# CFD Investigation of the Effect of Particle Size of A Fixed-Bed Adsorption Column for Removal of Ferrous Iron ($Fe^{2+}$) in Groundwater Using Activated Carbon

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DOI: 10.56201/ijemt.v8.no4.2022.pg1.11

***Abstract***
*Predictive model equations of a "fixed-bed adsorption column" packed with particles and the Langmuir adsorption isotherm equilibrium model were considered. A Computational Fluid Dynamic (CFD) simulation using COMSOL Multiphysics sofware of the adsorption column for the removal of iron from groundwater was carried out. "The results were presented in a line graph. The effect of particle size on the breakthrough curve was investigated for particle sizes of 0.001m, 0.002m, 0.003m and 0.004m. Simulated results showed that as the particle size increases the adsorption capacity of the bed decreases and about 28 days operative performance of the bed could be achieved for a bed weight of 1500kg and particle size of 0.001m". Predicted results were compared with results presented by Ruthven, 1984 and World Health Organization standards and the results were very acceptable.*

***Key words**: CFD Simulation, Particle size, Fixed-Bed, Adsorption column, Ferrous Iron*

## 1. Introduction

Clean water is becoming an increasingly scarce resource in our time. "Heavy metal pollution of groundwater is a problem that is caused by industrial discharges in many occasions, causing ground water poisoning. Therefore, the rising incident of deadly ailments such as diabetes mellitus and liver cirrhosis following the consumption of iron polluted water is an increasing concern (Mittal, 2006). Majority of studies on heavy metal removals from groundwater were done under batch operations which are easy in application and had also shown to be efficient in the processing of waste water in small scale. But results and data coming from batch systems are not too dependable for most treatment processes. This is due to the fact that the contact time is too short to establish a state of equilibrium in the column. Whereas a continuous system is flexible and also cost effective in its operation, and therefore fit in the present study" (Noureddine *et al*., 2016).

The empirical design of the adsorption column through extensive experimentation tends to be expensive and time consuming (Knepper, 1981). "There is therefore need for a simulated predictive model that will assist us in computing and improving on the dynamic efficiency of the adsorption column with little or no cost implications. This is why the development of a mathematical model is required to allow the simulation of the iron breakthrough behavior of the bed of packed adsorbents which will establish the basis for the adsorption column design. Simulation model for the adsorption unit is needed to optimize the key variables of the separation unit, such as the operating time of the bed and particle size etc. (Babu and Gupta, 2005). Fixed-bed adsorption is typically an unsteady state but a largely controlled process. And as time increases, the adsorbent gets saturated where the concentration of iron at any particular point in the bed changes with time and position (Azizian, 2004). Consequently, if the concentration of liquid feed (water) is analyzed at time zero and at some final time, it would be observed that the solute concentration in the effluent stream has dropped drastically".

Adsorption occurs only in a particular region of the bed called "the mass transfer zone (MTZ) which moves through the bed. After a while, the MTZ, the portion where the separation of iron present in the water takes place eventually exits the end of the adsorption column and the breakthrough of iron is said to have occurred (Ruthven and Ching, 1989). Now, at this point, the concentration of iron in the feed stream equals that in the exit stream, which is an indication that the bed is ready for regeneration or replacement. In chemical process industries, adsorption technology plays a vital role in the separation of valuable materials from process streams. It also has application in chemical purification science. Fixed-bed adsorption separation techniques require the continuous interaction of a fluid phase and a packed bed of adsorbents in which the transport of a solute component occurs naturally from a liquid or gaseous phase onto the surface of an adsorbent as a result of a difference in concentration between the two phases of interest (Babu and Gupta, 2005)".

In the treatment of groundwater to produce drinking water, the principle of adsorption is utilized in the removal of heavy metal constituents like iron. "This method of separation could be batch-wise, or easily set-up as continuous flow process in packed beds, which is relatively simple in design and scale up (Babu and Gupta, 2005). The importance of portable water in our daily living cannot be over-emphasized following the growing population of people and advances in modern technology. As a result, there is need for the availability of improved facilities including access to clean water. Water sourced from the ground comes with high concentrations of iron which must be reduced to an acceptable level for the purpose of drinking. It was established that the development of red blood cells required a little amount of iron present in water. However, high concentrations of iron in drinking water poses challenging health problems, and also causing environmental degradation. This drawback makes the removal of iron in water a vital step in every water purification unit (Nassar *et al*., 2003)".

