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F.E.M. Analysis for Carbon Dioxide Gas Entrapment into Zeolite

[1]Shanmukh Sarode, [2]Jaghadeeshwaran R, [3]Puneet Sharma, [4]Dr. Vijay Mishra
[1], [2], [3], [4] Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, Karnataka, India
[1]shanmukhsarode50@gmail.com, [2]eshwar.jags@gmail.com, [3]puneet@cense.iisc.ernet.in

Abstract— **Carbon dioxide is one of the major gases responsible for the greenhouse effect. Extracting CO_2 from various exhaust emission sources is becoming an effective way to reduce the greenhouse effect and in turn global warming. Adsorption is one of a potential method through which this can be accomplished. The following computational study quantitatively studies the adsorption of carbon dioxide gas using micro porous zeolite 5A, which is derived from aluminosilicate family of zeolites. The concentration of the gas adsorbed in the bed is plotted along its length after different time intervals. The study also gives a rough estimate of the volume of gas which can be extracted using desorption after particular time intervals. The effective life span of the adsorbent bed is estimated from the extent of adsorption for different time intervals.**

***Index terms*: Adsorption, Carbon dioxide, Entrapment, Global Warming, Zeolite 5A**

I. INTRODUCTION

Global warming and greenhouse effect are major environmental issues catching the attention of people because of the climatic changes. There are many causes of the greenhouse effect. The exhaust from automobiles and industrial emissions are the major source of CO2 emissions. Emission of the exhaust gases directly into the atmosphere is one of the primary concerns, which has gained much attention over the years. Carbon dioxide gas is considered as one of the biggest heat absorber on the earth which absorbs heat from sun rays and remains to be the prime contributor to the greenhouse effect. Carbon dioxide isn't only affecting the atmosphere, it has also been responsible for making the oceans more acidic, affecting the aquatic life greatly.

Hence, it is clear that carbon capture and sequestration should be encouraged in reducing the exhaust gas emissions. Modern technologies are needed to be harnessed to control the increasing carbon dioxide emissions. Environmental hazards from CO2 emissions provide the clearest possible rationale for reducing the emissions without delay.

In this study, a method to trap the carbon dioxide before it is emitted into the atmosphere using adsorption has been scrutinized. Adsorption of CO2 has been achieved by designing a bed containing the adsorbent, Zeolite 5A. The adsorption process is studied using Finite element analysis on COMSOL Multiphysics. Finite element analysis (FEA) or the finite element method (FEM) is a computer based method of modelling and simulation in which the behaviour of a structure or fluid is studied under a variety of conditions. It is an advanced tool, used primarily to replace experimental testing. In the finite element method, the model is divided into miniature entities called mesh and an iterative mathematical model is used to determine the solution of the problem. In this study, the volume of CO2 adsorbed in the adsorbent is simulated and studied. The study of adsorption for different time intervals is used to predict the effective life span of the adsorbent bed.

II. SELECTION OF MATERIAL

Several factors such as pressure drop, storage capacity, structural and chemical stability, performance at optimal temperatures and its commercial availability are considered before selecting the suitable adsorbent for CO2 -. By considering the above mentioned factors and after an intensive study about the properties of the selected adsorbents, Zeolites are found to exhibit most of the factors considered perfectly. Zeolite is a type of molecular sieve, highly crystalline material with an anionic framework of microporous and crystalline structure. It is an effective adsorbent of gases. Zeolites are the most effective and one of the recent technologies used to control CO2 emissions. It is the world's only mineral with a naturally-occurring negative charge**. [1]** It simply locks and holds onto positive ions. Hence, making the adsorption of CO2 and other similar gases easier. The Fig. 2 shows the entrapment mechanism of the zeolite.

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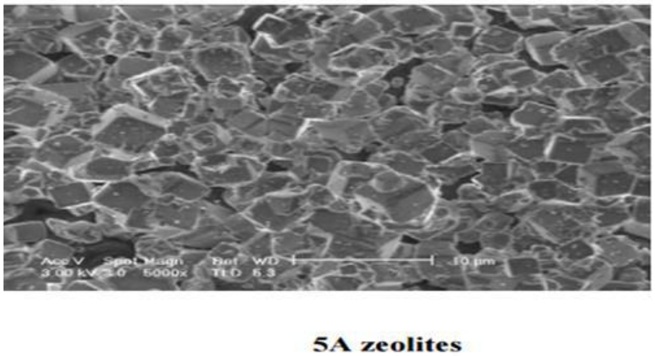

Figure 1: Zeolite microstructure

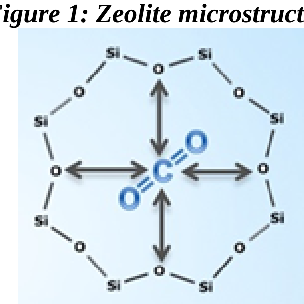

Figure 2: Entrapment mechanism (Image courtesy: NIST Center for Neutron research)

Among the various Zeolites considered, Zeolite 5A exhibited good results for the effective adsorption of CO2. They also have the potential to achieve specific separation of other gases like N2 as well. **[2]** The exhaust gases majorly consist of Nitrogen apart from the dioxides and monoxides of several elements. The carbon dioxide adsorption can be achieved by selective adsorption in an adsorbent bed of Zeolite 5A material. Selective adsorption involves maintaining specific conditions conducive for adsorption of a particular gas in the adsorption media.

