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# Design and Performance Assessment of Zeolite 13X Based Adsorber Bed for Carbon Capture under Atmospheric Conditions

Tirtharaj Babre[a], B. Kiran Naik[a*]

[a]*Sustainable Thermal Energy Systems Laboratory (STESL), Department of Mechanical Engineering, National Institute of Technology Rourkela, Rourkela, Odisha – 769008, India*

**Abstract**

Anthropogenic $CO_2$ emissions to the atmosphere are one of the most concerning climate issues in the modern era. This triggers the researchers to look forward to carbon capture technologies. They are many technologies available for carbon capture such as distillation process, cryogenic treatment, ad/absorption process, biosynthesis etc. Among these, for high quantity of carbon capture, low operating and maintenance costs, faster $CO_2$ capture rate and industry-oriented applications, adsorption-based carbon capture technology was found to be prominent. Thus, in the present investigation, the design and performance assessment of Zeolite 13X based adsorber bed for carbon capture is analyzed analytically under atmospheric conditions. Here, a finite difference-based analytical model is developed for design and performance analyses of adsorber bed. The developed model is validated with the experimental data available in the literature and found to match well with a maximum probable error of ±15%. Further, this analytical model has also been validated against the temperature swing adsorption (TSA) models for signifying the accuracy of the proposed model. The design and performance parameters chosen for the present study are adsorber bed length, temperature, $CO_2$ concentration variation with respect to time, $CO_2$ adsorption effectiveness, purity and recovery of CO2 with adsorption time. Employing the above-mentioned parameters, Zeolite 13X based adsorber bed design and performance analyses are evaluated. From the present study, it is observed that 28.46 % decrement in concentration ratio as temperature increase from 393.13 K to 303.15 K and 15% more $CO_2$ can be adsorbed by increasing the length of the bed from 2.4 m to 0.8 m.

*Keywords: Adsorption; TSA; Zeolite 13X; Analytical Model; $CO_2$ purity.*

## 1. Introduction

Despite the debate surrounding its primary cause, global warming is genuine. Greenhouse gases are linked to the rise in temperature, either as a cause or as a result of climate change [1]. The fact that atmospheric carbon dioxide ($CO_2$) levels are continuously growing, whether manmade or natural, necessitates immediate action [1,2]. The consequences of this worldwide impact are much too big to ignore, far too difficult to forecast, and far too late to address when we finally do. As a result, the scientific and political capital should be deployed right away to avoid and reduce $CO_2$ levels. The high-efficiency absorption of $CO_2$ from flue gas by amine scrubbing in fossil-fuel-fired power plants is a conventional approach that is currently in use [3]. However, numerous disadvantages of the amine scrubbing approach, such as corrosion of mechanical parts, release of poisonous compounds and fumes, and high energy requirements for regeneration, have limited its use. Adsorption is a more efficient alternative to amine-based absorption for $CO_2$ capture and could eventually replace it. [4] Metal-organic frameworks (MOF), porous carbons, zeolites 13X, and other solid porous sorbents are utilized in adsorption [4,5]. These adsorbents are low-cost, ecologically sound, have a large surface area, and are moisture and chemical resistant.

Lu Wang et al. [6] were investigated successful $CO_2$/ $N_2$ tests in a pallet of column full of zeolite 13X-APG. The kinetic adsorption parameters of $CO_2$ and $N_2$, respectively, at ambient temperature and ambient pressure, were determined using a mathematical model relying on bi-LDF mass transfer estimates, and the VTSA process was investigated. Yahui Lian et al. [7] have developed a method included in the simulation process that filtered firstly, and the numerical computation is carried out with a research study on Mg-MOF-74. Three cases with varying length and diameter combinations are explored under the constant surface area condition. Rached Ben-Mansour et al. [8] used Mg-MOF-74 to separate a mixture of $CO_2$ and $CO_2$/$N_2$ using temperature swing adsorption (TSA) combined with four phases (feed, washing, heating, and cooling). UDF coupled to Ansys Fluent software were used to improve the computer model's implementation and are used to validate two and three-dimensional CFD models. Dantas TL et al. [9] used the Linear Driving Force (LDF) approach to build a breakthrough curve for $N_2$/$CO_2$ capture utilizing an activated carbon adsorbent bed at varying temperatures of 301,