In adsorption science, "very important features like the adsorbent capacity and its operating life span play a key role in ensuring the effective operation of the column. In addition, a basic knowledge on adsorption dynamics and modeling are required (Kaczmark *et al*., 1997). The important question to be answered in this study is, of what effect is the amount of adsorbent on the fixed-bed column performance in a quest to establish the actual time for bed regeneration and replacement. A CFD simulation is useful in revealing how the performance or efficiency of the adsorption column is dictated by the fluid dynamics. It has been documented as a reliable tool in modeling and simulation of hydrodynamic systems, giving a deeper understanding into adsorption studies (Babu and Gupta, 2005). In view of the above, this work employs a computational fluid dynamics apparatus in COMSOL Multiphysics software to simulate the equilibrium and dynamic behavior of the adsorption column in order to accurately predict the effect of particle size in the performance of the fixed-bed adsorption column".

## 2. Methodology

### 2.1 Materials

Figure 1 shows the "fixed-bed column" considered.

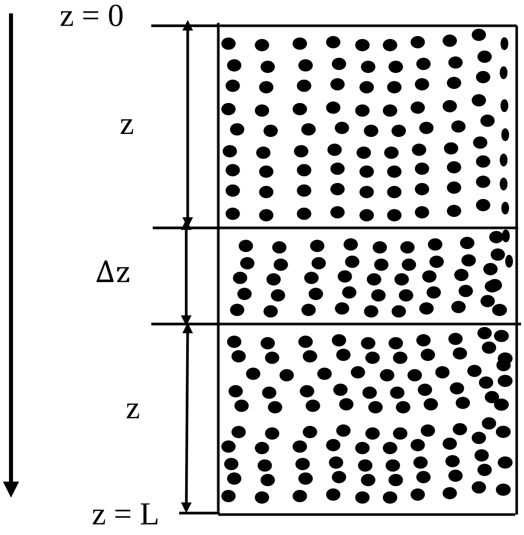


Figure 1: Differential element of fixed-bed adsorption column

In this study, "we considered the transport of material and energy through the adsorbent pellet to enable us study the distribution of material and energy within the pellet at different locations along length of the bed of adsorbent. The governing dynamic equations for the transport of material and energy through the fixed-bed was also considered for both transport in the axial direction by convection and in the radial direction by diffusion in a cylindrical coordinate system. The research methodology adopted to conduct this study was extensively established in the COMSOL Multiphysics software in simulating the adsorption bed.

The key assumptions made during the study are:

I. The adsorption equilibrium relationship is non-linear as described by the Langmuir isotherm.
II. The adsorbent particles are spherical in shape and homogenous in size and density.
III. The adsorption column was operated under isothermal conditions".

### 2.2 The Adsorption Column Model Development

This study considered only a single component adsorption of iron (Fe) in water on activated carbon and it is assumed to follow this simple stoichiometry expression shown in equation (1):

$$Fe + S \longleftrightarrow Fe.S \qquad (1)$$

"Where
*S* is adsorbent and,
*Fe* is iron molecule.
The equilibrium loading of the adsorbent is assumed to follow the two parameter Langmuir adsorption isotherm for single component adsorption neglecting any side interaction between the adsorbed particles for a monolayer adsorption. The expression is given in equation (2) (Ruthven and Douglas (1984):

$$q = q_m \frac{KC_i^{'}}{1+KC_i^{'}} \quad (2)$$

Where
$q$ = Adsorption loading of the adsorbent
$q_m$ =Equilibrium loading of the adsorbent
$K$ =Adsorption equilibrium constant
$C_i^{'}$ =Concentration of species within the pellet"

**Mole balance for the adsorbate distribution through the bed**

The "mole balance" for the adsorbate distribution through "the bed" is shown in equation (3)

| | | | | | |
|---|---|---|---|---|---|
| Accumulation of species in differential volume with time | = | Net flux of species into the differential volume | - | Depletion of species from differential volume due to adsorption loading of species into adsorbent pellet | (3) |

