International Journal of Academic Multidisciplinary Research (IJAMR)
ISSN: 2643-9670
Vol. 10 Issue 2 February - 2026, Pages: 426-433

Purification Of Industrial Waste Water Using Fixed-Bed Column

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Abstract *The implicit backward Euler finite difference scheme was used to develop and numerically solve a mathematical model for a fixed-bed adsorption column. MATLAB R2012a was used to implement the simulations. The work systematically assessed both the design and operational characteristics of the column for the treatment of industrial wastewater and successfully produced the corresponding breakthrough curve. Results from the parametric study indicated that a decrease in bed porosity shortens the solute residence time within the column, thereby improving the adsorption rate. In addition, smaller particle sizes were found to reduce the breakthrough time, whereas higher flow rates led to a more rapid increase in the adsorbate concentration ratio. These behaviors are in close agreement with trends reported in previous studies on similar adsorption processes. The findings demonstrate that the proposed model accurately represents the performance of a fixed-bed adsorption column and is suitable for analyzing its behavior under isothermal conditions.*

Keywords: Metal Contaminants, Fixed-Bed, Adsorption, Wastewater

INTRODUCTION

Heavy metals represent a significant environmental and public health concern due to their persistence, toxic nature, and strong tendency to bioaccumulate. Industrial wastewater has been widely recognized as the main source of heavy metal pollution, thereby necessitating effective treatment before such effluents are discharged into natural water bodies, including rivers, streams, and oceans [1].

In contrast to many other hazardous pollutants, metals are non-biodegradable and readily accumulate within living organisms, often leading to severe health complications and chronic diseases [2]. Beyond environmental considerations, the extraction and recovery of metals from industrial wastewater are also important from both technological and economic viewpoints. Since metals are finite resources and natural reserves are steadily declining, their removal from wastewater offers an opportunity for recycling and reuse in industrial processes. Conventional treatment methods, such as chemical precipitation and oxidation or reduction, can reduce high concentrations of heavy metals in wastewater [3]. Unfortunately, these standard methods often fall short, resulting in treated water that still fails to meet strict environmental standards. To bridge this gap, plants must turn to more advanced, tertiary treatments. These can include processes like ion exchange and adsorption, or sophisticated membrane technologies, from electrolysis and ultrafiltration to nanofiltration and reverse osmosis, that polish the water to a required level of purity.

[4], [5].

Among the available treatment techniques, fixed-bed adsorption is one of the most commonly employed methods for the purification of liquid mixtures, particularly industrial wastewater effluents. Over the past two decades, activated carbon has been extensively utilized in water and wastewater treatment, with its application increasingly extended to large-scale separation processes [6]. Mathematical modeling of adsorption systems plays a vital role in understanding system behavior, as it enables the prediction of breakthrough curves that are widely used in the treatment of industrial wastewater containing organic contaminants [7]. The effective design of fixed-bed adsorption systems requires comprehensive knowledge of adsorption kinetics and bed dynamics.

The modeling and performance evaluation of fixed-bed adsorption columns have been studied by a number of researchers. An isothermal adsorption column loaded with porous spherical particles and exposed to a step change in the intake solute concentration was examined by Raghavan et al. [8]. In their study, liquid-solid equilibrium was represented by a linear isotherm, and the governing equations were solved using the orthogonal collocation method after being simplified by a set of assumptions. Similar to this, Suresh et al. [9] developed a kinetic model that incorporated axial fluctuations in fluid velocity down the column, internal and external mass-transfer resistances, and deviations from ideal plug flow to assess the impact of key operating factors on fixed-bed adsorption behavior.

Industrial wastewater discharge continues to be a major source of water pollution worldwide. Over the past century, substantial quantities of industrial effluents have been released into rivers, lakes, and coastal regions, resulting in serious environmental degradation and adverse effects on ecosystems and human health [5]. Globally, pollution arising from food-processing and related industries has become a serious threat to plants, animals, and ultimately the quality of human life [10]. A well-documented example is the Minamata disease incident in Japan in 1956, which was caused by the discharge of industrial effluents contaminated with methyl mercury and resulted in severe neurological damage and fatalities [10]. In addition, the rate of industrial wastewater generation is reported to be higher in developing countries, such as Nigeria, than in developed nations [11].