* Corresponding author. Tel.: +919435686059.
*E-mail address:* naikkb@nitrkl.ac.in; k.bukke@gmail.com

306, 323, 373, and 423 K. Motoyuki Suzuki et al. [10] investigated the adsorption of fifteen different types of volatile organics from aqueous solution on activated carbon in a batch technique. It was considered that intraparticle surface diffusion and the effective surface diffusion coefficient governed the rate of adsorption, and so it was calculated. Guoxiong Zhan et al. [11] used dynamic process simulation and optimization to remove $CO_2$ from limited space with pressure and temperature swing adsorption. This study uses two distinct adsorbents, Zeolite 13X and NaUSY, to demonstrate a PTSA method for low $CO_2$ concentration separation in a limited environment. This paper is used to validate the results which show good agreement.

As per the literature, only a few experimental and computational studies on $CO_2$ adsorption have been performed. However, none of them proposed the analytical approach to evaluate $CO_2$ adsorption in zeolite 13X using an unsteady state-based model. For the evaluation of performance parameters, an unsteady state-based one dimensional analytical model employing the finite difference method Euler's approach is proposed. Further, by choosing concentration ratio ($C/C_o$), adsorption effectiveness, purity and recovery of $CO_2$ variation with respect to time for different temperatures and length of the bed is analyzed.

## 2. Analytical model

The modeling of the adsorbent bed is done analytically to get the performance characteristics. In order to get the concentration profile for the adsorbent, consider a rectangular pack of fixed adsorbent bed having length L of 0.8 m, which is placed under inlet conditions of 303.15 K temperature and 1.0 bar pressure. The feed gas rate of 500 $Nm^3$/day is provided which contains 0.7 mole fraction of $CO_2$. Following assumptions are made while writing the governing equations.

- One Dimensional, unsteady-state without internal heat generation.
- Gas-phase obeys ideal gas law.
- No association and Dissociation are considered during the whole process.
- Thermo-physical property is considered as constant.

### *2.1. Governing equation*

The following governing equations for analysing concentration profile and temperature profile are formulated using the assumptions stated above:

Concentration profile: $$\frac{\partial^2 C}{\partial x^2} = \frac{1}{D}\frac{\partial C}{\partial t} \tag{1}$$

Temperature Profile: $$\frac{\partial^2 T}{\partial x^2} + \frac{G(t)}{k} = \frac{1}{\alpha}\frac{\partial T}{\partial t}, \text{ where } G(t) = \rho H \frac{\partial \omega}{\partial t} \tag{2}$$

Boundary Condition: $$x=0,\ \frac{\partial C}{\partial x}=0;\quad x=L,\ C=C_o;\ x=0,\ \frac{\partial T}{\partial x}=0;\ x=L,\ T=T_o \tag{3}$$

Initial Boundary condition: $$t=0,\ C=C_i;\ \ t=0,\ T=T_i \Rightarrow T_{amb} \tag{4}$$

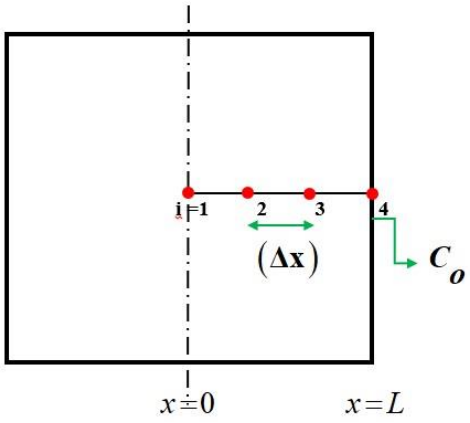


Fig. 1. Schematic diagram of computational domain

Governing equation after discretization equation (1) and (2)

