet:** The upper boundary of the coal matrix is taken as the inlet and the pressure is applied to it through which the gas will be flown in to the whole matrix. The inlet pressure given in the upper boundary is 1000 Pa. The inflow velocity at the inlet is 5 m/s. The properties of fluids are taken as input according to Table-2 and Table-3.

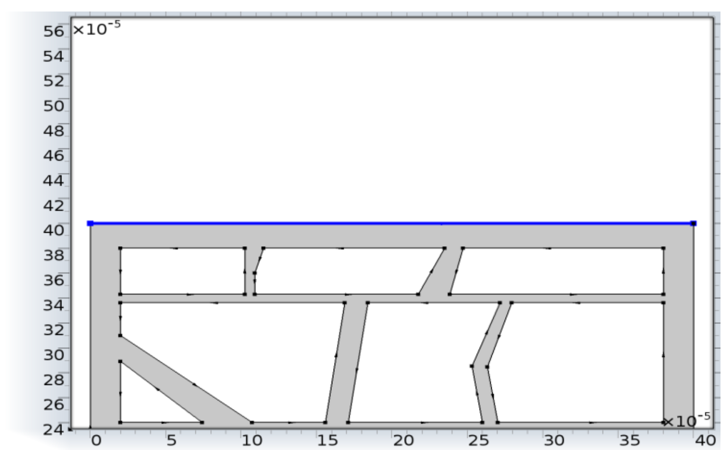

Fig 9. Inlet of cleat structure

3. **Outlet:** The bottom most boundary is taken as the outlet boundary and the output pressure is obtained in this outlet boundary after the completion of the flow of gas through it. Initially, the pressure at the outlet boundary is taken as zero.

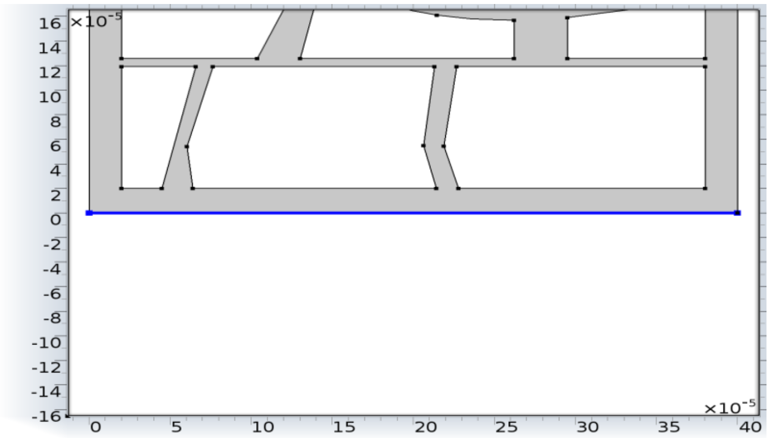

Fig 10. Outlet of cleat structure

4. **No Flux:** Under no flux condition, the flow of the fluid is confined inside the highlighted blue (i.e. within the area marked as grey) boundaries as shown in figure. The fluid will not pass beyond the boundaries (the area marked as white) in any case.

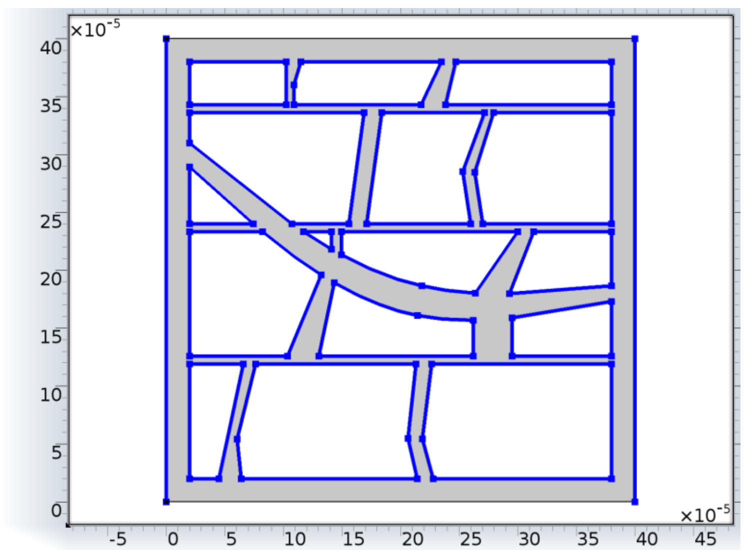

Fig 11. No flux condition in cleat structure

5. **Meshing:** Finer meshing is done under physics-controlled condition.

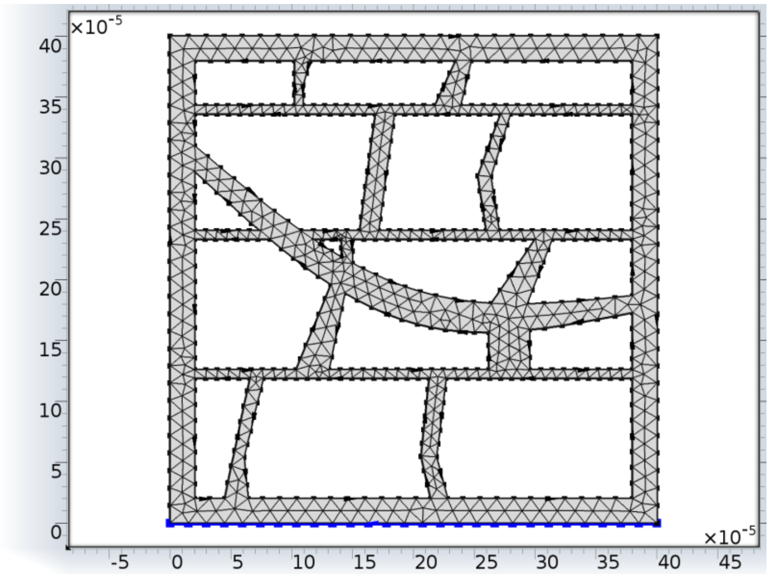

Fig 12. Meshing in cleat structure

6. **Study & Result Analysis:** Comsol gives output in form velocity and pressure distribution. Fig. shows velocity and pressure distribution model of coal matrix in the form of different colors.