These observations suggest that the burden of industrial wastewater pollution has gradually shifted from developed to developing regions. As a result, the increasing demand for clean and safe water necessitates the development of efficient, reliable, and sustainable treatment technologies capable of ensuring environmentally safe effluent discharge. Physico-chemical treatment methods, particularly fixed-bed adsorption columns, have demonstrated considerable effectiveness in addressing these challenges.

The design and operation of a fixed-bed adsorption column for the removal of hazardous metals from industrial wastewater are made simple and practical by this study. This kind of wastewater poses major threats to public health and ecosystems if left untreated. The study methodically investigates the effects of important operational parameters on the breakthrough behavior of the column, such as flow rate, adsorbent particle size, and bed porosity. The results provide engineers and operators with useful information to maximize the effectiveness and practical implementation of these crucial treatment systems by illustrating the impact of these parameters.

DEVELOPMENT OF MATHEMATICAL MODEL

In this work, a mathematical model of a fixed-bed adsorption column is created by carefully taking into account important variables that influence its performance, especially the fluid velocity variation along the bed. This variation is crucial to the column's operation and design. The resulting model can be used to treat a variety of pollutants, including organic compounds and inorganic contaminants like metal ions. It also offers a useful means of comprehending and forecasting the dynamic behavior of fixed-bed adsorption systems.
Currently, numerous mathematical models exist for describing and predicting the breakthrough characteristics of adsorption columns operating in either liquid or gaseous phases. In the case of a liquid–solid adsorption column, the modeling procedure generally involves decomposing the overall process into four basic steps [13]:
1. Mass transfer in the liquid phase, including molecular diffusion and convective mass transfer,
2. Interface diffusion (also known as film diffusion) between the liquid phase and the adsorbent's exterior surface,
3. Intra-pellet mass transfer involving surface and pore diffusion, and
4. The adsorption-desorption process To create a mathematical model to explain the dynamics of a fixed bed adsorption column, let's look at Fig. 1.

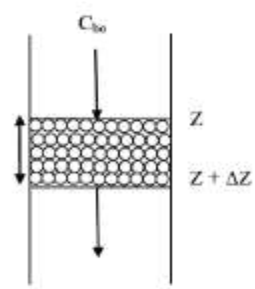

Fig. 1: Mass Balance in the Elements of a Fixed Bed

From the principle of conservation of mass to fluid and pore phases in the column; we have:

Rate of material in − Rate of material out
± Rate of material generation by adsorption
= Rate of material accumulation.

The following presumptions guided the development of the system's mathematical model:

1. It is assumed that the system functions in an isothermal (constant temperature) environment.
2. A non-linear Langmuir isotherm is used to depict adsorption equilibrium.
3. The pore diffusion coefficient, DPD_PDP, is a measure of the mass transfer that takes place within the adsorbent particles by Fickian diffusion.
4. Mass transfer resistance in the fluid film surrounding the particles is described using the external film mass transfer coefficient, RRR.
5. The adsorbent particles are thought to be spherical, homogeneous in density, and uniform in size.
6. An axial dispersion plug flow technique is used to represent fluid flow through the bed.

7. It is assumed that the axial fluid velocity will not change during the bed's length.
8. A pseudo single-component adsorption technique is applied to the system.

These assumptions simplify the modeling process while capturing the essential behavior of the fixed-bed adsorption system, making it practical for simulation and design analysis.

