
A STUDY OF THE BEHAVIOUR OF A FIXED-BED ADSORPTION COLUMN FOR REMOVAL OF FERROUS IRON (Fe^{2+}) IN GROUNDWATER USING ACTIVATED CARBON

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ABSTRACT

The Langmuir adsorption isotherm equilibrium model and the fixed-bed adsorption models were used. A Computational Fluid Dynamic (CFD) simulation of an adsorption column for the removal of iron from groundwater was carried out. CFD solution model was developed in COMSOL Multiphysics which provided detailed facts about the fixed-bed adsorption column and offers enhanced design perception. The line graph and the 2D surface plots were generated. Simulated results indicated 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 very acceptable when compared with World Health Organization Standards for drinking water.

Keywords: *Fixed-Bed, Adsorption column, Ferrous Iron, Groundwater, Activated Carbon, Concentration*

INTRODUCTION

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). Adsorption had been known to be an effective separation process for the removal of heavy metal fractions like those of iron and mercury from polluted water sources.

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). A majority of the studies on heavy metal removal 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).

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. Based on previous studies to analyze the performance of fixed-bed adsorption systems, this work focuses on the performance analysis of a fixed-bed adsorption unit filled with activated carbon for a down flow configuration. 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 concentration of ferrous iron along the bed at different times or days.

PROBLEM STATEMENT

Groundwater pollution has become a major problem worldwide. In the Yenagoa metropolis of Bayelsa state of Nigeria, in the rural and semi-urban areas, the major source of drinking water is groundwater. Groundwater which is less susceptible to bacterial contamination has severe problems with metal contamination which occurs in the cracks of sedimentary rocks present in high concentrations. The pollution of groundwater with excess amount of iron is a great problem because it is not safe for drinking. Although iron is an essential mineral in the transportation of oxygen in the blood, the presence of iron in water above a concentration level of 0.03mol/m^3 will render it unhealthy for use due to its metallic sense of taste, odour and staining of surfaces (Das *et al.*, 2007).

Lauffer (1992) had established that the excessive accumulation of iron in human body caused ailments. The human body has limited ways of eliminating the over dose iron that is present in water after consumption; it therefore accumulates in certain body organs like the liver, the bone marrow and pancreases, thereby causing malfunctioning of the body. The iron deposits in the liver and in the pancreases cause liver cirrhosis and diabetes mellitus (Lauffer, 1992). Hence, this research work seeks to simulate the equilibrium and dynamic behavior of a fixed bed adsorption column for iron removal using finite element method (FEM) in COMSOL Multiphysics software, to accurately predict the optimum amount of adsorbent (activated carbon), the time required for adsorption bed regeneration upon complete saturation with iron. The simulation process also established the diameter and the length of the fixed-bed adsorption column.

MATERIALS AND METHODS

Materials

In this chapter the governing dynamic equations for the transport of material and energy through the fixed-bed was developed considering both transport in the axial direction by convection and in the radial direction by diffusion in a cylindrical coordinate system. In the study, we also considered 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 research methodology adopted to conduct this study was extensively established in the COMSOL Multiphysics software in simulating the adsorption bed.

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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.
- A dynamic model formulation in the fixed-bed column leads to the formation of a coupled system of partial differential equations (PDEs) with more than one dependent variable influencing the behavior of column.

In simulating the models to study the dynamic behavior of the adsorption column, a mathematical algorithm in solving the coupled PDEs was set up and implemented in COMSOL Multiphysics software-a graphical programming environment. This package was employed because of its high level of stability and being relatively fast in calculations, capable of handling both Neumann and Dirichlet boundary conditions with the application of the finite element method (FEM) in COMSOL. Some process parameters and constants for the purpose of simulating the models were extracted from works by Bautista *et al.*, 2003 which are given in Table 3.1.

A step-by-step presentation of how the software was used achieve the objectives of the present study is outlined elsewhere (Ali, 2021).

Methods

The Adsorption Column Model Development

The adsorption column is shown in Figure 3.1

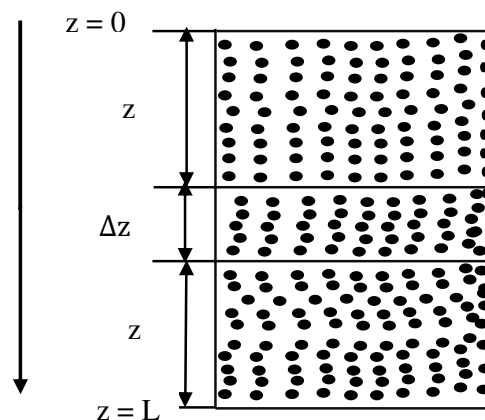


Figure 3.1: Differential element of fixed-bed adsorption column

Stoichiometry of the adsorption process

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 (3.1):



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 (3.2) (Ruthven and Douglas (1984):

$$q = q_m \frac{KC_i}{1 + KC_i} \quad (3.2)$$

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

$$\left[\begin{array}{l} \text{Accumulation} \\ \text{of species in} \\ \text{differential volume} \\ \text{with time} \end{array} \right] = \left[\begin{array}{l} \text{Net flux of} \\ \text{species into} \\ \text{the differential} \\ \text{volume} \end{array} \right] - \left[\begin{array}{l} \text{Depletion of Species} \\ \text{from differential} \\ \text{volume due to adsorption} \\ \text{loading of species into} \\ \text{adsorbent pellet} \end{array} \right] \quad (3.3)$$

Equation (3.3) is simplified as

$$A = F_z + F_r - D \quad (3.4)$$

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

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The change in volume occupied by the liquid and solid phase respectively expressed in terms of the overall change in volume of the adsorption bed is given as:

$$\Delta V_l = \varepsilon_b \Delta V_o \quad (3.5)$$

$$V_s = (1 - \varepsilon_b) \Delta V_o \quad (3.6)$$

$$\Delta V_o = r \Delta \theta \Delta r \Delta z \quad (3.7)$$

where ΔV_l = Change in volume occupied by liquid

ΔV_o = Change in total volume of adsorber

ΔV_s = Change in volume occupied by solid

ε_b = Bed porosity

r = Radial direction

Δr = Change in the radial direction

$\Delta \theta$ = Change in the angular direction

and Δz = Change in the axial direction.