6.1 Pressure profile: After the simulation, it has been found that when the fluid moves with in the cleats then the variation of pressure takes place as per the cleat structure. As the fluid moves away from the inlet the pressure gradually decreases in value and the value of pressure at different sections of the cleat is shown by different colors as depicted in the figure.

The highest pressure is found to be around 27.5 MPa around the inlet area which is highlighted by dark red color in the figure. In the middle portion of the cleat structure the value of pressure becomes average and the value is found to be around 15 MPa which is shown by yellow and somewhat green color and towards the outlet the pressure decreases to zero as indicated by the dark blue color in the figure.

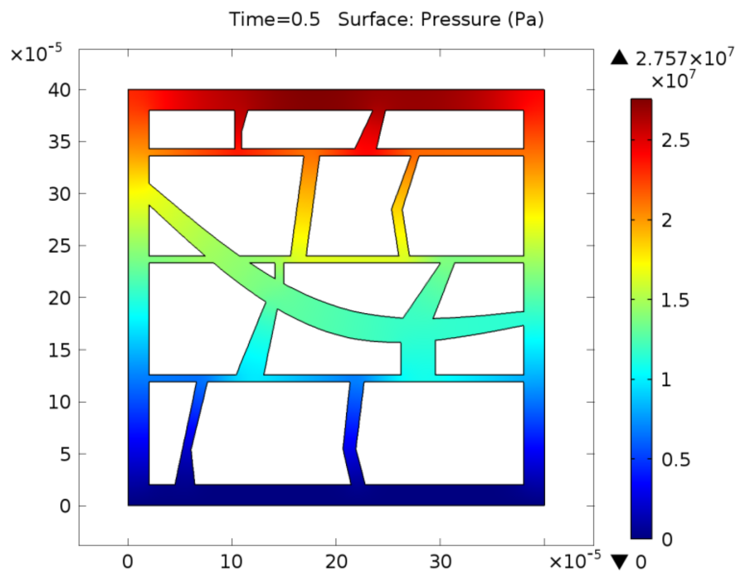

Fig 13. Pressure profile for cleat structure

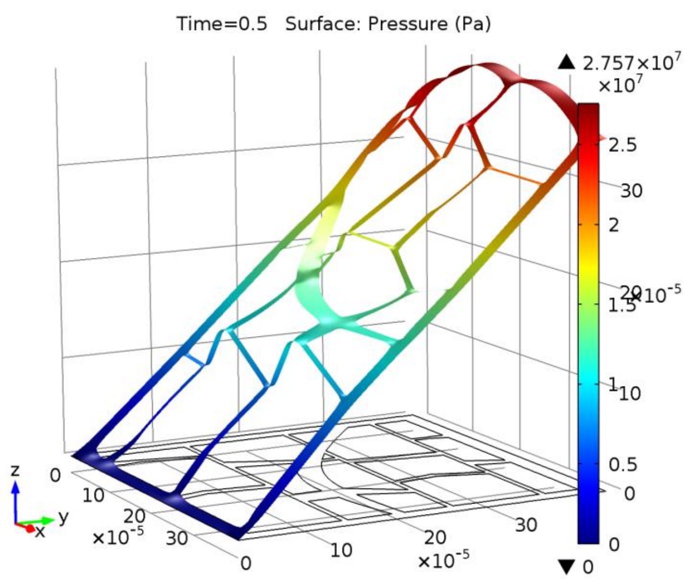

Fig 14. Height expression for pressure profile of cleat structure

This Figure shows height expression and pressure contour. Pressure contour shows variation of gas pressure in coal matrix. Different color line shows different values of pressure in whole coal matrix. These all lines form pressure profile of whole coal matrix.

6.2 Pressure vs X-axis at the "Inlet" boundary: From this graph, it is clear that the pressure at the inlet boundary increases first and then gradually decreases. There are two peaks appearing in the graph one between the coordinates (150, 0) and (200, 0) µm and another peak between the coordinates (250, 0) and (300, 0) µm. This is because of presence of one narrow cleat pathway between the coordinate (150, 0) and (200, 0) µm and another one between the coordinates (250, 0) and (300, 0) µm in the geometry itself. Near these narrow cleats, the inlet the pressure is becoming very high which attains a peak value of 27.5 MPa and 27 MPa respectively. Beyond that zone the pressure gradually decreases to a value of around 24 MPa.

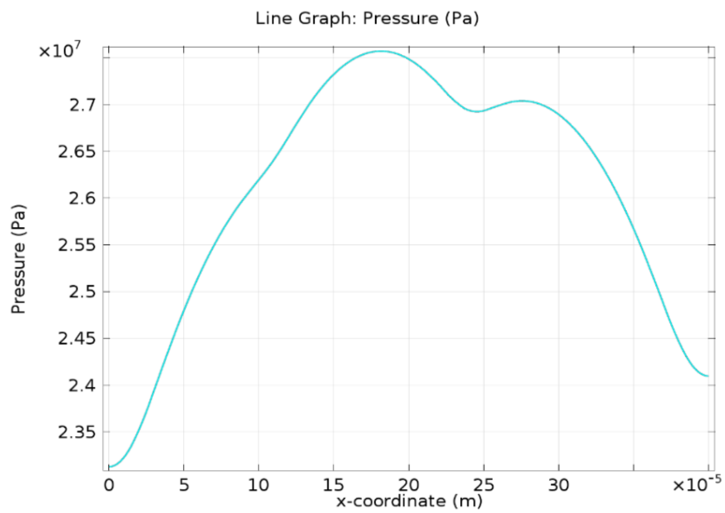

Fig 15. Plot between Pressure vs X-axis at the "Inlet" boundary

6.3 Velocity profile: After simulation by COMSOL, it has been found that the velocity varies considerably throughout the whole cleat structure as shown in the figure. The velocity varies from 0-60 m/sec throughout the cleat as per the width of passage for the flow of fluid. As per the equation of continuity of fluid flow,

$$A*V = \text{Constant}$$

Where, A is area and V is velocity respectively.

As per this law area of passage is inversely proportional to velocity of fluid flow throughout the structure. Where the area of the passage decreases the velocity increases. Hence, the velocity magnitude is very high in the narrowest portions and sharp edges of the cleats structure which is of the order of 60 m/s. and, the velocity is nearly zero in the very wide pathways of fluid flow.

On an average the velocity is around 30-40 m/s in the pathways of moderate width. The highest velocity is indicated by red color and the least is shown by blue color in the figure.