Concentration profile: $\frac{C_i^{p+1}-C_i^p}{(\Delta t)}=D\left[\frac{C_{i-1}^p-2C_i^p+C_{i+1}^p}{(\Delta x)^2}\right]$ (5)

Temperature Profile: $\frac{T_i^{p+1}-T_i^p}{(\Delta t)}=\left(\frac{\alpha}{1-\alpha B}\right)\left[\frac{T_{i-1}^p-2T_i^p+T_{i+1}^p}{(\Delta x)^2}\right]$, where $\frac{1.0784C_P\rho H}{kH_L}=B$ (6)

Boundary Condition: $i=1,\ \frac{C_{i+1}^p-C_{i-1}^p}{2(\Delta x)}=0\Rightarrow C_0^p=C_2^p\ ;\ x=L,\ C=C_o\Rightarrow C_4=0$ (7)

$$i=1,\ \frac{T_{i+1}^p-T_{i-1}^p}{2(\Delta x)}=0\Rightarrow T_0^p=T_2^p\ ;\ x=L,\ T=T_o\Rightarrow T_4 \quad (8)$$

Initial Boundary Condition: $t=0,\ C=C_i\ ;\ t=0,\ T=T_i\Rightarrow T_{amb}$ (9)

The above equation (5) and (6) can be solved by finite difference method where 3 number of division take with equal grid spacing shown in Fig. 1. There are different types of discretization methods, particularly for solving this equation Euler's approach (Explicit method) is used. Both the governing equation is discretized in forward in time and central in space (FTCS) as shown on Fig. 2.

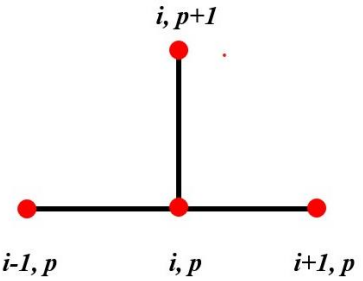


Fig. 2. Forward time central space scheme

Concentration profile: $C_i^{p+1}-C_i^p=\beta\left[C_{i-1}^p-2C_i^p+C_{i+1}^p\right]$ (10)

Where $\frac{D(\Delta t)}{(\Delta x)^2}=\beta$, for stability condition $\beta\le 0.5$ and $D=4.31\times10^{-4}\,e^{\left(\frac{-E_a}{RT}\right)}$

Temperature Profile: $T_i^{p+1}=\left(1-\frac{2\beta}{1-\alpha B}\right)T_i^p+\left(\frac{\beta}{1-\alpha B}\right)\left[T_{i-1}^p+T_{i+1}^p\right]$ (11)

Where C is concentration ratio ($C/C_o$) ($mole_{adsorbate}/mole_{adsorbent}$), D is diffusivity coefficient of adsorbent ($m^2/s$), $E_a$ is activation energy of adsorbent (kJ/mole), R is universal gas constant (J/K mole), T is temperature (K), ρ is adsorbent density ($kg/m^3$), k is adsorbent thermal conductivity (W/m K), H is adsorption enthalpy (kJ/kg), α is thermal diffusivity (m2/s), $C_p$ is adsorbent specific heat capacity (kJ/kg K), $H_L$ is vaporization enthalpy (kJ/kg), β stability constant, B is constant, Δx is space between two grid point (m).

Table 1. Physical properties of Zeolite 13X [11,12]

| Parameters | Unit | Value |
|---|---|---|
| Diameter | m | 0.2 |
| Height | m | 0.8 |
| Activation Energy | kJ/mole | 29.38 |
| Density | $kg/m^3$ | 666.5 |
| Thermal conductivity | W/m K | 0.27 |
| Adsorbent Enthalpy | kJ/kg | 550 |
| Specific Heat at constant pressure | J/kg K | 880 |