Accumulation of species (adsorbate) in differential volume between the interval t and $t + \Delta t$ is given by:

$$C_i \varepsilon_b \Delta V_o \Big|_{t+\Delta t} - C_i \varepsilon_b \Delta V_o \Big|_t \quad (3.8)$$

where t = Time and Δt = Change in time.

Net flux of material in the axial direction in the interval Δt

$$\varepsilon_b r \Delta \theta \Delta r \Delta t N_i \Big|_{z+\Delta z} - \varepsilon_b r \Delta \theta \Delta r \Delta t N_i \Big|_z \quad (3.9)$$

where z is the axial direction and N_i is the molar flux of species.

Net flux of material in the radial direction in the interval Δt

$$\varepsilon_b r \Delta \theta \Delta z \Delta t N_i \Big|_{r+\Delta r} - \varepsilon_b r \Delta \theta \Delta z \Delta t N_i \Big|_r \quad (3.10)$$

Let the rate of adsorbent loading be expressed in terms of the rate of external mass transfer of the adsorbate to the surface of a single adsorbent pellet given as,

$$\frac{A_p}{V_p} (1 - \varepsilon_b) \Delta V_o \Delta t k_m (C_i - C_i') \quad (3.11)$$

Where A_p = Surface area of adsorbent pellet

V_p = Volume of adsorbent pellet

k_m = External mass transfer coefficient

C_i = Concentration of species along the bed

For a spherical pellet:

$$\frac{A_p}{V_p} = \frac{6}{d_p} \tag{3.12}$$

d_p =Diameter of adsorbent pellet

Therefore, we have

$$\frac{6}{d_p}(1-\varepsilon_b)\Delta V_o\Delta t k_m(C_i-C_i') \tag{3.13}$$

Substituting(3.8), (3.9), (3.10), (3.13) into(3.4) we have

$$\begin{aligned} \varepsilon_b\Delta V_o(C_i|_{t+\Delta t} - C_i|_t) &= \varepsilon_b r\Delta\theta\Delta r\Delta t(N_i|_{z+\Delta z} - N_i|_z) + \varepsilon_b r\Delta\theta\Delta z\Delta t(N_i|_{r+\Delta r} - N_i|_r) \\ &\quad - \frac{6}{d_p}(1-\varepsilon_b)\Delta t\Delta V_o k_m(C_i - C_i') \end{aligned} \tag{3.14}$$

Dividing (3.14) by $\varepsilon_b\Delta\Delta V_o$ we have

$$\begin{aligned} \frac{(C_i|_{t+\Delta t} - C_i|_t)}{\Delta t} &= \frac{r\Delta\theta\Delta r(N_i|_{z+\Delta z} - N_i|_z)}{\Delta V_o} + \frac{r\Delta\theta\Delta z(N_i|_{r+\Delta r} - N_i|_r)}{\Delta V_o} \\ &\quad - \frac{6(1-\varepsilon_b)}{d_p\varepsilon_b}k_m(C_i - C_i') \end{aligned} \tag{3.15}$$

Substituting equation (3.7)

$$\begin{aligned} \frac{(C_i|_{t+\Delta t} - C_i|_t)}{\Delta t} &= \frac{r\Delta\theta\Delta r(N_i|_{z+\Delta z} - N_i|_z)}{r\Delta\theta\Delta r\Delta z} + \frac{r\Delta\theta\Delta z(N_i|_{r+\Delta r} - N_i|_r)}{r\Delta\theta\Delta r\Delta z} \\ &\quad - \frac{6(1-\varepsilon_b)}{d_p\varepsilon_b}k_m(C_i - C_i') \end{aligned} \tag{3.16}$$

Taking limits on (3.16) as $\Delta t, \Delta z, \Delta r$ tends to zero and canceling out appropriately gives

$$\begin{aligned} \lim_{\Delta t \rightarrow 0} \frac{(C_i|_{t+\Delta t} - C_i|_t)}{\Delta t} &= \Delta\theta\Delta r \lim_{\Delta z \rightarrow 0} \frac{r(N_i|_{z+\Delta z} - N_i|_z)}{r\Delta\theta\Delta r\Delta z} + \frac{r\Delta\theta\Delta z(N_i|_{z+\Delta z} - N_i|_z)}{r\Delta\theta\Delta r\Delta z} - \frac{6(1-\varepsilon_b)}{d_p\varepsilon_b}k_m(C_i - C_i') \\ \frac{\partial C_i}{\partial t} &= \frac{\partial N_i}{\partial z} + \frac{1}{r} \frac{\partial(rN_i)}{\partial r} - \frac{6(1-\varepsilon_b)}{d_p\varepsilon_b}k_m(C_i - C_i') \end{aligned} \tag{3.17}$$

The net flux is a combination of the diffusion flux according to Fick's law and convective flux thus we have (Fogler, 2012):

$$N_i = -D_i \frac{\partial C_i}{\partial z} + C_i v \tag{3.18}$$

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where D_i = Diffusivity or effective dispersion coefficient of species i

v = Fluid flow velocity,

And other variables remain as earlier presented.

Substituting (3.18) into (3.17) we have

$$\frac{\partial C_i}{\partial t} = -D_z \frac{\partial^2 C_i}{\partial z^2} + v_z \frac{\partial C_i}{\partial z} - D_r \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_i}{\partial r} \right) + v_r \frac{1}{r} \frac{\partial (r C_i)}{\partial r} - \frac{6}{d_p} \frac{(1-\varepsilon_b)}{\varepsilon_b} k_m (C_i - C_i') \quad (3.19)$$

Neglecting the diffusion in the axial direction and the velocity in the radial direction the equation reduces to

$$\frac{\partial C_i}{\partial t} = -D_r \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_i}{\partial r} \right) + v_z \frac{\partial C_i}{\partial z} - \frac{6}{d_p} \frac{(1-\varepsilon_b)}{\varepsilon_b} k_m (C_i - C_i') \quad (3.20)$$