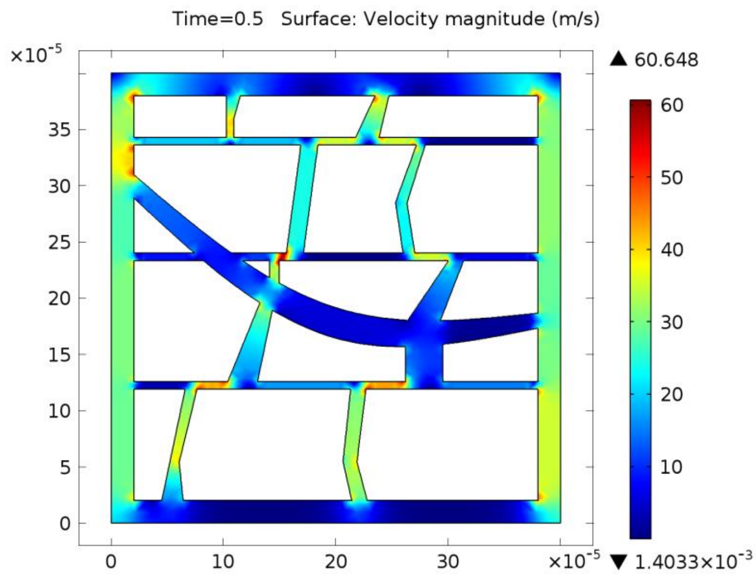

Fig 16. Velocity profile for cleat structure

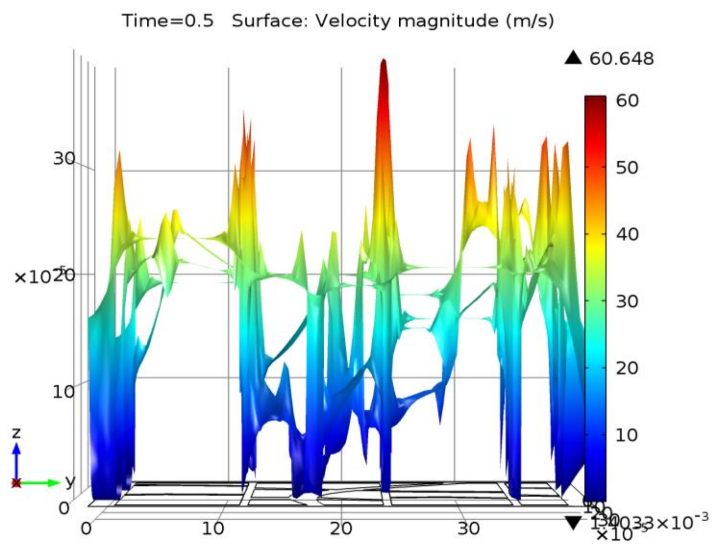

Fig 17. Height expression for velocity profile of cleat structure

This figure shows the velocity height profile in the cleat structure. Here, the velocity is shown as a projection up on the cleat structure and here we can get the velocity profile quite accurately.

The highest velocity is shown by the sharp tip that is shown by the red color in the profile which is around 60.648 m/s in value.

6.4 Velocity vs X-axis at "Inlet" boundary: The velocity varies along the inlet boundary according to the narrow pathways present near it. The velocity increases from 0 to 25 m/sec between the coordinates (0, 0) and (50, 0) µm because of the presence of sharp corners and narrow pathways within this region. After that it decreases as the flow region is wider and again getting peak of 14 m/sec because of presence of another corner between the coordinates (100,0) and (150,0) µm. again the velocity decreases due to wider path then increases between (200,0) and (250,0) µm and attains a value of around 10 m/sec and then continuously goes on increasing up to 22 m/sec within (350,0) and (400,0) µm due to presence of very sharp corner in the region.

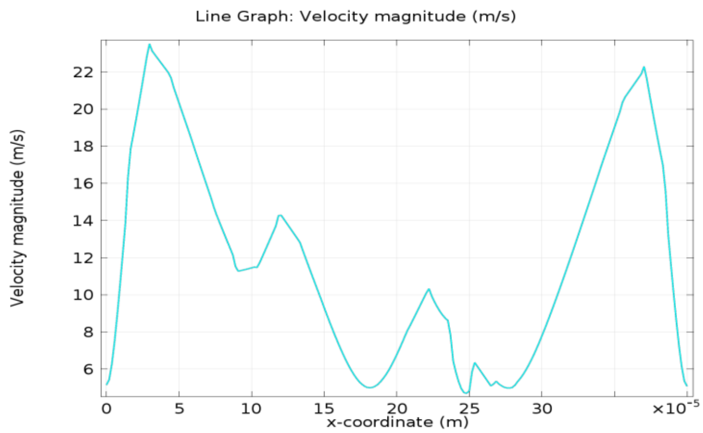

Fig 18. Plot between Velocity vs X-axis at "Inlet" boundary

6.5 Velocity vs X-axis at "Outlet" boundary: This graph shows the variation of velocity of fluid along the outlet boundary and there are three high peaks of velocity of around 22 m/sec initially at the (0, 0) µm and another peak in between (20, 0) and (25, 0) µm of around 10 m/sec and the last peak velocity of around 26 m/sec can be seen at finishing corner of boundary at (40, 0) µm. These peaks are generated because of the presence of sharp corners.

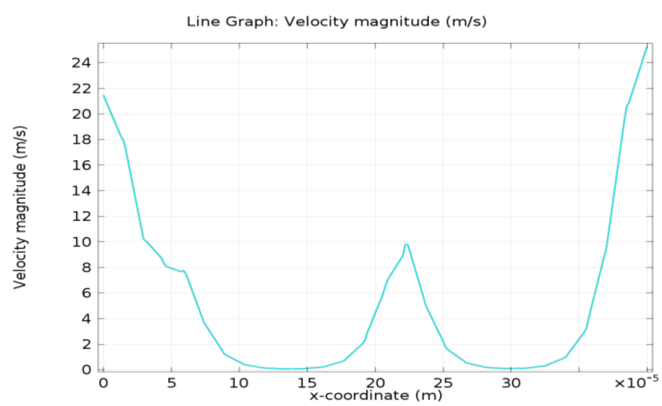

Fig 19. Plot between Velocity vs X-axis at "Outlet" boundary

4.2 Fluid Flow behavior in porous structure of coal

1. **Geometry:** This is a rectangular 2-Dimensional structure representing a porous medium of dimension 600 µm * 325 µm. The primary zone of interest is the rectangular region with lower left corner at (0,-300) µm and lower right coordinate at (600, -300) µm. The porous structure of above specification has been imported as a dxf file to COMSOL Multiphysics. The properties of coal are taken as input according to TABLE-1.