*2.2. Algorithm*

In the present analytical model, finite difference method is used to solve the equation for each grid point in the computational domain which is depicted in Fig. 1. having three number of division. Fig. 3. shows the basic algorithm to solve both concentration and temperature profile equation. For solving one dimensional unsteady state equation Euler's method (Explicit) is used which easy among the all other method and gives better result. This method conditionally stable so need to check stability condition which is denoted by $\beta$. The value of $\beta$ should be less than 0.5. If it is not then stop check again and verify. First discretize both the governing equation forward in time and central in space (FTCS). By applying boundary conditions to discretize the form of equation check stability condition. With the help of inlet condition calculate concentration ratio at each grid point of the computational domain from i=1 to i=3 ($C_1$, $C_2$, $C_3$) for the next time step in terms of three simultaneous equations. Three equations with three unknowns can be solved and get actual value of concentration ratio for the next time step. One loop is created whether the saturation is achieved or not. After it reached to final concentration, it stop the iteration process otherwise loop will continue and iterate for the second time step. The previous time step's output is used as the input for the following time step, allowing the loop to continue until saturation is reached.

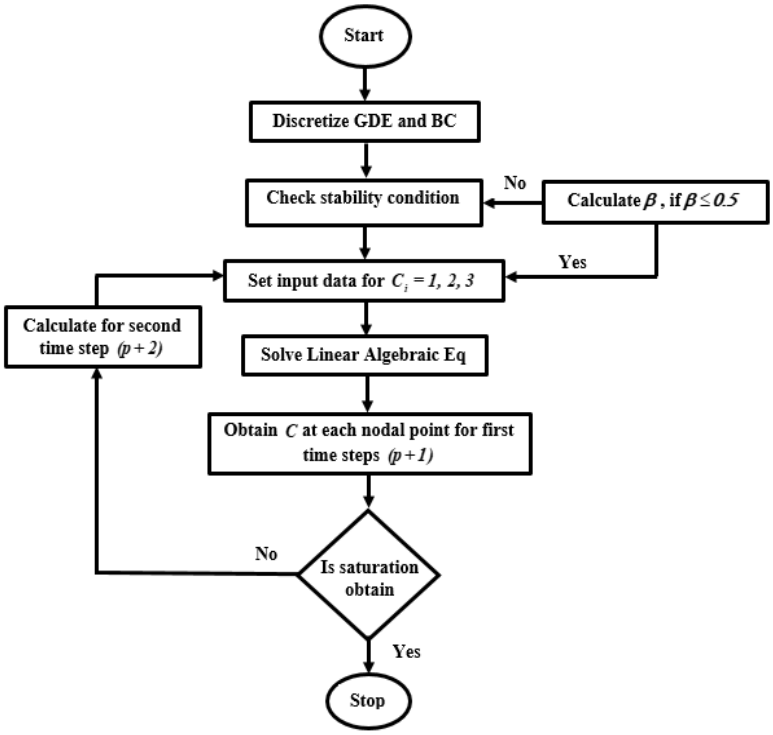


Fig. 3. Algorithm for solving FDM equation

## 3. Performance parameters of adsorbent

Performance parameter of the adsorbent is tried to formulate after getting the solution of the differential equation analytically. The performance parameters depict the important kinetics of the adsorbent to understand the behaviour and feasibility.

### *3.1. Concentration Ratio ($C/C_o$)*

Concentration ratio is how much $CO_2$ is adsorbed by adsorbent used. Its unit is mole of adsorbate per mole of adsorbent. With variation of temperature, amount of $CO_2$ get absorbed at different interval of time. It can be obtained with the help of equation (12).

$$C_i^{p+1} = (1-2\beta)C_i^p + \beta\left[C_{i-1}^p + C_{i+1}^p\right] \tag{12}$$

### *3.2. Adsorption Effectiveness*

It mainly determines how much adsorption occurs for the given time compared to maximum adsorption possible. By knowing this parameters, an effective operating temperature can be selected which will give better Adsorption Effectiveness. It can be given as,

$$Adsorption\ Effectiveness\ =\ \frac{CO_2\ Cocentration\ at\ any\ time\ (t)}{Maximum\ CO_2\ Cocentration\ possible} = \frac{C(t)}{C_{\max}} \tag{13}$$