Equation (3) is simplified as

$$A = F_z + F_r - D \quad (4)$$

where
$A$ = accumulation of species in differential volume
$F_Z$ = Net flux of material in the axial direction
$F_r$ = Net flux of material in the radial direction
$D$ = Rate of adsorbent loading
There are many other equations that were used for the simulation that are not presented here but are found elsewhere (Ali, 2021; Forgler, 2012; Knepper, 1981; Seader and Earnest, 2010; Warren *et al*., 2001; Yousuo et al., 2022). Such equations account for the following:

i. Change in volume occupied by liquid
ii. Change in total volume of adsorber
iii. Change in volume occupied by solid
iv. Bed porosity
v. Radial direction
vi. Change in the radial direction
vii. Change in the angular direction
viii. Change in the axial direction.
ix. Time and change in time.
x. Net flux of material in the axial direction in the interval, Net flux of material in the radial direction in
xi. the interval, Diffusivity or effective dispersion coefficient of species, Fluid flow velocity
xii. Surface area of adsorbent pellet, Volume of adsorbent pellet, External mass transfer coefficient,
xiii. Concentration of species along the bed, Diameter of adsorbent pellet.
xiv. Diffusivity of the species within the pellet and the crystal particle density.
xv. Energy Balance through the Bed for a Cylindrical Geometry, Energy Balance through the
xvi. Adsorbent Pellet for a Spherical Geometry
xvii. Pressure Drop through the Bed

### 2.3 Comsol Multiphysics modus operandi

The governing models which included the adsorption isotherm model, the fixed bed model, the Particle model, the bed pressure drop equation and the energy balance model were solved using the finite element method in
COMSOL Multiphysics (Ali, 2021; Babu and Gupta, 2004; Yousuo et al., 2022). The steps taken in solving the models using COMSOL Multiphysics software are shown elsewhere (Ali, 2021; Yousuo et al., 2022). "COMSOL Multiphysics is a cross-platform finite element analysis, solver and Multiphysics simulation software. It permits conventional physics-based user interfaces and the numerical solutions of coupled systems of partial differential equations (PDEs). COMSOL provides a unified workflow which shows the user how to carry out a COMSOL Multiphysics simulation".

"The workflow is as follows:

I. Set-up the model environment
II. Specify material properties
III. Define physics and boundary conditions
IV. Create the mesh
V. Run the simulation
VI. Post-process the results"

### 2.4 Parameters used for the Simulation

The parameters used for the simulation are shown in Table 1 and Table 2. The use of the parameters for the simulation using the COMSOL Multiphysics is shown elsewhere (Ali, 2021; Yousuo et al., 2022).

Table 1: "Model parameters for the simulation" (Bautista et al., 2003).

| Property | Value |
|---|---|
| Density of water | 1000 $kg/m^3$ |
| Molar mass of activated carbon | 0.012 kg/mol |
| Molar mass of water | 0.018 kg/mol |
| Porosity of adsorbent particle | 0.3 |
| Diameter of particle | 0.001m |
| Thermal conductivity of column wall | 50 W/(m.K) |
| Particle density | 2100 $kg/m^3$ |

Table 2: "Model parameters for the simulation in the simulation environment.

| Name | Expression | Value | Description |
|---|---|---|---|
| Rhop | 2100[kg/m^3] | 2100 $kg/m^3$ | Particle density |
| Qm | 8.492[mg/g]/MFe | 0.053175 mol/kg | Maximum equilibrium loading of adsorbent |
| K | 0.234[L/mg]*MFe | 37.37 $m^3/mol$ | Equilibrium Adsorption constant |
| Ep | 0.3 | 0.3 | porosity of particle |
| Eb | 0.4 | 0.4 | Porosity of Bed |
| Dp | 0.001[m] | 0.001 m | Diameter of particles |
| Rp | dp/2 | 5E−4 m | Radius of particle |
| rhoH2O | 1000[kg/m^3] | 1000 $kg/m^3$ | Density of water |
| visH2O | 1.787E-3[Pa*s] | 0.001787 Pa·s | Viscosity of water |
| Mfe | 159.7[g/mol] | 0.1597 kg/mol | Molar Mass of Iron |
| MH2O | 18[g/mol] | 0.018 kg/mol | Molar mass of water |
| MC | 12[g/mol] | 0.012 kg/mol | Molar mass of activated carbon |