Expressing in terms of the adsorbate iron we have that

$$\frac{\partial C_{Fe}}{\partial t} = -D_{rFe} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_{Fe}}{\partial r} \right) + v_z \frac{\partial C_{Fe}}{\partial z} - \frac{6}{d_p} \frac{(1-\varepsilon_b)}{\varepsilon_b} k_m (C_i - C_i') \quad (3.21)$$

Initial and Boundary conditions:

The models given below define the boundary conditions that are required to solve the coupled partial differential equation, (3.21).

$$At \quad t = 0, \quad C_{Fe}(0, z) = 0$$

$$At \quad z = 0, \quad C_{Fe}(t, 0) = C_{Fein}$$

$$At \quad z = L, \quad \left. \frac{\partial C_{Fe}}{\partial z} \right|_{z=L} = 0$$

Mole Balance within the Adsorbent Pellet

Also considering only transport in the radial direction for a spherical geometry gives (Knepper, 1981):

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \varepsilon_p D_{pi} \frac{\partial^2 C_i'}{\partial r^2} \right] - \rho_s \frac{\partial q}{\partial t} = \frac{\partial C_i'}{\partial t} \varepsilon_p \quad (3.22)$$

Where D_{pi} is the diffusivity of the species within the pellet and ρ_s is the crystal particle density.

From elementary calculus, we have that (Forgler, 2012)

$$\frac{\partial q}{\partial t} = \frac{\partial C_i'}{\partial t} \frac{\partial q}{\partial C_i'} \quad (3.23)$$

Substituting (3.23) into (3.22) gives

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \varepsilon_p D_{pi} \frac{\partial^2 C'_i}{\partial r} \right] - \rho_s \frac{\partial C'_i}{\partial t} \frac{\partial q}{\partial C'_i} = \frac{\partial C'_i}{\partial t} \varepsilon_p \quad (3.24)$$

The crystal density of the particle is related to the density of the particle by the following expression (Seader and Earnest, 2010).

$$\rho_s = (1 - \varepsilon_p) \rho_p \quad (3.25)$$

Where ρ_p is the density of the particle and ε_p is the particle porosity.

Differentiating (3.2) with respect to C'_i gives

$$\frac{dq}{dC'_i} = \frac{q_m K}{(1 + KC'_i)^2} \quad (3.26)$$

Substituting (3.25) and (3.26) into (3.24), we have that

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \varepsilon_p D_{pi} \frac{\partial^2 C'_i}{\partial r} \right] - (1 - \varepsilon_p) \rho_p \frac{q_m K}{(1 + KC'_i)^2} \frac{\partial C'_i}{\partial t} = \frac{\partial C'_i}{\partial t} \varepsilon_p \quad (3.27)$$

Dividing (3.27) by ε_p and factorizing, we have

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 D_{pi} \frac{\partial^2 C'_i}{\partial r} \right] - \left[1 + \frac{(1 - \varepsilon_p)}{\varepsilon_p} \rho_p \frac{q_m K}{(1 + KC'_i)^2} \right] \frac{\partial C'_i}{\partial t} = 0 \quad (3.28)$$

Expressing in terms of Iron we have

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 D_{pFe} \frac{\partial^2 C'_{Fe}}{\partial r} \right] - \left[1 + \frac{(1 - \varepsilon_p)}{\varepsilon_p} \rho_p \frac{q_m K}{(1 + KC'_{Fe})^2} \right] \frac{\partial C'_{Fe}}{\partial t} = 0 \quad (3.29)$$

Initial and boundary condition:

The models given below define the boundary conditions that are required to solve the coupled partial differential equation of (3.29)

$$\begin{aligned} At \quad t = 0, \quad C'_{Fe}(0, r) &= 0 \\ At \quad r = 0, \quad \left. \frac{\partial C'_{Fe}}{\partial r} \right|_{r=0} &= 0 \\ At \quad r = R_p, \quad C'_{Fe}(t, R_p) &= C'_{Fein} \end{aligned}$$

Energy Balance through the Bed for a Cylindrical Geometry

$$\left[\begin{array}{l} \text{Rate of Increase} \\ \text{of Kinetic and} \\ \text{internal energy} \\ \text{in the differential} \\ \text{volume} \end{array} \right] = \left[\begin{array}{l} \text{Net rate of} \\ \text{kinetic and} \\ \text{internal energy} \\ \text{addition by} \\ \text{convection} \end{array} \right] + \left[\begin{array}{l} \text{Net rate of} \\ \text{heat added} \\ \text{by molecular} \\ \text{transport} \\ \text{conduction} \end{array} \right] + \left[\begin{array}{l} \text{Heat} \\ \text{generated} \\ \text{due to} \\ \text{chemical} \\ \text{reaction} \end{array} \right] + \left[\begin{array}{l} \text{Heat} \\ \text{transferred} \\ \text{from} \\ \text{fluid stream} \end{array} \right] \quad (3.30)$$

The parameters in equation (3.30) are defined as follows:

First parameter: Measures the energy increase within the adsorber.

Second parameter: Indicates the heat addition (kinetic and internal) as the water flows through the adsorption column in the axial direction.

Third parameter: A term that measures heat transfer due to molecular diffusion.

Fourth parameter: Heat energy added due to reactive adsorption in the column.

Fifth parameter: Heat flow from bulk fluid to the wall of the adsorber.

Neglecting the change in kinetic energy of the system, the rate of increase of internal energy of the system is given as

$$\rho_i \varepsilon_b \Delta V_o U \Big|_{t+\Delta t} - \rho_i \varepsilon_b \Delta V_o U \Big|_t \quad (3.31)$$

where U = Internal energy

and ρ_i = Density of adsorbate species, i

Net rate of heat addition by conduction and convection in the axial direction in the interval Δt

$$r \Delta \theta \Delta r \Delta t (Q_{con} + Q_{cov}) \Big|_{z+\Delta z} - r \Delta \theta \Delta r \Delta t (Q_{con} + Q_{cov}) \Big|_z \quad (3.32)$$

where Q_{con} is the heat addition by conduction and Q_{cov} , the heat addition by convection.