### *3.3. Purity of $CO_2$*

The most vital criterion of adsorption process is $CO_2$ purity. It is defined as a ratio of the amount of pure $CO_2$ content to the produced $CO_2$ inside the adsorbent bed. It shows level of purity that is obtained during capturing of $CO_2$. Mathematically it can be written as

$$Purity\ of\ CO_2\ =\ \frac{\int C_{CO_2}\,dt}{\sum_i \int C_{CO_2}\,dt} \tag{14}$$

### *3.4. Recovery of $CO_2$*

Recovery of $CO_2$ signifies that at the outlet how much $CO_2$ is adsorbed to bed as compared to how much it feeds at the staring. It is defined as the ratio of the amount of produced carbon dioxide to that fed to the adsorbent bed.

$$Recovery\ of\ CO_2\ =\ \frac{Amount\ of\ produced\ \ CO_2}{Feed\ to\ adsorbent\ bed} \tag{15}$$

## 4. Model Validation

In this study adsorbent zeolite 13X is chosen as this is better adsorbent for $CO_2$ capture as compared to others because of its properties. Most of the researcher analysed this material and get the best result to get output. This adsorbent shows appreciable results for the practical application.

The adsorbent thermos-physical characteristics considered for this study are listed in Table 1. By using zeolite 13X as the adsorbent, a comparison is done between the estimated data and experimental data present in the literature [11] to examine the accuracy of the proposed analytical approach. Concentration ratio, adsorption effectiveness, purity and recovery $CO_2$ are used as performance parameters. Fig. 4.(a) shows the validation findings and the proposed technique has been found to be reliable, with an adequate precision of 15%. It is observed that for a particular inlet condition, adsorption of $CO_2$ by adsorbent for a temperature of 393.15 K increases to a certain extent and then becomes steady as adsorption time increases. This implies that as time passes, the adsorbent's adsorption capacity becomes saturated. Zeolite 13X adsorbed 0.699 of $CO_2$ within a time of 704 sec and beyond 704 sec it reached saturation condition. Furthermore, during the process of adsorption, the temperature is increased from 303.15 K to 314.26 K within a time of 1300 sec which is shown in Fig. 4.(b). Temperature variation with respect to time curve closely matches with experimental one which shows that the analytical model is correct.

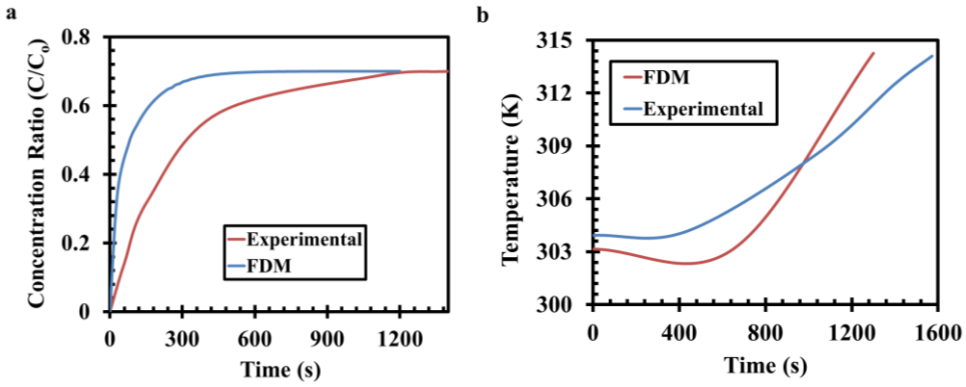


Fig. 4. (a) Concentration ratio ($C/C_0$) variation validated at 393.15 K; (b) Temperature variation validation

## 5. Results and Discussion

### *5.1. Adsorption Effectiveness*

It is observed from Fig. 5.(a) that the maximum possible adsorption effectiveness of zeolite 13X for different temperature range is 0.35. Whereas the adsorption effectiveness is decreases as time is increases. For temperature 303.15 K which is atmospheric temperature, the adsorption effectiveness is 0.203 at maximum possible time as compared to other operating temperature. In case of higher temperature effectiveness is decreased quickly that is in 432 sec. This happened because temperature is function of diffusivity coefficient which is deciding factor for adsorption effectiveness.