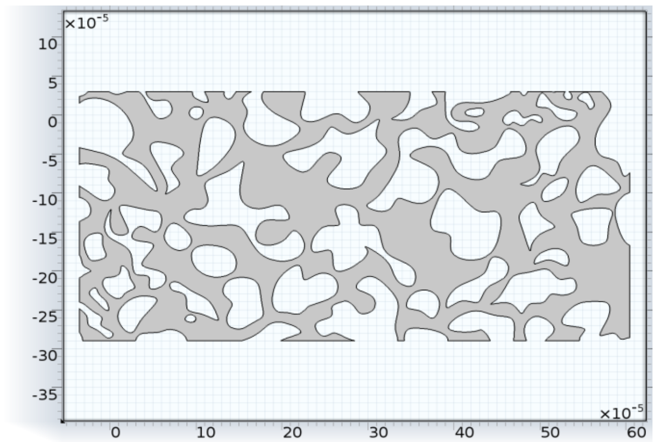

Fig 20. Geometry of porous structure of coal

2. **Inlet:** The right side boundary of the coal porous structure is taken as the inlet and the pressure is applied to it through which the gas will be flown inside via the pores throughout the whole structure. The inlet pressure given in the inlet boundary is 1000 Pa. The inflow velocity at the inlet is 5 m/s. Also, the properties of fluids are taken as input according to Table-2 and Table-3.

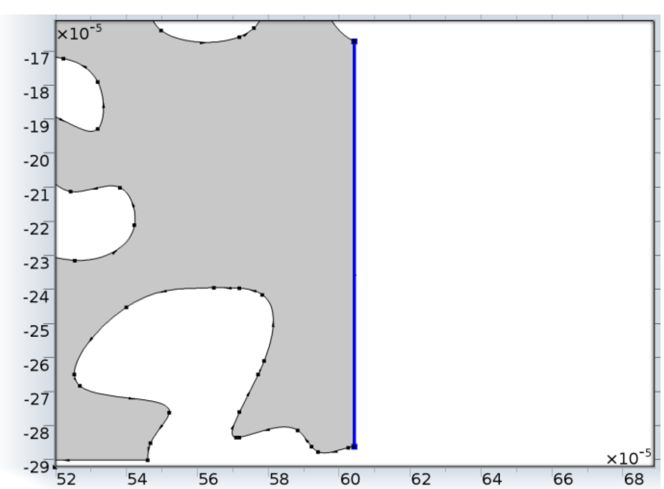

Fig 21. Inlet of porous structure

3. **Outlet:** The left most boundary is taken as the outlet boundary and the output pressure is obtained in this outlet boundary after the completion of the flow of gas through it. Initially, the pressure at the outlet boundary is taken as zero.

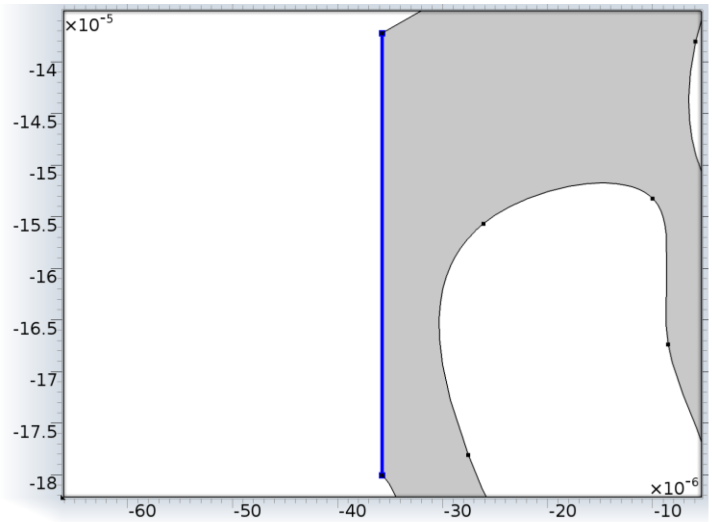

Fig 22. Outlet of porous structure

4. **No Flux:** Under no flux condition, the flow of the fluid is confined inside the highlighted blue (i.e. within the area marked as grey) boundaries as shown in figure. The fluid will not pass beyond the boundaries (the area marked as white) in any case. So under no flux condition, the fluid will be confined inside the micropores and the macropores only.

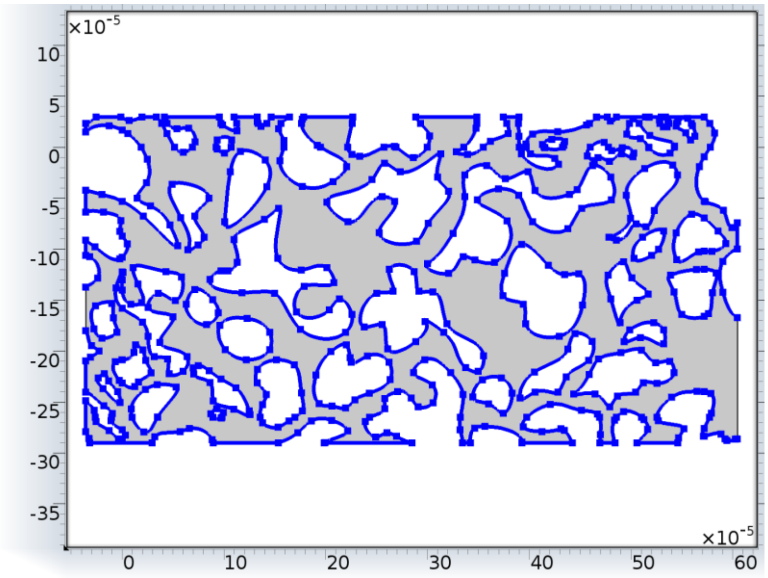

Fig 23. No flux condition in porous structure

5. **Meshing:** Finer meshing is done under physics-controlled condition.