Material Balance for Adsorption Column

Subject to the assumptions above, the following parameters can be deduced from the system:

a. Convective Mass transfer across the boundary layer is given by: -

$$U\frac{\partial C_b}{\partial z}$$

Where; Z = Axial coordinate, m, C_b = Adsorbate concentration in the mobile phaseU = Superficial Velocity, ms-1 , mgL-1,

b. Axial dispersion is given by:

$$D_L\frac{\partial^2 c_b}{\partial z^2}$$

Where; DL = Axial dispersion coefficient, m2s-1

$$\varepsilon\frac{\partial c}{\partial t}+ u\frac{\partial c}{\partial z}+(1-\varepsilon)\rho_a\frac{\partial q}{\partial t}= D_2\frac{\partial^2 c}{\partial z^2}$$

Where initial and boundary conditions are:

$$t=0\rightarrow C(=,t)=0$$
$$t=0\rightarrow q(=,t)=0$$
$$z=0\rightarrow c_b(0,t=,0),c_b(0,t>0)= c_{bo}$$
$$z=H\rightarrow\frac{\partial C}{\partial z}=0$$

When the axial dispersion is ignored, equation 1 becomes:

$$\varepsilon\frac{\partial c}{\partial t}+ u\frac{\partial c}{\partial z}+(1-\varepsilon)\rho_3\frac{\partial q}{\partial t}= 0$$

The initial and boundary conditions turn to:

$$t=0\rightarrow C(z,t)=0$$
$$z=0\rightarrow c_b=c_{bo}+\frac{D_{zz}\partial c_b}{\partial z}$$
$$z=H\rightarrow\frac{\partial C}{\partial z}= 0$$

Where H is the bed height, ε is the bed porosity, p_o or p_p the particle or adsorbent density, t is the time, C_{bo},

c. Materials absorbed by the adsorbent is given by:

$$(1-\varepsilon)\rho_a\frac{\partial q_t}{\partial t}$$

Where; , t = Time, sec p_a = Density of adsorbent or particle, kgm-3,ε = Bed porosity, q_t = Average solid phase adsorbate concentration, mgg-1

d. Accumulation of the adsorbate is given by:

$$\varepsilon\frac{\partial c_b}{\partial t}$$

Using the previously outlined principle of mass conservation, an overall material balance for the column may be determined based on the four groups of factors mentioned above. Equation (1) is the result of this method.

Consequently, the following expression [6] represents the material balance for the fluid phase inside the adsorption column:

$$-D_L\frac{\partial^2 C_b}{\partial z^2}+U\frac{\partial C_b}{\partial t}+\frac{\partial C_b}{\partial t}+\left(\frac{1-\varepsilon}{\partial t}\right)t_3\frac{\partial q_1}{\partial t}=0$$

We can introduce some dimensionless variables for conveniences as shown below;

$$\widetilde{C_b}=\frac{C_b}{C_{bo}},X=\frac{z}{L},\tau=\frac{Ua^t}{L},\breve{q_\tau}= q_\tau,\breve{u}=\frac{u}{u_a}$$

Substitute the dimensionless variables into the equation (2), we have:

$$\frac{1}{\rho_t}\frac{\partial^2\bar{C}_3}{\partial x^2}+\frac{\overline{\partial C}_3}{\partial x}+\frac{\overline{\partial C}_3}{\partial x}+\left(\frac{1-\varepsilon}{\varepsilon}\right)\frac{t_3}{C_b}\frac{\bar{q}}{\partial y}=0$$

where, $P_e = Peclet\ number\ \frac{ul}{D_L}$

The interphase mass transfer rate may be expressed in terms of the concentration driving force across the bounding film to give:

$$l_3 \frac{\partial q_1}{\partial f} = \frac{3k_f}{a_f}(c_3 - c_1)$$

Where; $l_3(1 - \varepsilon_f)l_2$

Substituting equation (4) into (5) gives

$$\frac{\partial q}{\partial t} = 3\frac{k_f(1-\varepsilon_p)}{l_p a_p}$$

Introducing the appropriate dimensionless variables stated above, we have:

$$\frac{\partial \bar{q}}{\partial t} = \frac{3k_f L(1-\varepsilon_P)}{U_l a_p l_f} c_{bo}\left(\bar{c}_b - \frac{c_f}{c_{bo}}\right)$$