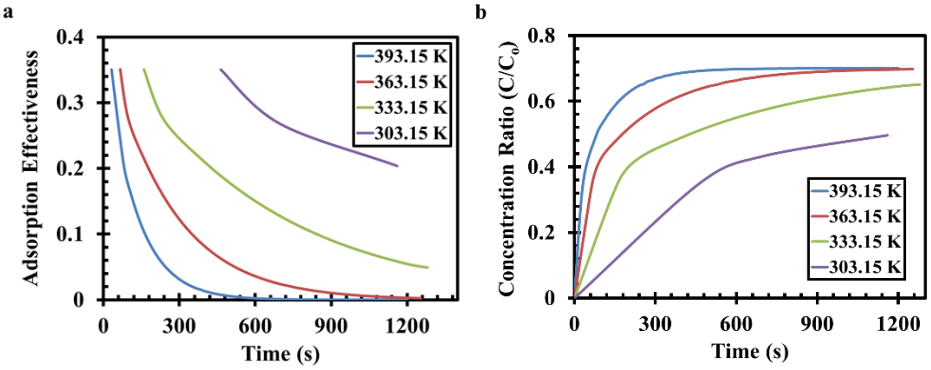


Fig. 5. (a) Adsorption Effectiveness of adsorbent; (b) Concentration Ratio ($C/C_o$) at different temperature

### *5.2. Concentration ratio ($C/C_o$)*

The variation of concentration ratio with variation of temperature is shown in Fig. 5.(b). Concentration ratio ($C/C_o$) of zeolite 13X is found to be 0.699 and attains saturation at 704 sec for temperature of 393.15 K but at the same time the concentration ratio for temperature 363.15 K is 0.676. For temperature 333.15 K and 303.15 K, adsorption of $CO_2$ is 0.645 and 0.5 respectively within 1200 sec time period because of different diffusivity coefficient which is vary according to temperature. With decrease in temperature, the diffusivity coefficient decreases therefore concentration ratio decreases.

### *5.3. Purity of $CO_2$*

From Fig. 6.(a) it can be inferred that purity of $CO_2$ of zeolite 13X adsorbent is 98.95 % for temperature 393.15 K and it becomes constant after some time. In more detail, it can be concluded that there is 1.04 % of drop in purity within given period of time. Simlarly for temperature 363.15 K, 333.15 K, 303.15K the purity of $CO_2$ is 98.25 %, 96.826 %, 94.34%. As the temperature increases the purity of $CO_2$ improve upto certain extent but it always less than 100%.

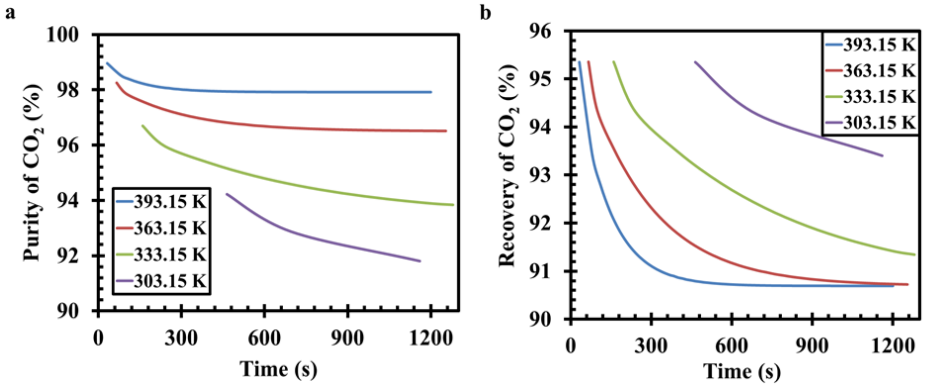


Fig. 6. (a) Purity of $CO_2$; (b) Recovery of $CO_2$

*5.4. Recovery of $CO_2$*

As compare to purity, recovery of $CO_2$ is slightly less by comparing both Fig. 6.(a) and (b). For all temperature, recovery of $CO_2$ is 95.35% for first time step but gradually decrease as per their operating temperature. Within 1200 sec of time recovery of $CO_2$ drop to 90.69 %, 90.72%, 91.34 %, and 93.40 % for temperature 393.15 K, 363.15 K, 333.15 K and 303.15 K respectively. From percentage drop in recovery, it is understood that as time passes we cannot get the maximum recovery of $CO_2$.