| Name | Expression | Value | Description |
|---|---|---|---|
| mFein | 7e-6[kg/L] | 0.007 kg/m³ | Inlet mass concentration of iron in water * |
| cFein | mFein/Mfe | 0.043832 mol/m³ | Inlet molar concentration of iron in water * |
| Tau | 1.5[min] | 90 s | Residence time * |
| Fl | (1 - eb)*Vr/tau | 0.0079365 m³/s | Volumetric flow rate of water |
| Rr | 0.5[m] | 0.5 m | Radius of adsorption column |
| Ar | pi*Rr^2 | 0.7854 m² | Cross sectional area of adsorber |
| Vr | Ar*Lr | 1.1905 m³ | volume of adsorber |
| Lr | Wc/(Ar*rhob) | 1.5158 m | Height of adsorption unit * |
| rhoH2Oin | rhoH2O*Fl*1[s] | 7.9365 kg | Inlet mass density of water * |
| cH2Oin | rhoH2Oin/(MH2O* Vr) | 370.37 mol/m³ | inlet molar concentration of water |
| Vin | Fl/Ar | 0.010105 m/s | Inlet velocity of water |
| Rhob | rhop*(1 - eb) | 1260 kg/m³ | Particle bed density |
| Wb | 1500[kg] | 1500 kg | Weight of adsorbent bed |
| Tin | 298.15[K] | 298.15 K | Inlet temperature of fluid * |
| Kw | 50[W/(m*K)] | 50 W/(m·K) | Thermal Conductivity of Column Wall * |
| Dx | 0.5[cm] | 0.005 m | Thickness of wall material * |
| Ts | 295.18[K] | 295.18 K | Temperature of the surrounding * |

Note: The values of those parameters with asterisk (*) are assumed".

## 3 Results and Discussion

As stated in the introduction, "the aim of the study is to employ a CFD COMSOL Multiphysics software to simulate the equilibrium and dynamic behavior of the adsorption column in order to accurately predict the effect of particle size in the performance of the fixed-bed adsorption column. Therefore, this section presents results and the discussion of the results.

### 3.1 The effect of particle size

The effect of particle size is observed in Figure 1. It shows that as the particle size increases the adsorption capacity of the bed decreases. Higher adsorption was found at smaller particle sizes; particles with 0.001 m were more in the adsorption capacity than 0.003m and 0.004m because the rate of adsorption in the column increases with decrease in particle size. Mehmet (2007) reported similar results during his studies on heavy metal adsorption by modified oak sawdust.

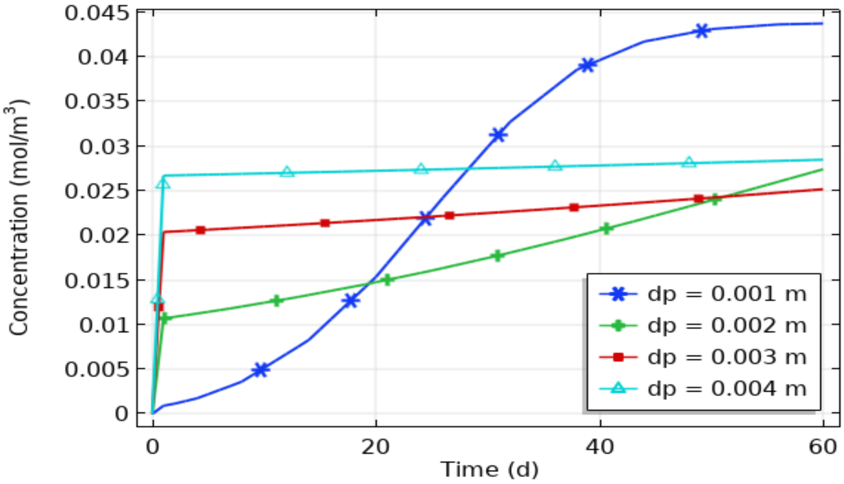


Figure 1: Breakthrough curve of ferrous iron concentration at the end of the bed".