Net rate of heat addition by conduction and convection in the radial direction in the interval Δt

$$r \Delta \theta \Delta z \Delta t (Q_{con} + Q_{cov}) \Big|_{r+\Delta r} - r \Delta \theta \Delta z \Delta t (Q_{con} + Q_{cov}) \Big|_r \quad (3.33)$$

Heat transferred from liquid to solid by convection in the interval Δt

$$\frac{A_p}{V_p} h(1 - \varepsilon_b) \Delta V_o \Delta t (T_f - T_s) \quad (3.34)$$

where h = Heat transfer coefficient

T_f = Fluid temperature

T_s = Temperature of adsorbent solid

Heat generated within differential volume by adsorption

$$\frac{A_p}{V_p} (1 - \varepsilon_b) \Delta V_o \Delta H_{ads} \Delta t k_m (C_i - C_i') \quad (3.35)$$

where ΔH_{ads} = Change in heat of adsorption.

Heat lost to the surrounding in the interval Δt

$$\frac{4h(1 - \varepsilon_b)}{D_r} \Delta V_o \Delta t (T_f - T_w) \quad (3.36)$$

where T_w = Temperature of adsorption column wall

D_r = Diameter of adsorption unit

Therefore, we have:

$$\begin{aligned} \rho_i \varepsilon_b \Delta V_o (U|_{t+\Delta t} - U|_t) = & \varepsilon_b r \Delta \theta \Delta r \Delta t \left((Q_{con} + Q_{cov})|_{z+\Delta z} - (Q_{con} + Q_{cov})|_z \right) \\ & + \varepsilon_b r \Delta \theta \Delta z \Delta t \left((Q_{con} + Q_{cov})|_{r+\Delta r} - (Q_{con} + Q_{cov})|_r \right) \\ & + \frac{A_p}{V_p} (1 - \varepsilon_b) \Delta V_o \Delta t \left(h(T_s - T_f) + \Delta H_{ads} k_m (C_i - C_i') \right) \\ & + \frac{4h(1 - \varepsilon_b)}{D_r} \Delta V_o \Delta t (T_f - T_w) \end{aligned} \quad (3.37)$$

Dividing (3.37) by $\Delta V_o \Delta t \varepsilon_b$ gives

$$\begin{aligned} \frac{\rho_i (U|_{t+\Delta t} - U|_t)}{\Delta t} = & \frac{r \Delta \theta \Delta r \left((Q_{con} + Q_{cov})|_{z+\Delta z} - (Q_{con} + Q_{cov})|_z \right)}{\Delta V_o} \\ & + \frac{r \Delta \theta \Delta z \left((Q_{con} + Q_{cov})|_{r+\Delta r} - (Q_{con} + Q_{cov})|_r \right)}{\Delta V_o} \\ & + \frac{A_p (1 - \varepsilon_b)}{V_p \varepsilon_b} \left(h(T_s - T_f) + \Delta H_{ads} k_m (C_i - C_i') \right) \\ & + \frac{4h(1 - \varepsilon_b)}{D_r \varepsilon_b} (T_f - T_w) \end{aligned} \quad (3.38)$$

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From (3.7) for a cylindrical coordinate system we have that

$$\begin{aligned} \frac{\rho_i (U|_{r+\Delta r} - U|_r)}{\Delta t} = & \frac{r\Delta\theta\Delta r \left((Q_{con} + Q_{cov})|_{z+\Delta z} - (Q_{con} + Q_{cov})|_z \right)}{r\Delta\theta\Delta r\Delta z} \\ & + \frac{r\Delta\theta\Delta z \left((Q_{con} + Q_{cov})|_{r+\Delta r} - (Q_{con} + Q_{cov})|_r \right)}{r\Delta\theta\Delta r\Delta z} \\ & + \frac{A_p (1-\varepsilon_b)}{V_p \varepsilon_b} \left(h(T_s - T_f) + \Delta H_{ads} k_m (C_i - C'_i) \right) \\ & + \frac{4h(1-\varepsilon_b)}{D_r \varepsilon_b} (T_f - T_w) \end{aligned} \quad (3.39)$$

Taking limits on (3.39) as $\Delta t, \Delta z, \Delta r$ approaches zero and canceling out appropriately gives

$$\begin{aligned} \frac{\rho_i \partial U}{\partial t} = & \frac{\partial (Q_{con} + Q_{cov})}{\partial z} + \frac{1}{r} \frac{\partial (r(Q_{con} + Q_{cov}))}{\partial r} \\ & + \frac{A_p (1-\varepsilon_b)}{V_p \varepsilon_b} \left(h(T_s - T_f) + \Delta H_{ads} k_m (C_i - C'_i) \right) \\ & + \frac{4h(1-\varepsilon_b)}{D_r \varepsilon_b} (T_f - T_w) \end{aligned} \quad (3.40)$$

Expressing in terms of temperature, the change in internal energy is given as (Hoy, 2004):

$$\partial U = C_p \partial T \quad (3.41)$$

where C_p is the specific heat capacity at constant pressure.

The conduction term is expressed using Fourier law of heat conduction (McKay and Hoy, 1999):

$$Q_{con} = -\lambda \frac{\partial T}{\partial z} \quad (3.42)$$

where λ is the thermal conductivity.

The convection term due to velocity of species is given as (Knepper, 1981):

$$Q_{cov} = v C_p \rho T \quad (3.43)$$

Therefore, we have

$$\rho C_p \frac{\partial T_f}{\partial t} = \frac{\partial \left(-\lambda \frac{\partial T_f}{\partial z} \right)}{\partial z} + \rho C_p v_z \frac{\partial T_f}{\partial z} + \frac{1}{r} \frac{\partial \left(-r \lambda \frac{\partial T_f}{\partial z} \right)}{\partial r} + \frac{\rho C_p v_r}{r} \frac{\partial (r T_f)}{\partial r} + \frac{A_p (1-\varepsilon_b)}{V_p \varepsilon_b} \left(h(T_s - T_f) + \Delta H_{ads} k_m (C_i - C_i') \right) + \frac{4h(1-\varepsilon_b)}{D_r \varepsilon_b} (T_f - T_w) \quad (3.44)$$