Table I: Conditions necessary for adsorption of different gases. **[3]**

Gas	Temperature °C	Pressure kPa	Max. Adsorption mol/kg
N_2	25	81	0.58
CO_2	25	91	5.48

III. MATHEMATICAL MODELS

The Transport of Diluted Species in Porous Media interface is used to compute the species concentration and transport in free and porous media. It includes reaction rate expressions and solute sources for modeling of solute transport. The physics interface includes species transport through diffusion, convection, dispersion, adsorption and volatilization in saturated or partially saturated porous media.

The physics interface can be used for both stationary and time-dependent analysis**. [4]**

Mathematics involved in flow through transport media

$$P_{1,i}\frac{\partial c_i}{\partial t} + P_{2,i} + \nabla.\boldsymbol{\Gamma}_i + u.\nabla c_i = R_i + S_i$$

$$P_{1,i} = (\varepsilon_p + \rho k_{P,i})$$

$$P_{2,i} = (c_i - \rho_P c_{P,i})\frac{\partial \epsilon_p}{\partial t}, \quad \rho_P = \frac{\rho}{(1-\epsilon_p)}$$

$$N_i = \boldsymbol{\Gamma}_i + \boldsymbol{u}c_i = -(D_{D,i} + D_{e,i})\nabla c_i + \boldsymbol{u}c_i$$

Mathematics involved in reaction simulation

$$\frac{\partial c_i}{\partial t} + \nabla.(-D_i\nabla c_i) + u.\nabla c_i = R_i$$

All symbols used are standard denotations as used in COMSOL Multiphysics.

IV. MODELLING AND SIMULATION

For simplicity of computation and harnessing the symmetry in the geometry, the analysis was done for 2D geometry only.

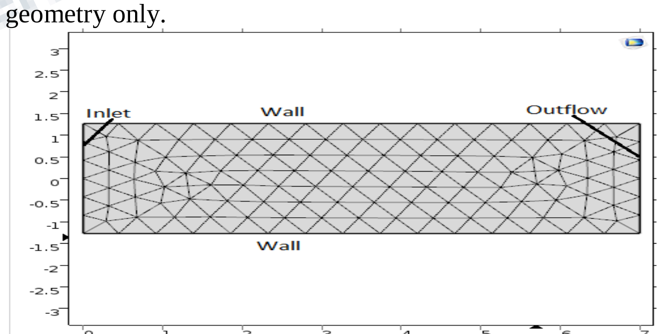

Figure 3: Geometrical representation of adsorbent bed with boundary conditions

The simulation was carried out in COMSOL Multiphysics 5.0 using Transport of diluted species through Porous media physics. The dimensions for the geometry was arbitrarily selected as 2.54 cm x 7 cm. The gas of unit concentration is made to enter the adsorbent bed with unit normal velocity from the left as shown in Fig. 3 and leaves

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the adsorbent bed from the other side. A time dependant study was undertaken using Transport of Diluted species in Porous media with a reaction.
A blank material was assigned to the entire domain and the following required properties of zeolite were given to it

Table II: Properties of zeolite [5][6]

Property	Zeolite 5A	Unit
Porosity	0.5	1
Density	2200	kg/m^3

Carbon dioxide was assigned as the continuous phase. The adsorption phenomenon is studied using Langmuir isotherm and the adsorption is assumed to follow first order kinetics. The rate constant was calculated using Arrhenius's relation from the data available. **[7]** The various constants required for simulation of the flow of diluted species through a porous media with reaction are stated below in Table III.

Table III: Data required for simulation for CO2 adsorption in Zeolite 5A [2][3]

Property	Value	Unit
Diffusion coefficient	1.48×10^{-11}	m^2/s
Langmuir adsorption constant	0.76	m^3/kg
Maximum adsorption	0.122	mol/kg
Rate constant	2.06×10^{-3}	mol/s

All the initial values were kept zero throughout the domain. The default normal size mesh was used for the simulation. The study is carried out for three different time intervals and a domain probe was inserted to study variation of the adsorbed gas concentrations along the length.