### 3.2 Other Graphs

The line graph (Figure 2) showing the concentration of ferrous ion along the bed at different times (days). "The results showed that about 28days effective performance of the bed was achieved for a bed weight of 1500kg. A detailed discussion is given in our work elsewhere (Ali, 2021; Yousuo et al., 2022)

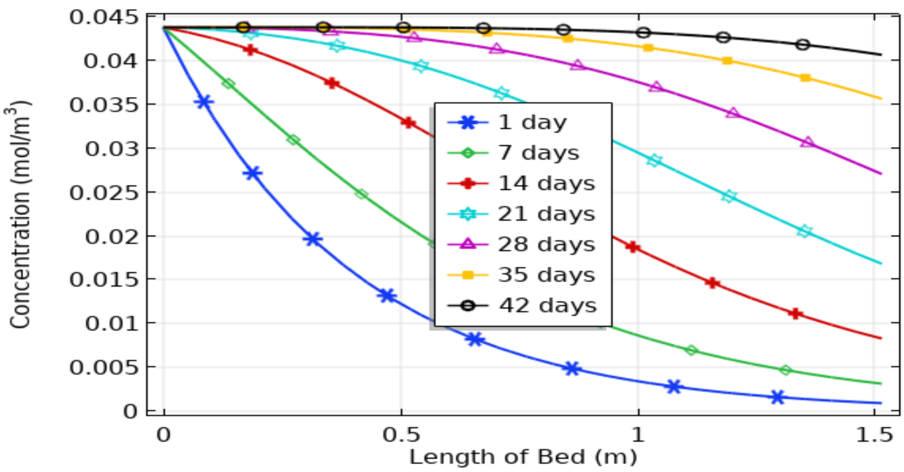


Figure 2: Line graph of ferrous iron concentration along the bed at different times (days)".

"Comsol Multiphysics software can represent the performance of the adsorption column in a 2D surface plot as shown in Figures 3-9. In the 2D surface plot the red color indicates the level of iron concentration in the bed, the change in colour down the bed shows a drop in the iron concentration in the water. As the days increased, there was increased intensity of the red colour which means the bed was now filled with iron and ready for regeneration'. A detailed discussion is given in our work elsewhere (Ali, 2021; Yousuo et al., 2022)"

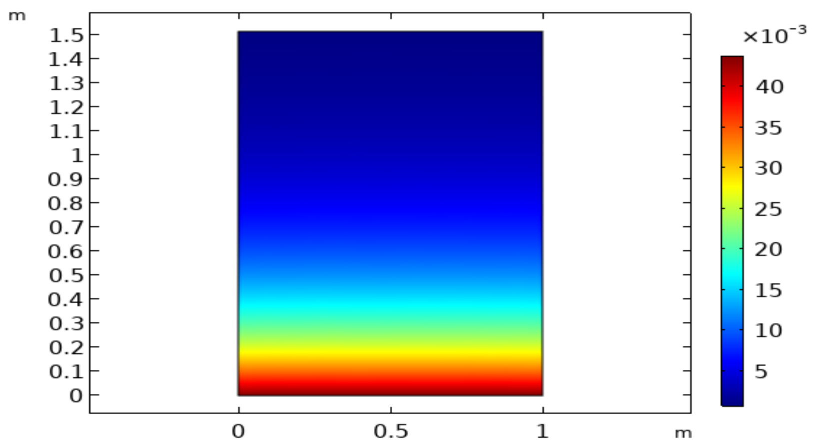


Figure 3: 2D surface plot of ferrous iron concentration along the bed at the end of the 1st day.

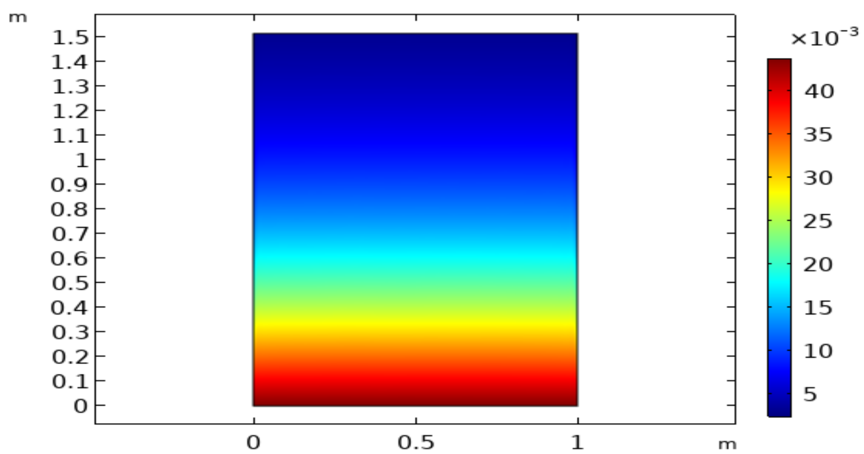


Figure 4: 2D surface plot of ferrous iron concentration along the bed at the end of 7 days