From (3.12) for a spherical pellet we have

$$\rho C_p \frac{\partial T_f}{\partial t} = \frac{\partial \left(-\lambda \frac{\partial T_f}{\partial z} \right)}{\partial z} + \rho C_p v_z \frac{\partial T_f}{\partial z} + \frac{1}{r} \frac{\partial \left(-r \lambda \frac{\partial T_f}{\partial z} \right)}{\partial r} + \frac{\rho C_p v_r}{r} \frac{\partial (r T_f)}{\partial r} + \frac{6(1-\varepsilon_b)}{d_p \varepsilon_b} \left(h(T_s - T_f) + \Delta H_{ads} k_m (C_i - C_i') \right) + \frac{4h(1-\varepsilon_b)}{D_r \varepsilon_b} (T_f - T_w) \quad (3.45)$$

Expressing for the solid phase with zero velocity gradient we have;

$$\rho_s C_{ps} \frac{\partial T_s}{\partial t} = \frac{\partial \left(-\lambda_s \frac{\partial T_s}{\partial z} \right)}{\partial z} + \frac{1}{r} \frac{\partial \left(-r \lambda_s \frac{\partial T_s}{\partial z} \right)}{\partial r} + \frac{6(1-\varepsilon_b)}{d_p \varepsilon_b} \left(h(T_s - T_f) + \Delta H_{ads} k_m (C_{Fe} - C_{Fe}') \right) + \frac{4h(1-\varepsilon_b)}{D_r \varepsilon_b} (T_f - T_w) \quad (3.46)$$

Expressing for the Fluid phase with zero velocity in the radial direction we have

$$\rho_f C_{pf} \frac{\partial T_f}{\partial t} = \frac{\partial \left(-\lambda_f \frac{\partial T_f}{\partial z} \right)}{\partial z} + \rho_f C_{pf} v_z \frac{\partial T_f}{\partial z} + \frac{1}{r} \frac{\partial \left(-r \lambda_f \frac{\partial T_f}{\partial z} \right)}{\partial r} + \frac{6(1-\varepsilon_b)}{d_p \varepsilon_b} \left(h(T_s - T_f) + \Delta H_{ads} k_m (C_{Fe} - C_{Fe}') \right) + \frac{4h(1-\varepsilon_b)}{D_r \varepsilon_b} (T_f - T_w) \quad (3.47)$$

Boundary conditions:

The boundary conditions are established at the inlet and outlet of the adsorption column, and will be employed in solving the resulting coupled Partial Differential Equations

$$\begin{aligned} At \quad z = 0, \quad T_f &= T_f^{in}, & T_s &= T_s^{in} \\ At \quad z = L, \quad \frac{\partial T_f}{\partial z} \Big|_{z=L} &= 0, & \frac{\partial T_s}{\partial z} \Big|_{z=L} &= 0 \\ At \quad r = 0, \quad \frac{\partial T_f}{\partial r} \Big|_{r=0} &= 0, & \frac{\partial T_s}{\partial r} \Big|_{r=0} &= 0 \\ At \quad r = R_r, \quad \lambda_L \frac{\partial T_f}{\partial r} \Big|_{r=R_r} &= h(T_f - T_w), & \lambda_s \frac{\partial T_s}{\partial r} \Big|_{r=R_r} &= h(T_s - T_w) \end{aligned}$$

Energy Balance through the Adsorbent Pellet for a Spherical Geometry

This was modelled assuming that both the solid and the fluid at every point in the pellet have the same temperature (Warren *et al.*, 2001):

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \lambda_{ep} \frac{\partial^2 T_p}{\partial r^2} \right] - \Delta H_{ads} \rho_s \frac{\partial q}{\partial t} = \rho_s C_p \frac{\partial T_p}{\partial t} \quad (3.48)$$

Applying (3.23), (3.25), (3.26) we have

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \lambda_p \frac{\partial^2 T_p}{\partial r^2} \right] - \Delta H_{ads} \rho_p (1 - \varepsilon_p) k_m (C_{Fe} - C'_{Fe}) = \rho_p (1 - \varepsilon_p) C_p \frac{\partial T_p}{\partial t} \quad (3.49)$$

Boundary and initial conditions:

$$\begin{aligned} At \quad t = 0, \quad T_p &= 0 \\ At \quad r = 0, \quad \frac{\partial T_p}{\partial r} \Big|_{r=0} &= 0, \\ At \quad r = R_p, \quad T_p &= T_s, \end{aligned}$$

Pressure Drop through the Bed

The pressure drop through the bed is modelled following the Ergun's equation in (3.50) (Warren *et al.*, 2001):

$$\frac{dp}{dz} = - \frac{G}{\rho g_c d_p} \left(\frac{1 - \varepsilon_b}{\varepsilon_b^3} \right) \left[\frac{150(1 - \varepsilon_b) \mu}{d_p} + 1.75G \right] \quad (3.50)$$

where G = Mass velocity of fluid approaching particle

ρ = Fluid density

dp = Pressure drop in packed bed

μ = Absolute viscosity of fluid

d_p = Diameter of adsorbent pellet

g_c = Newton's law proportionality factor

This equation is capable to handle both laminar and turbulent flows.

Solution Technique for the Adsorption Model

The governing models which included the adsorption isotherm model (3.2), the fixed bed model (3.21), the Particle model (3.29), the bed pressure drop (3.50) and the energy balance model (3.47) were solved using the finite element method in COMSOL Multiphysics. The

adsorption isotherm data was taken from the works of Babu and Gupta (2004).

The Steps taken in using the Comsol Multiphysics Software in solving the Models

The steps taken in solving the models using COMSOL Multiphysics software are shown elsewhere (Ali, 2021)

The working of COMSOL Multiphysics: 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 develop and execute a multiphysics simulation from start to finish.

The workflow is as follows:

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

Parameters used for the Simulation

The parameters used for the simulation are shown in Table 3.1 and Table 3.2. The use of the parameters for the simulation using the COMSOL Multiphysics is shown elsewhere (Ali, 2021).