The adsorption equilibrium is described by Langmuir Isotherm [9]:

$$q_1 = \frac{q_m bc}{1+bc}$$

Where (fluid phase concentration in equilibrium with on the surface of the pellet

After re-arrangement and substitution of for c, equation 8 becomes:

$$c_3 = \frac{q_1}{(q_m b - q_1 b)}$$

Put equation 9 into equation 3, we have:

$$\frac{1}{\rho_e}\frac{\partial^2 c_b}{\partial x^2} + \frac{\partial \bar{c}_b}{\partial x} + \frac{\partial \bar{c}_3}{\partial x} + \frac{3k_f L(1-\varepsilon_F)}{\partial z}\left(\bar{\varepsilon}_b - \frac{q_1}{c_{bo}(q_{mb} - q_{cb})}\right) = 0$$

Initial and boundary condition The initial and boundary condition to be employed for fluid phase model are: Initial condition:

$$\tau \le 0, X = 0, \bar{c}_b = 1$$
$$\tau < 0, 0 < X < L_{t,}\bar{c}_b = 0$$

Boundary condition:

$$1 - \bar{c}_b + \frac{1}{P_f}\frac{\partial \bar{c}_b}{\partial x} = , X = 0, \tau > 0$$
$$\frac{\partial \bar{c}_b}{\partial x} = 0, X = L, \tau \ge 0$$

Material Balance for Pore Diffusion Control Phase [10]: Subject to the aforementioned assumptions and equation 1, the material balance for diffusion into spherical pellet is written.

Differentiating the left-hand side term, we have:

$$\frac{D_l}{r^2}\varepsilon_p\left[\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}\right] = \varepsilon_p\frac{\partial c}{\partial t} + (\varepsilon_p)l_p\frac{\partial_f}{\partial t}$$

Assuming instantaneous equilibrium

$$\frac{\partial q}{\partial t} = \frac{\partial c}{\partial t} x \frac{\partial q}{\partial c}[1]$$

By substitution and rearrangement, we have:

$$D_l\varepsilon_p\left[\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}\right] = \frac{\partial c}{\partial t}[+(1-\varepsilon_p)l_p\frac{\partial_q}{\partial c}]$$
$$\frac{\partial c}{\partial t} = \frac{1}{\left[1 + l_p\left(\frac{1-\varepsilon_p}{\varepsilon_p}\right)\frac{\partial q}{\partial c}\right]} D_f\left(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}\right)$$

Where is the derivative of adsorption isotherm differentiating Langmuir Isotherm (equation 8).

$$\frac{\partial q}{\partial c} = \frac{q_m b}{(1+bc)^2}$$

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Substituting equation 19 into equation 18, we have;

$$\frac{\partial c}{\partial t} = \frac{1}{\left(1 + l_p(\frac{1 - l_p}{\varepsilon_p}) \frac{q_m b}{(1 + bc)^2}\right)} D_l \left(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}\right)$$

The diffusion-controlled model is described by equation (19). The proper beginning and boundary conditions were established for this kind of numerical problem.

The mathematical model developed to assess the fixed-bed adsorption system's performance under isothermal operating conditions is shown in equation (20).

RESULTS AND DISCUSSION

The implicit backward Euler finite-difference approach was used to solve the system of partial differential equations given in Equations (1)–(20) numerically by converting them into a set of ordinary differential equations. This strategy was used to deal with the model's non-linear adsorption isotherm. Because of its numerical stability and compatibility with the specified boundary conditions, the finite-difference technique was chosen.

To solve the resulting coupled equations, a computational approach was created in MATLAB and put into practice as a simulation software. The simulations' model parameters were taken from Crittenden and Weber [14]. To evaluate their impact on fixed-bed adsorption performance, important operating factors such particle diameter, bed porosity, initial solute concentration, and fluid flow rate were methodically changed.