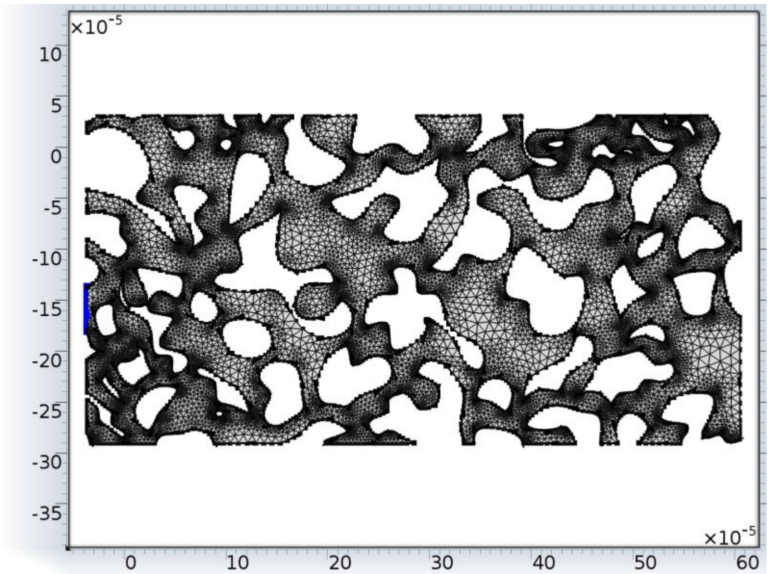

Fig 24. Meshing in porous structure

6. **Study & Result Analysis:** Comsol give output in forms of velocity and pressure distribution. Figure shows velocity and pressure distribution model of coal matrix in the form of different colors.

6.1 Pressure profile: After the simulation, it has been found that when the fluid moves with in the porous medium, then the variation of pressure takes place as per the location and size of the pores. As the fluid moves away from the inlet, the pressure gradually decreases in value and the value of pressure at different sections of the porous medium is shown by different colors as depicted in the figure.

The highest pressure is found to be around 14MPa around the inlet area which is highlighted by dark red color in the figure. In the middle portion of the porous structure, the value of pressure becomes average and the value is found to be around 6-8 MPa which is shown by yellow and somewhat green color and towards the outlet the pressure decreases to zero as indicated by the dark blue color in the figure. Hence, the pressure varies from around 13 MPa at the inlet boundary up to nearly zero MPa at the outlet boundary.

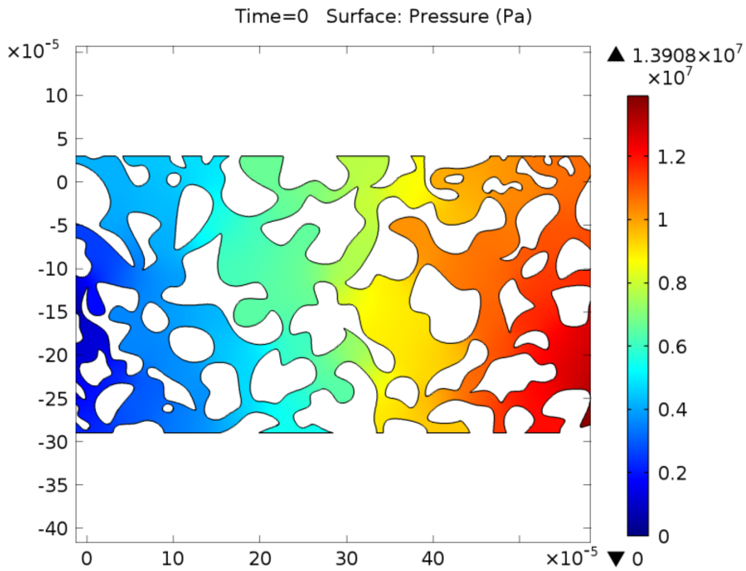

Fig 25. Pressure profile for Porous structure

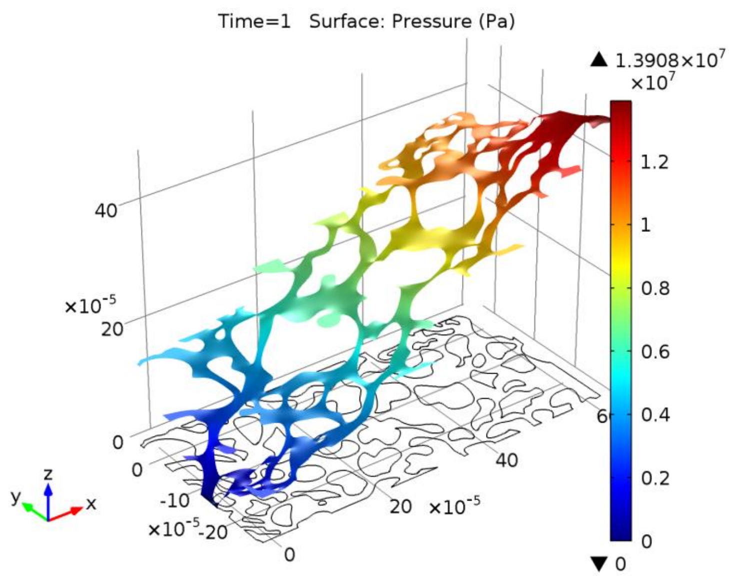

Fig 26. Height expression for pressure profile of porous structure

Figure shows height expression and pressure contour. Pressure contour shows variation of gas pressure in coal layer. Different color line shows different values of pressure in whole coal layer. These all lines form pressure profile of whole coal porous layer.

6.2 Pressure vs Y-axis at "Inlet" boundary: The inlet boundary is taken in between the coordinates (500,-280) µm and (500,-170) µm. and the graphical analysis shows that the value of pressure decreases from 13.8 MPa to 12.9 MPa at a uniform rate throughout the inlet region. The variation of pressure is due to the presence of nearby pores.