V. RESULTS

The results obtained show a non-linear decrease in the concentration of the gas adsorbed along the length after a particular time interval. The data sets were generated for adsorbed gas concentration, using the domain probe values in the steps of 0.5 cm along the length for all the three time intervals. The variations were plotted using MS Excel. The area under the curve was calculated by Reimann's method in order to determine the amount of gas adsorbed in the bed. The area under the curve is suitably multiplied with Avogadro's molar volume to obtain the volume of gas adsorbed per unit depth. The simulation results obtained are stated below along with the plots.

5.1. Case 1

Time interval = 1000000 seconds = 11.57 days

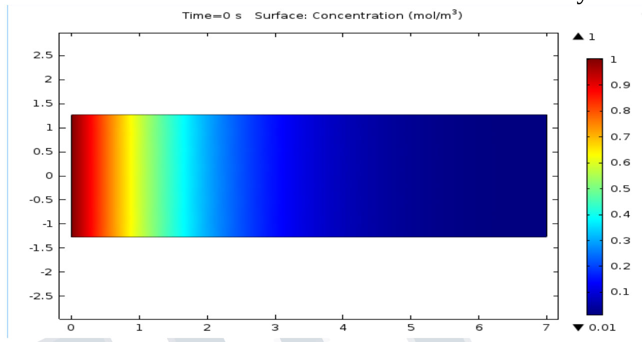

Figure 4: COMSOL simulation results

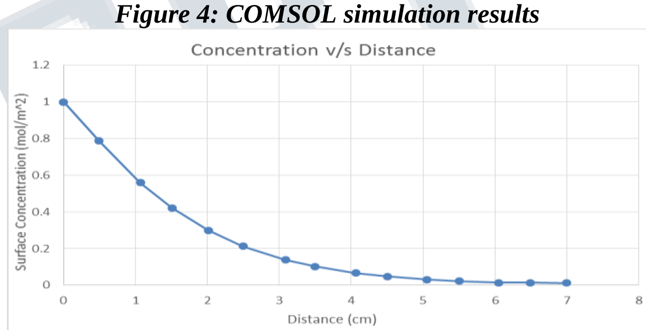

Figure 5: Adsorbed gas concentration variation along the length

Area under the curve = *0.01632* mol/m
Using Avogadro's molar volume,
Volume of CO2 adsorbed = *365* ml

5.2. Case 2

Time interval = 10000000 seconds = 115.7 days

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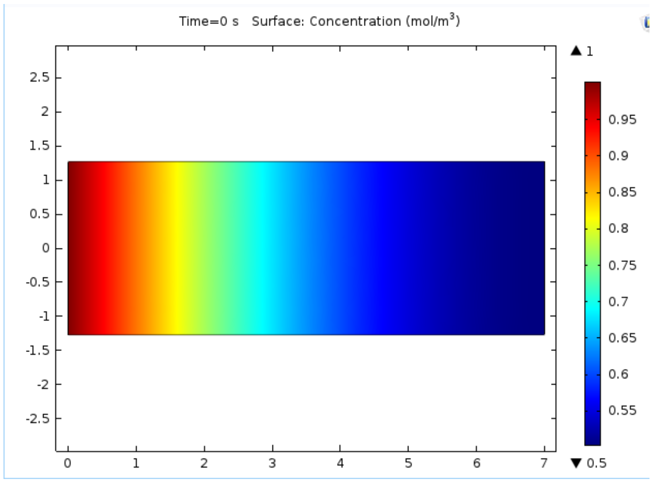

Figure 6: COMSOL simulation results

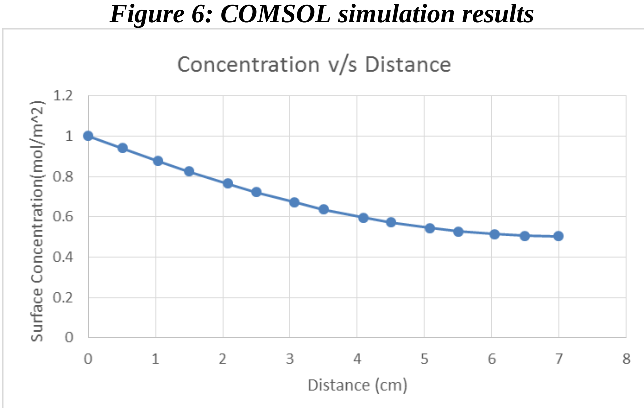

Figure 7: Adsorbed gas concentration variation along the length

Area under the curve = *0.04733* mol/m
Using Avogadro's Molar volume,
Volume of CO2 adsorbed = *1059.8* ml