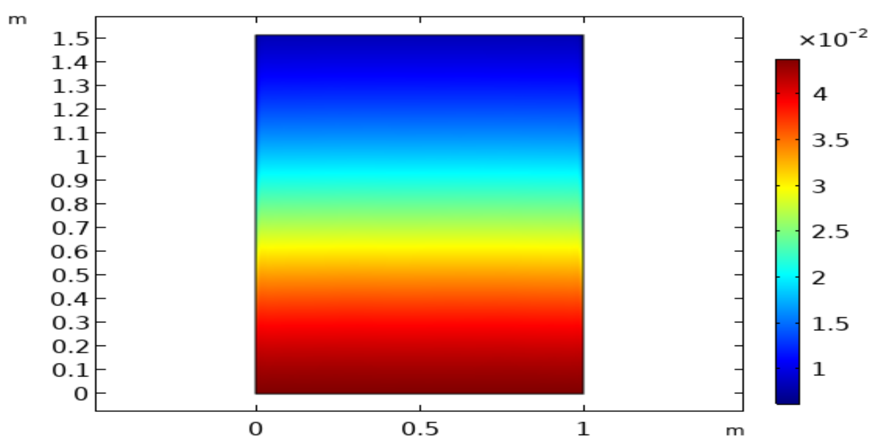

Figure 5: 2D surface plot of ferrous iron concentration along the bed at the end of 14 days

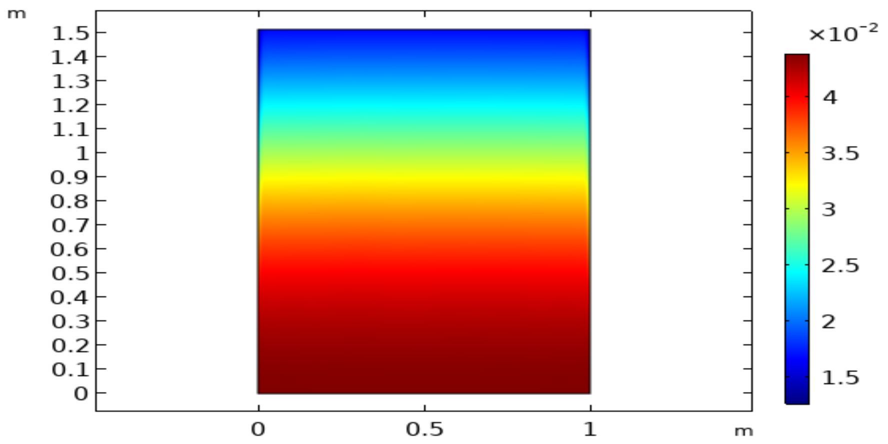


Figure 6: 2D surface plot of ferrous iron concentration along the bed at the end of 21 days

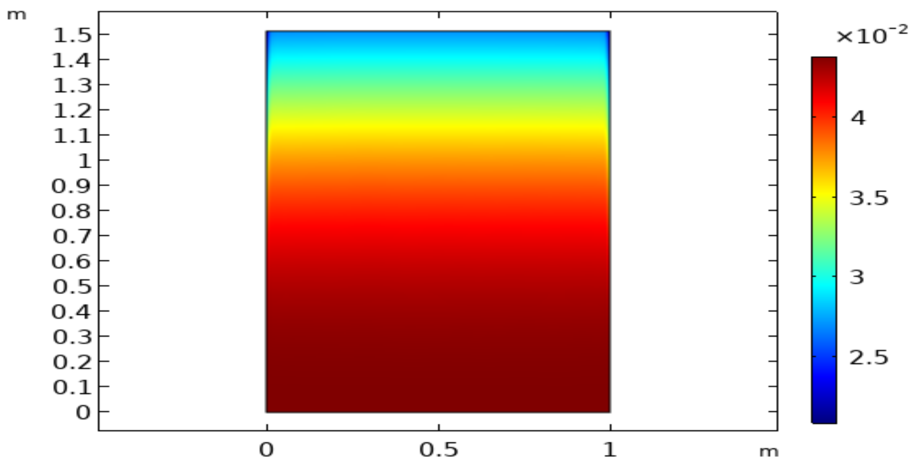


Figure 7: 2D surface plot of ferrous iron concentration along the bed at the end of 28 days