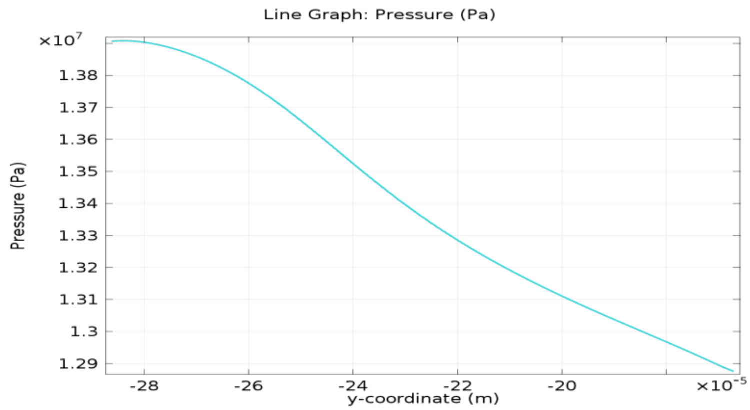

Fig 27. Plot between Pressure vs Y-axis at "Inlet" boundary

6.3 Velocity profile: After simulation by COMSOL, it has been found that the velocity varies considerably throughout the whole porous medium as shown in the figure. The velocity varies from 0-90 m/sec throughout the porous medium as per the size of the pores for the flow of fluid.

As per the equation of continuity of fluid flow, area of passage is inversely proportional to velocity of fluid flow throughout the structure. Where the area of the passage decreases, the velocity increases. Hence, the velocity magnitude is very high in very small pores or at intersection of these micropores within the structure, which is of the order of 90 m/s. and, the velocity is nearly zero in the macropores or in the wide portions of the porous structure during the fluid flow. On an average the velocity is around 20-30 m/s in the pathways of moderate width. The highest velocity is indicated by red color and the least is shown by very dark blue color in the figure. The highest velocity is found in a particular point in this simulation which is off the order of around 90 m/s and this is shown by zooming in that portion in the figure shown below.

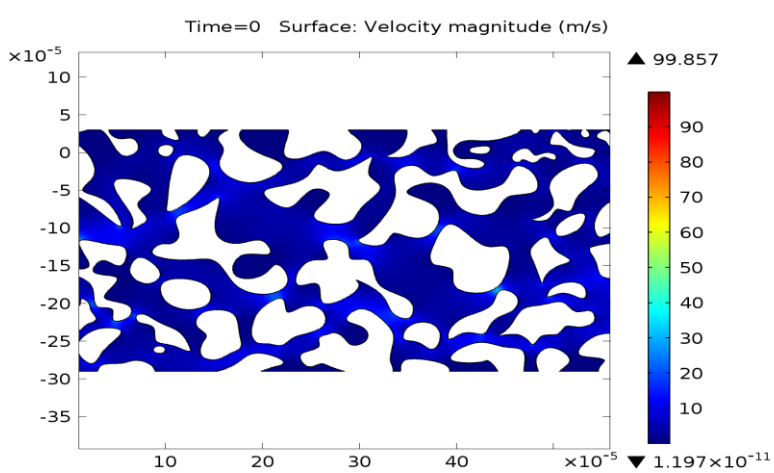

Fig 28. Velocity profile for porous structure

The next figure shows the velocity height profile in the porous medium. Here, the velocity is shown as a projection up on the porous structure and here, we can get the velocity profile quite accurately. The highest velocity is shown by the sharp pics that is shown by the red color in the profile which is around 90 m/s in value.

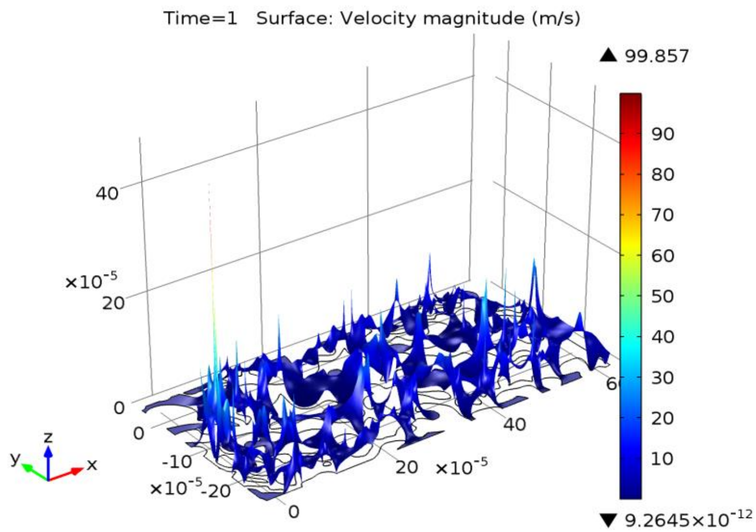

Fig 29. Height expression for velocity profile of porous structure

6.4 Velocity vs Y-axis at "Inlet" boundary: The initial velocity was give to be of 5 m/sec and after the simulation the graph shows the variation from 5 to 8.4 m/sec in velocity. And, there is a peak of around 8.4 m/sec corresponding to the Y-axis between (-260 to -240) µm because of a presence of narrow porous media. Hence, the velocity risen up due to the confined porous space.

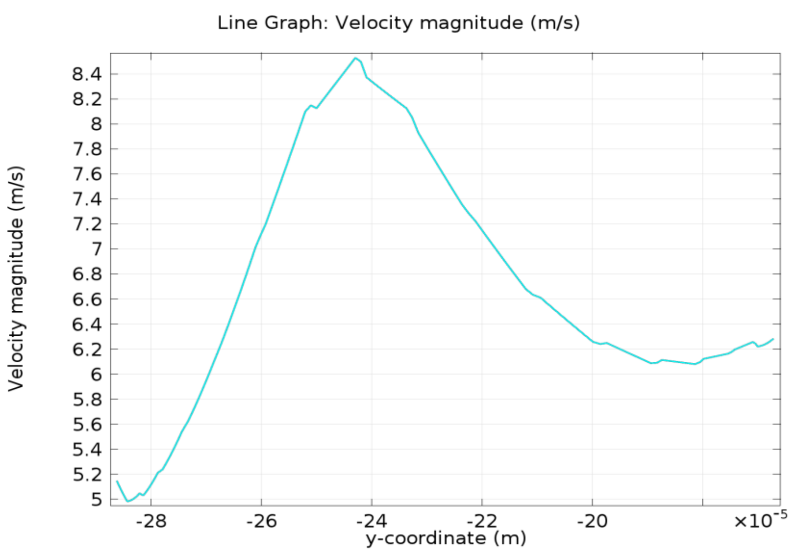

Fig 30. Plot between Velocity vs Y-axis at "Inlet" boundary

6.5 Velocity vs Y-axis at "Outlet" boundary: The velocity at the outlet boundary decreases first and then increases. The decrease in velocity is due to the open space along the boundary where the fluid gets enough space to move around and the velocity decreases whereas, at the end points of boundary, where fluid doesn't get much space for movement, the velocity goes on increasing.