5.3. Case 3

Time interval = 20000000 seconds = 231.5 days

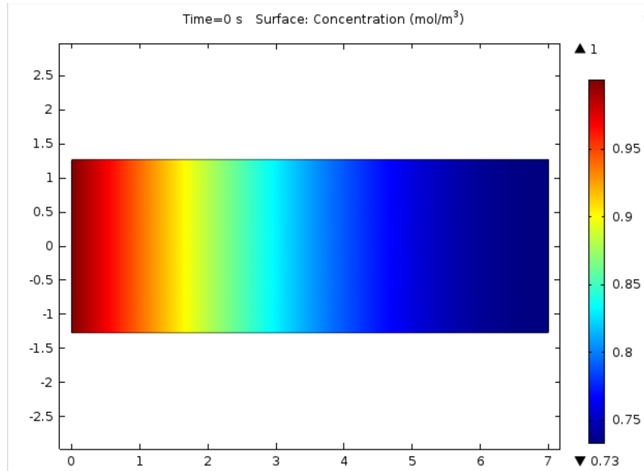

Figure 8: COMSOL simulation results

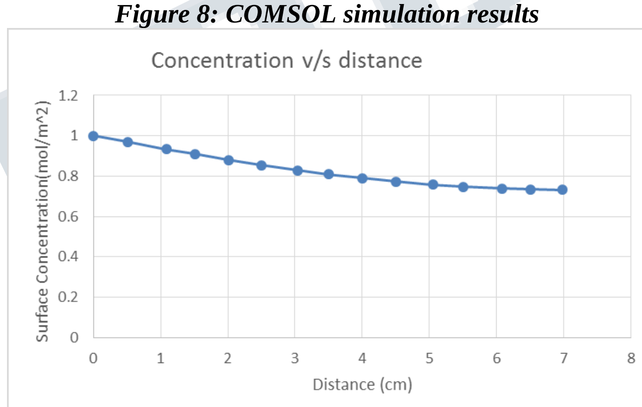

Figure 9: Adsorbed gas concentration variation along the length

Area under the curve = *0.05788* mol/m
Using Avogadro's Molar volume,
Volume of CO2 adsorbed = *1296.5* ml

5.4. Interpreting results

The following table summarizes the results obtained:

Table IV: Summary of simulation results

Time (days)	Volume (litres)
11.57	0.365
115.7	1.0591
231.4	1.296

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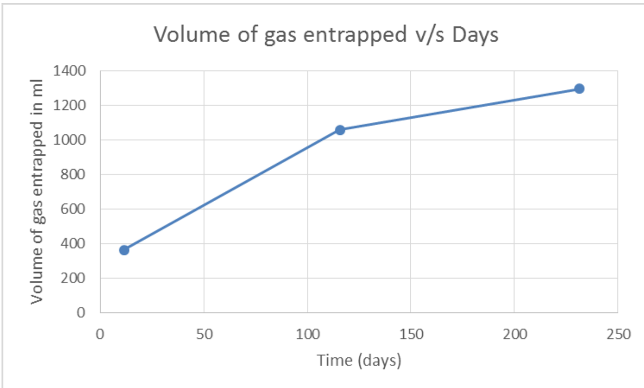

Figure 10: Variation of volume of gas entrapped with time

As seen in Figure 8, after 231.4 days the adsorbed gas concentration is above 73% throughout the domain. The amount of gas that can be adsorbed depends directly on the number of active sites present in the adsorbent bed. The number of active adsorption sites remaining after 231.5 days are just 27%. Even after extrapolating the results further to 347.1 days, the increase in volume of adsorbed gas is just 100 ml.

As seen in Figure 10, the volume of gas adsorbed per day decreases with increase in days. Therefore, it is recommended to desorb the gas as early as possible. There are various desorption techniques developed till date. Thermal desorption is the most basic method used for desorption of adsorbed gases. The adsorbent system is heated till the temperature is raised enough to break the temporary bonds formed during adsorption.**[7]** The desorbed carbon dioxide can be stored and used for further applications such as chemical reactions where the purity of carbon dioxide is not of utmost importance.

VI. CONCLUSION

From the analysis it can be concluded that the zeolite adsorbent bed can be used to adsorb CO2 from a mixture of gases. It is observed that the adsorbed gas concentration reduces as we go from the inlet to the outlet. The volume of gas adsorbed or the volume of gas obtained after desorption per day decreases as the number of days of gas exposure are increased.

The adsorbent bed is recommended to be desorbed regularly (before 230 days) if subjected to continuous inflow of CO2. The actual adsorbent bed size required would vary depending upon its specific application, the concentration of the gas to be adsorbed and the time of exposure. The amount of gas entrapped would increase with larger or concentrated emissions sources and with larger adsorbent beds.

VII. ACKNOWLEDGEMENTS

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