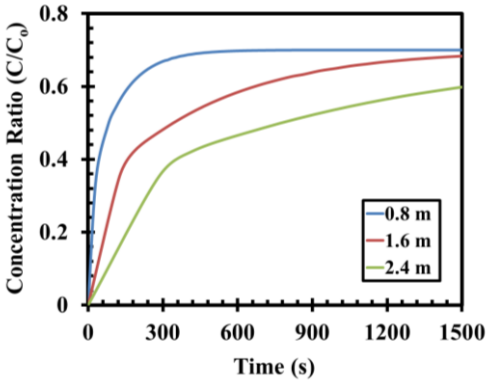


Fig. 7. Concentration Ratio ($C/C_o$) variation at different lengths of adsorbent bed

*5.5. Concentration ratio ($C/C_o$) at different length of bed*

Fig. 7. shows that the adsorption of $CO_2$ effect when the length of the bed is changed. Concentration ratio when operating temperature 393.15 K is 0.699, 0.68 and 0.59 for lengths of 0.8 m, 1.6 m, 2.4 m respectively. As the length of the bed is increases, large amount of adsorption of $CO_2$ takes place which can be easily inferred from Fig. 7. In case of 2.4 m length of bed, it can be adsorbed 15% more $CO_2$ as compared to 0.8 m length of the bed. Furthermore, in details 0.8m length bed reached to saturation condition with minimum time which is 704 sec but for 2.4 m length bed it takes some time to reach up to saturation condition.

## 6. Conclusions

In the present study, to estimate and analyse $CO_2$ adsorption, a one dimensional unsteady state analytical model is developed using the finite difference method. The proposed model has been validated by experimental data from the literature [11] by choosing concentration ratio, adsorption effectiveness, purity and recovery of $CO_2$ as performance parameters. From the validation analysis, it is observed that experimental and predicted data are in good agreement and found suitable for adsorption assessments for different lengths of bed and operating temperature. From the results obtained by analysing the performance evaluation parameters, following conclusions are drawn:

- Concentration ratio in case of temperature 393.15 K is high as compared to other three temperature which is 0.699 and attains saturation state very fast at 704 sec while for lowest temperature 303.15 K it shows very slow adsorption of

$CO_2$ which is found to be 0.5 within 1200 sec. There is 28.46 % decrement in concentration ratio as temperature increase from 393.13 K to 303.15 K.

- Due to increase in temperature, the adsorption effectiveness decreases from 0.35 to 0. The maximum possible effectiveness is found to be 0.35 but in case of 393.15 K, it reduced drastically but for 303.15 K still it does not become 0 within the given time. So by selecting the proper temperature the adsorption effectiveness can be improved.
- Purity of $CO_2$ for temperature 393.15 K is 98.95 % which is maximum among all other temperatures. As temperature decreases the purity level is reduced. There is 0.7 %, 1.424 %, 2.486 % drop in purity with respect to subsequent temperature range.
- As compared to purity, recovery of $CO_2$ is slightly less. Recovery of $CO_2$ by choosing zeolite 13X adsorbent for all temperatures is 95.35 % which is highest but decreases as time is increased. It is found from the result that for lower temperature still some more $CO_2$ can be adsorbed because it is 93.40 % at 1200 sec.
- By choosing three different lengths of bed it can be concluded that 2.4 m length bed take some time to reach up to saturation condition. If the length of adsorbent bed is double then the adsorption of $CO_2$ can be improved up to 4.14 % similarly if it became three-time then it reached to 18.45 %.

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