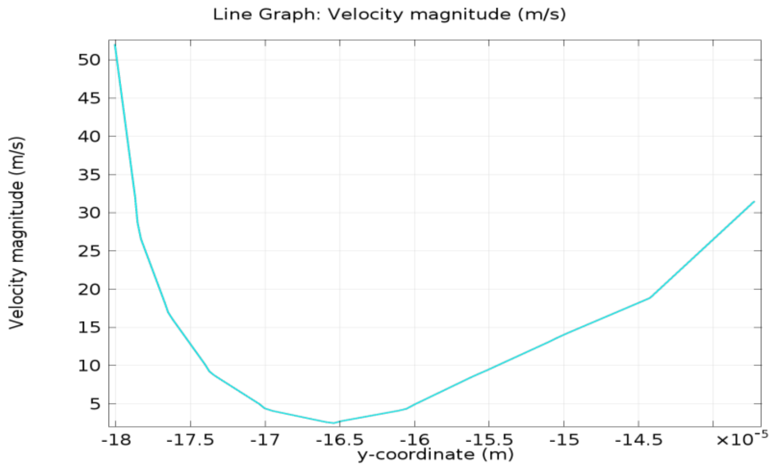

Fig 31. Plot between Velocity vs Y-axis at "Outlet" boundary

4.3 Fluid Flow behavior in 3-D structure of coal

1. **Geometry:** This is a cubical 3-D geometry generated in the CATIA software and imported as a (.stp extension) file in the COMSOL multiphysics for our simulation. Also, the properties of coal are taken as input to the geometry according to Table-1.

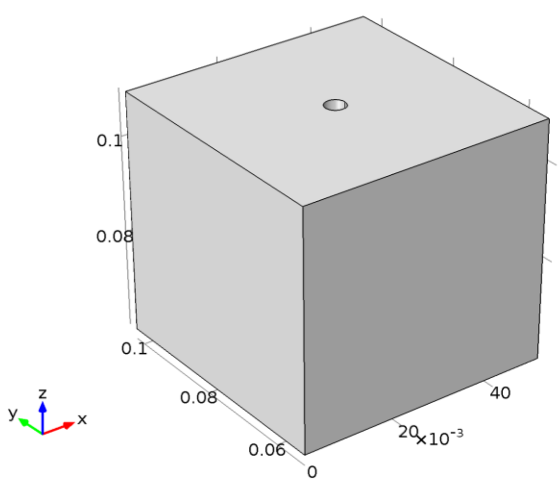

Fig 32. Geometry of 3D structure of coal

2. **Inlet:** A drill hole is made at centre of the top plane whose inside lateral surface as well as the base of the hole is taken as the inlet to inject fluid. The properties of fluids are taken as input according to Table-2 and Table-3.

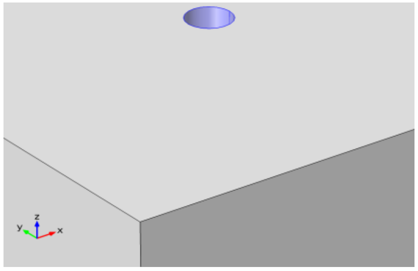

Fig 33. Inlet of 3D structure of coal

3. **Outlet:** The bottom surface of the geometry is taken as the outlet surface. And, initially the pressure at outlet boundary is set as zero.

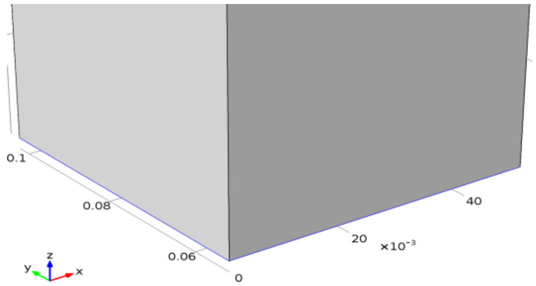

Fig 34. Outlet of 3D structure of coal

4. **No Flux:** Under no flux condition, the flow of the fluid is confined inside the highlighted blue boundaries (i.e. within the area marked as grey) boundaries as shown in figure. The fluid will not pass beyond the boundaries (the area marked as white) in any case.

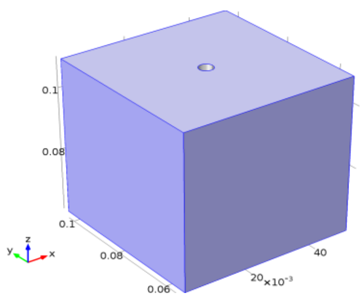

Fig 35. No flux condition in 3D structure of coal

5. **Meshing:** Normal meshing is done under physics-controlled condition.

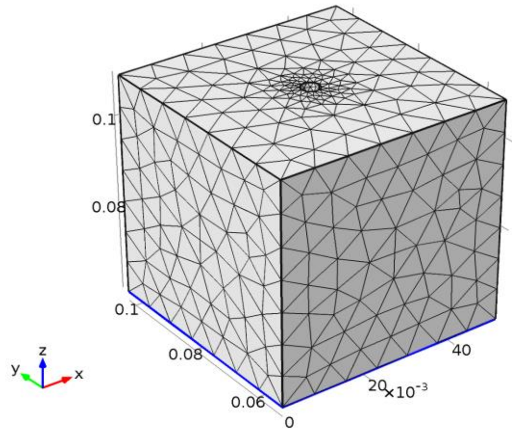

Fig 36. Meshing for 3D structure of coal

6. **Study & Result Analysis:** Comsol give output in form velocity and pressure distribution. Fig. shows velocity and pressure distribution model of coal matrix in the form of different colors.

6.1 Pressure profile: This pressure profile indicates that the high pressure zone is being created around the injection hole which is 86.5 MPa and after that the pressure gradually decreases as we move outwards from the injection hole laterally. The pressure value is varying from around 86 MPa to about 40 MPa in the lateral area around the injection hole. As we move downwards towards the outlet the pressure value tends to decrease and approaches to zero. The pressure variation is indicated by using 5-planes sectional view in the below figure.