Table 3.1: Model parameters for simulation of fixed bed adsorption column (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

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Table 3.2: Model parameters for simulation of fixed bed adsorption column 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
mFein	7e-6[kg/L]	0.007 kg/m ³	Inlet mass concentration of iron in water *
cFein	mFein/MFe	0.043832 mol/m ³	Inlet molar concentration of iron in water *
Tau	1.5[min]	90 s	Residence time *
Fl	(1 - eb)*Vr/tau	0.0079365 m ³ /s	Volumetric flow rate of water
Rr	0.5[m]	0.5 m	Radius of adsorption column
Ar	pi * Rr ²	0.7854 m ²	Cross sectional area of adsorber
Vr	Ar * Lr	1.1905 m ³	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/m ³	inlet molar concentration of water
Vin	Fl/Ar	0.010105 m/s	Inlet velocity of water
Rhob	rhop * (1 - eb)	1260 kg/m ³	Particle bed density
Wb	1500[kg]	1500 kg	Weight of adsorbent bed
Tim	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.

RESULTS AND DISCUSSION

As stated in the introduction, the aim of the study is to employ 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 concentration of ferrous iron along the bed at different times or days, establishing the

operating time of the adsorption unit and the optimum adsorbent dosage. Therefore, this section presents data showing how the aim was achieved in both graphs and content analysis. The solutions to the developed models along with the Langmuir adsorption isotherm were established using the finite element method in COMSOL Multiphysics software.

Graph of Concentration of Ferrous Ion along the Bed at Different Times (Days)

The concentration profile graph is shown in Figure 4.1. The concentration of iron ions was seen decreased exponentially along the length of adsorption column and the decreased for different days were also observed in the simulation. From the graph, it is observed that after 1 day of operation of the adsorption unit, the effluent concentration of iron was very close to zero at the exit of the bed. This was because the bed was still very fresh. After operating the unit for 7 days, it was noticed that, the effluent concentration increased slightly. It is also shown that for the different operating days (i.e., 1 day, 7 days, 14 days, 21 days, 28 days, 35 days, 42 days), it was also noticed that there was a corresponding increased in iron concentration at the end of the bed. The results showed that about 28 days' effective performance of the bed was achieved for a bed weight of 1500kg. Beyond 28 days operating time the effluent concentration of Fe^{2+} exceeded 0.03mol/m^3 , the limit recommended by the WHO. This result agrees with similar results reported by (Ruthven and Douglas, 1984).

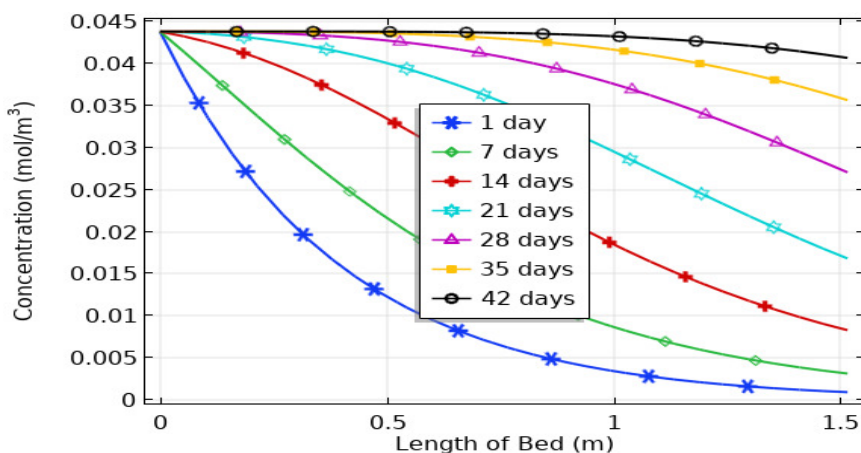


Figure 4.1: Line graph of ferrous iron concentration along the bed at different times.

D Surface Plot of Ferrous Ion Concentration For Different Times (Days)

The performance of the adsorption column, observing it at different days is well represented with a 2D surface plot when computational fluid mechanics tool was used. This is one major contribution of the present work which is new in the literature. The use of computational dynamic tools such as COMSOL Multiphysics gives better insight in the simulation and design of adsorption column. 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 concentration of the iron in the water. Now, as the number of days increased, there was increased intensity of the red colour which means the bed was now filled with iron and ready for regeneration. 2D surface plots showed that the iron concentration of the bed at various times can be observed in Figures 4.4 to Figures 4.10. The surface plot shows the region of the bed that was filled with ferrous ion particles and the region of the bed that is not completely filled. Also, the vertical colour bar by the right-hand side of the different 2D surface plots shows the changing iron concentration along the bed. Simulated result using surface plot indicates that the bed could have maximum adsorption capacity for up to 28 days and at days above 28, the bed must be regenerated. Thus, the surface plot obtained using CFD gave a good insight in the study of adsorption column.

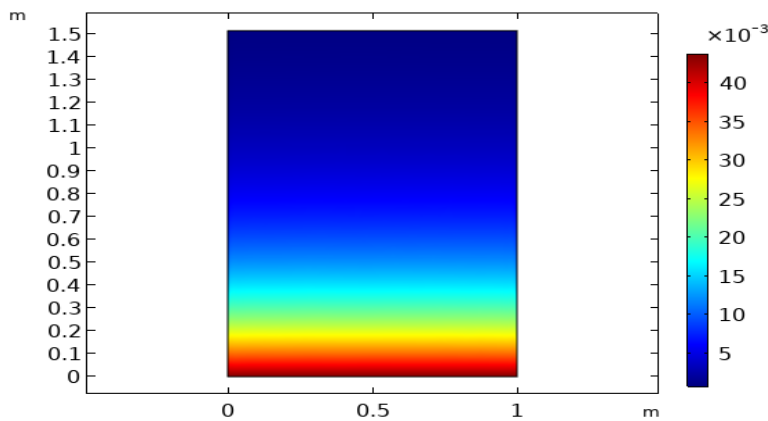


Figure 4.4: 2D surface plot of ferrous iron concentration along the bed at the end of the 1st day.