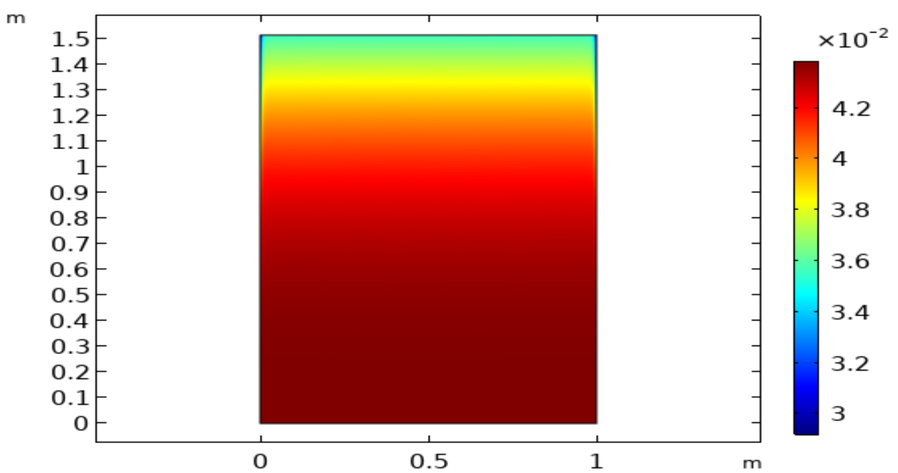

Figure 8: 2D surface plot of ferrous iron concentration along the bed at the end of 35 days.

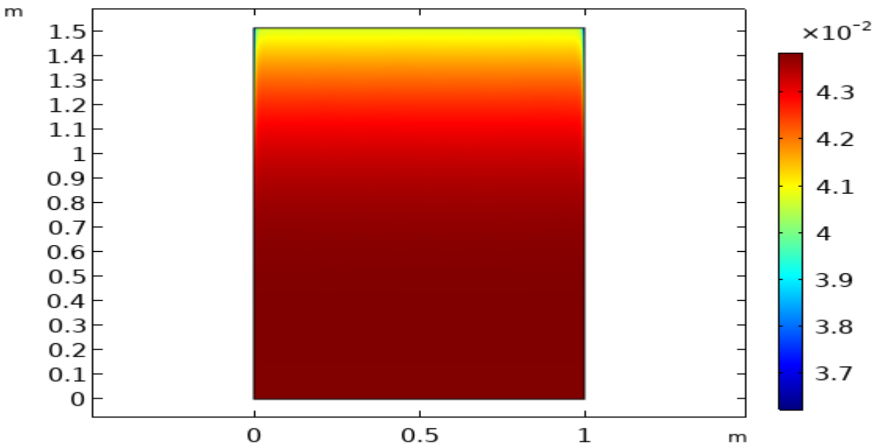


Figure 9: 2D surface plot of ferrous iron concentration along the bed at the end of 42 days.

### 3.3 Validation of simulated result with literatures

The CFD simulated effluent iron concentration was compared with literatures as shown in table 3. The result showed that the effluent iron concentration of this work is very acceptable.

Table 3: Comparing effluent concentration with literatures

| Parameter | This Work | Ruthven, 1984 | WHO |
|---|---|---|---|
| Effluent iron concentration ($mol/m^3$) | 0.028 | 0.029 | 0.03 |

### Conclusion

Model equations were used in COMSOL Multiphysics and the detail work is shown elsewhere (Ali, 2021; Yousuo et al., 2022). The results were presented in a line graph and also in 2D surface plots. A 2D model was developed to illustrate the iron concentration distribution for different days, which clearly showed the days for which the adsorbent was completely filled with iron.

The effect of particle size on the breakthrough curve was investigated for particle sizes of "0.001m, 0.002m, 0.003m and 0.004m'. Simulated results showed that as the particle size increases the adsorption capacity of the bed decreases. It was also observed that about 28 days operative performance of the bed could be achieved for a bed weight of 1500kg and particle size of 0.001m. Predicted results were compared with results presented by Ruthven, 1984 and World Health Organization standards".

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