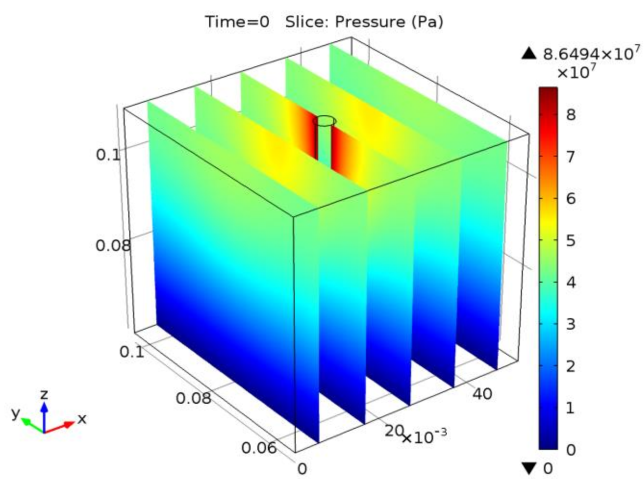

Fig 37. Pressure profile for 3D structure of coal

6.2 Pressure contour: The contour lines which are shown in this figure are the concentric circles indicating the same pressure value around the injection hole. The highest pressure is indicated by the red contour lines around the injection hole.

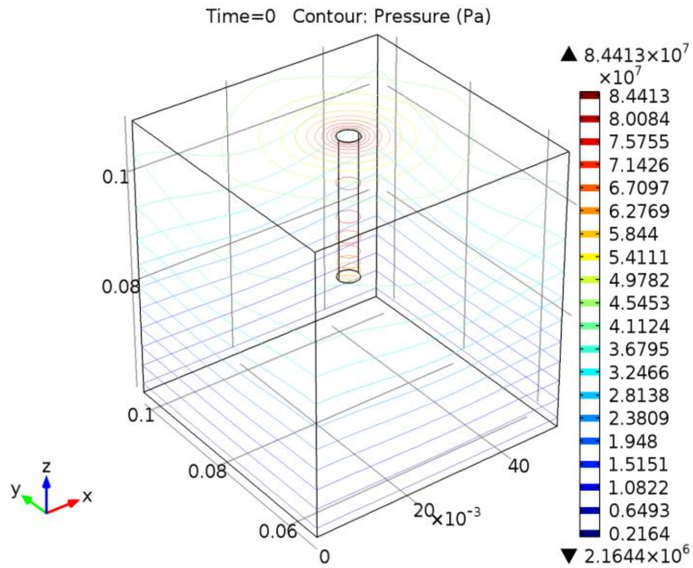

Fig 38. Pressure contour for 3D structure of coal

6.3 Velocity profile: This velocity profile indicates that the high velocity zone is being created around the injection hole which is at 6.03 m/sec and after that the velocity gradually decreases as we move outwards from the injection hole laterally. The velocity of fluid is varying from around 6.03 m/sec to about zero as we move away from the hole. The velocity variation is indicated by using 5-planes sectional view in the below figure.

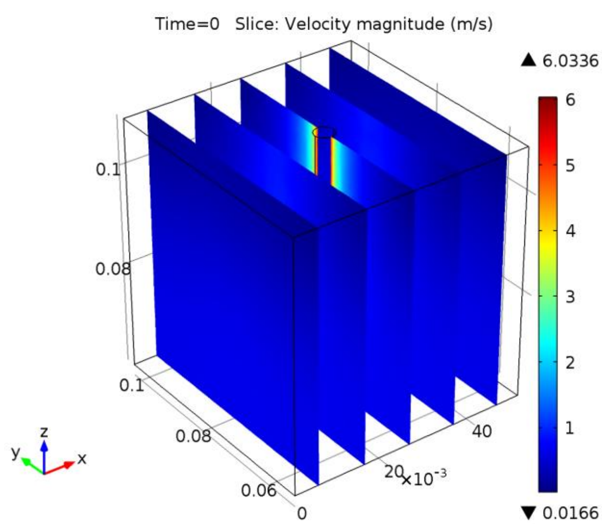

Fig 39. Velocity profile for 3D structure of coal

6.4 Velocity contour: The contour lines which are shown in this figure are the concentric circles indicating the same velocity of fluid around the injection hole. The highest velocity is indicated by the blue contour lines around the injection hole.

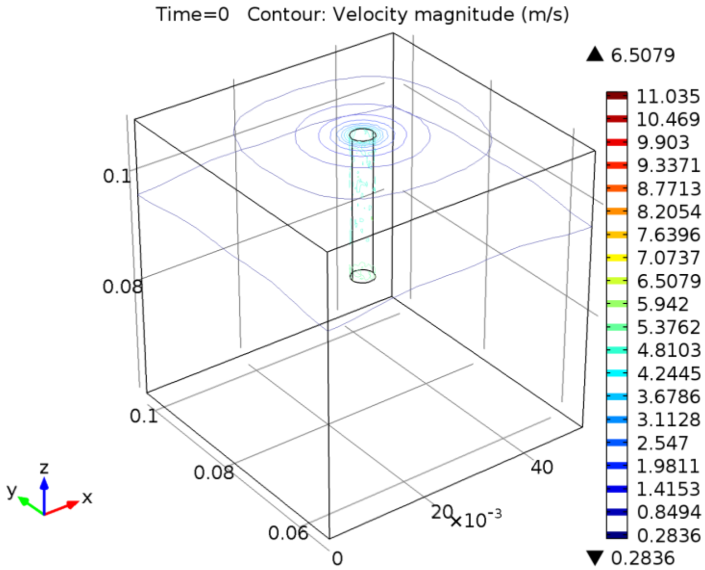

Fig 40. Velocity contour for 3D structure of coal

CONCLUSION

CONCLUSION

From the modelling & simulation we have got the following conclusions:

1. In both cleat and porous structure of coal the fluid moves from high pressure to low pressure zone as per Darcy law.
2. Maximum pressure is developed near the injection boundary and the pressure gradually decreases as we move away from it.
3. In both pore and cleat structure the velocity gradually decreases as we move away from the injection boundary.
4. In porous structure the size of pores are extremely small as compared to cleats so the maximum velocity obtained in pore structure is greater than the cleat structure.
5. The value of pressure and velocity is found to be high near the cleats and micropores.
6. In 3D modelling we have concluded that the variation of pressure is a uniform decreasing profile in the lateral section around the injection hole away from it and it almost tends to zero when the fluid moves below the injection hole.

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