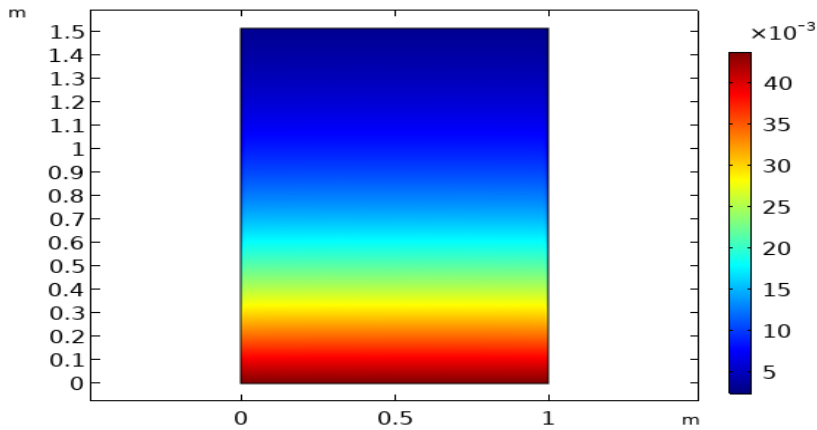


Figure 4.5: 2D surface plot of ferrous iron concentration along the bed at the end of 7 days

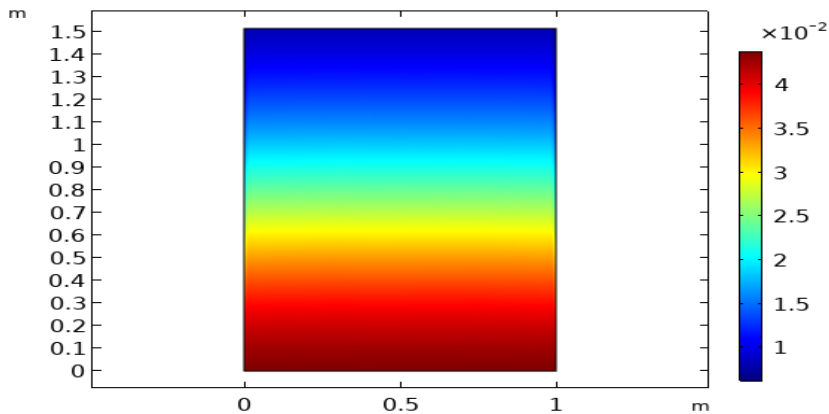


Figure 4.6: 2D surface plot of ferrous iron concentration along the bed at the end of 14 days

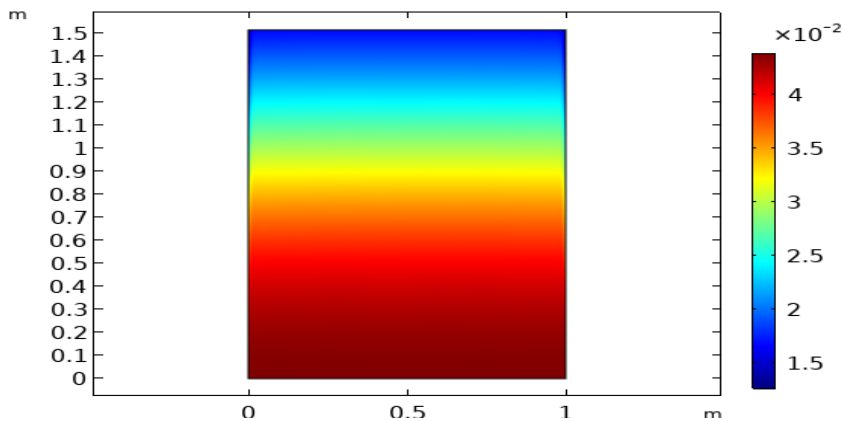


Figure 4.7: 2D surface plot of ferrous iron concentration along the bed at the end of 21 days

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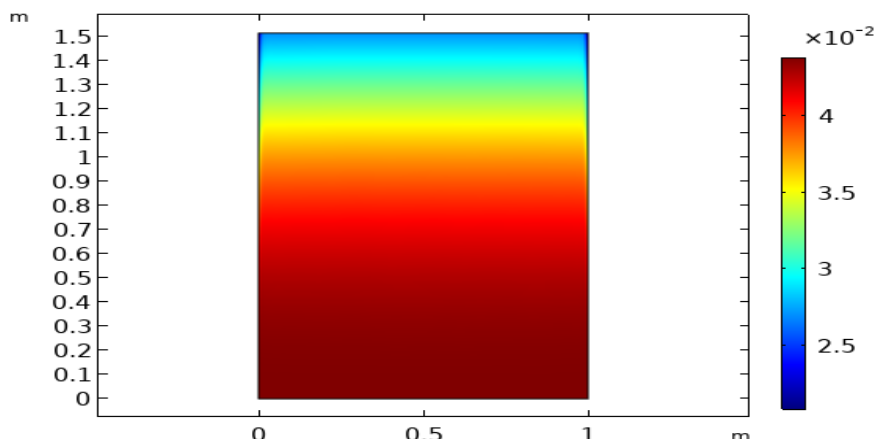


Figure 4.8: 2D surface plot of ferrous iron concentration along the bed at the end of 28 days

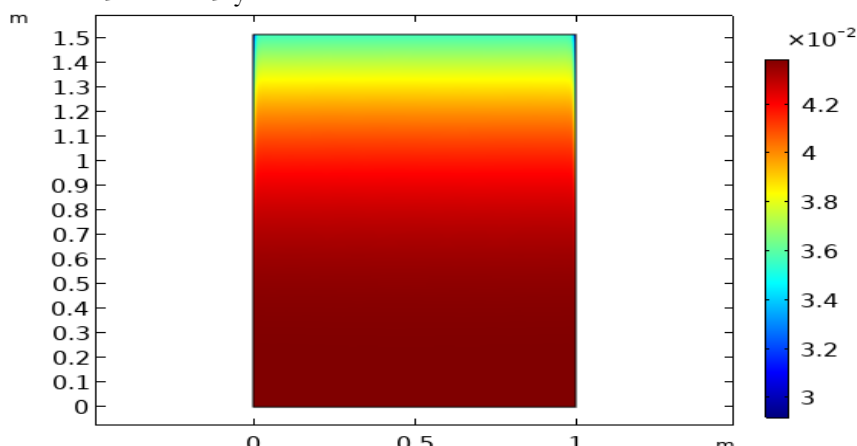


Figure 4.9: 2D surface plot of ferrous iron concentration along the bed at the end of 35 days.

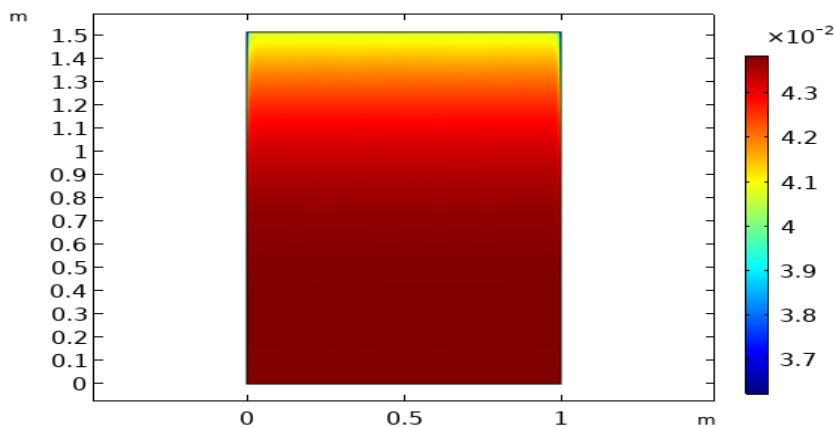


Figure 4.10: 2D surface plot of ferrous iron concentration along the bed at the end of 42 days.

Pressure Drop and Temperature Profile in the Adsorption Column

The pressure drop profile in the bed is shown in Figure 4.11 as a 2D surface plot; it was observed that the pressure drop across the column at constant flow rate condition increased (increasing colour intensity) as the water filtered down the adsorption column. The implication is that at high pressure drops the bed saturation rate is faster. The results conform to similar results presented by (McKay and Hoy, 1999).

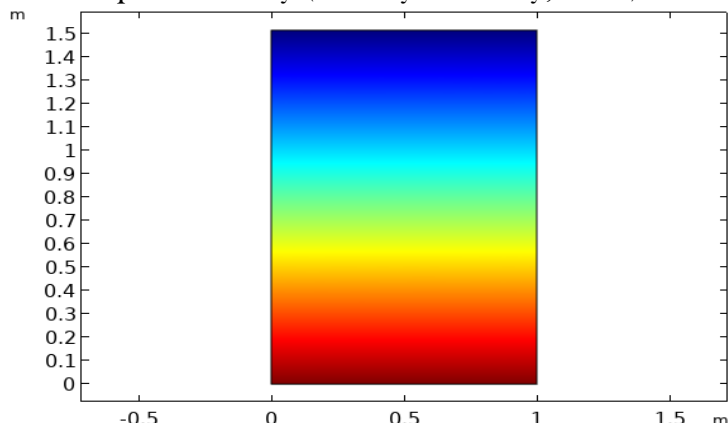


Figure 4.11: 2D surface plot of pressure drop along the bed.

The 2D surface plot of the temperature profile along the bed, presented in Figure 4.12, indicates that the temperature was uniform everywhere within the bed due to the fact that the bed was operated under isothermal conditions (neglecting the effect of temperature variation). It was for this condition the colour intensity of the bed was constant all through. Similar results were obtained by (McKay and Hoy, 1999).

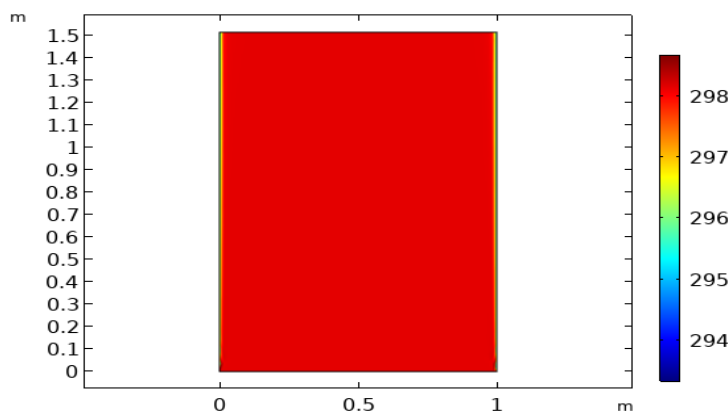


Figure 4.12: 2D surface plot of temperature along the bed

CONCLUSION

Detailed CFD models were developed in COMSOL Multiphysics to provide detailed information about the fixed-bed adsorption column, giving better design insight. Both the line graphs and the 2D surface plots were generated. A 2D model was developed to illustrate the iron concentration distribution for different days, clearly showed the days for which the adsorbent was completely filled with iron.

Simulated results showed that about 28 days optimum performance of the bed was achieved for a bed weight of 1500kg and particle size of 0.001m. The computed effluent iron concentration in the present study for 28 days operating time was approximately equal to 0.028 mol/m^3 . This result when compared with World Health Organization standards for iron concentration (0.003 mol/m^3) in drinking water is acceptable. sed understanding into fixed-bed adsorption studies.

The Study Limitations

One limitation of this work was the selection of small sample size in studying the effect of particle size on the efficiency of the adsorption unit. Centering our study in larger sample size could have produced more perfect results.

The scope and complexity of discussions in this study might have been compromised in many stages compared to the works of the proficient scholars due to lack of many years of experience of conducting researches and producing academic papers of such a large size.

The 2D modeling of the adsorption unit only explains the iron distribution profile in the bed, indicating the days for which the adsorber is ready for replacement or regeneration, but give no account of heat transfer effects.

RECOMMENDATIONS FUTURE WORK

Although very useful results were established for the simulation of the adsorption column model using finite element method in COMSOL Multiphysics, considering only 2D sectional view of the fixed-bed adsorption column, the following are recommendations for future work.

1. The effect of the weight of the bed on the breakthrough curve should be studied with CFD
2. The effect of particle size and adsorption capacity of the bed.

3. Future research should be devoted to the development of the 3D model for both rectangular and cylindrical coordinates in COMSOL Multiphysics. This takes account of the third coordinate, to gain insight into the complex heat exchange and flow path in the sorbent bed during desorption. The 3D modeling is expected to give better results for water purification studies; however, higher computation time and memory would be needed.

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