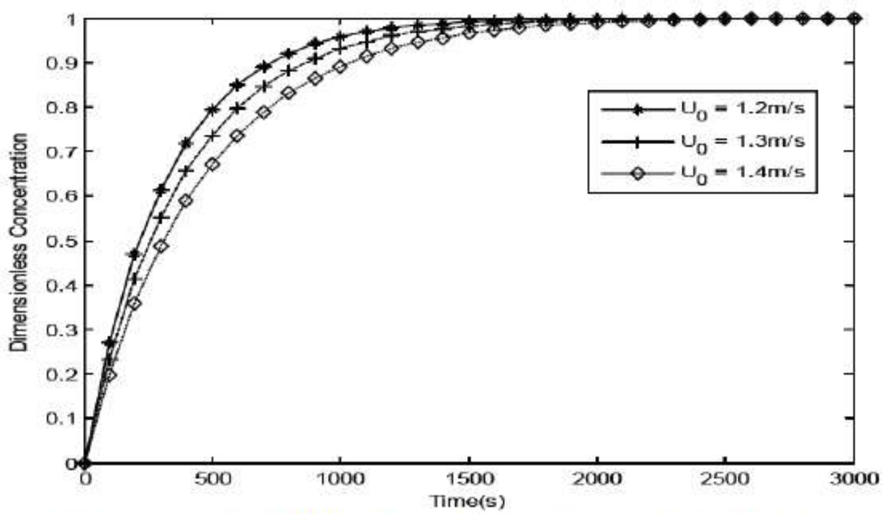

Fig. 1: Effect of Fluid Flow Rate on Simulated Breakthrough Curve \

With all other operating variables held constant, Figure 1 displays the results achieved at three different input flow rates. The breakthrough curve becomes visibly steeper as the flow rate rises, suggesting that the adsorbate exits the column before equilibrium is fully reached. Higher flow rates also shorten the time to reach bed saturation because the adsorption bed has a set saturation capacity under the same driving power.

Therefore, a key factor in the design and operation of fixed-beds is the wastewater flow rate through the adsorption column. It is important to carefully optimize operating parameters because increasing the flow rate typically results in a decrease in the overall removal effectiveness of pollutants. Furthermore, it is noted that when the flow rate increases, the time corresponding to the column's stoichiometric capacity decreases.

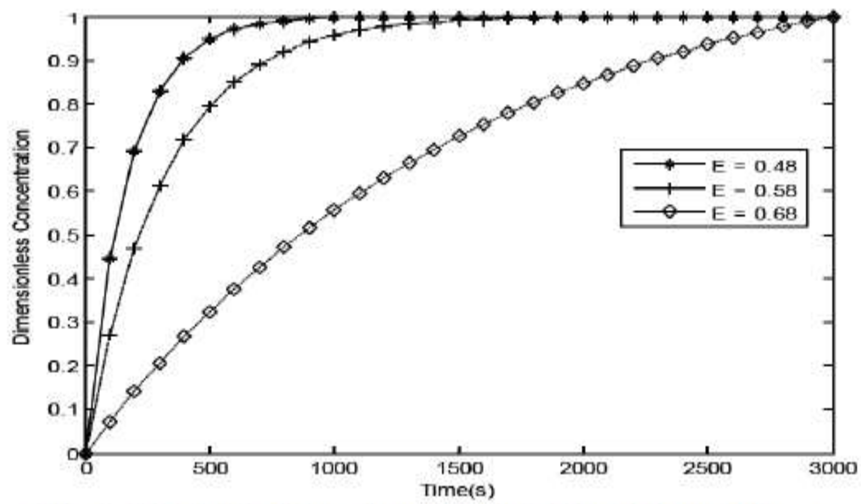

Fig. 2: Effect of Bed Porosity on Simulated Breakthrough Curve

Increasing the bed porosity results in a flatter breakthrough curve, which shows a decrease in the solute removal efficiency of the column (Figure 2). Lower bed porosity, on the other hand, lengthens the solute's contact time within the bed, increasing the adsorption rate and boosting the column's overall effectiveness.

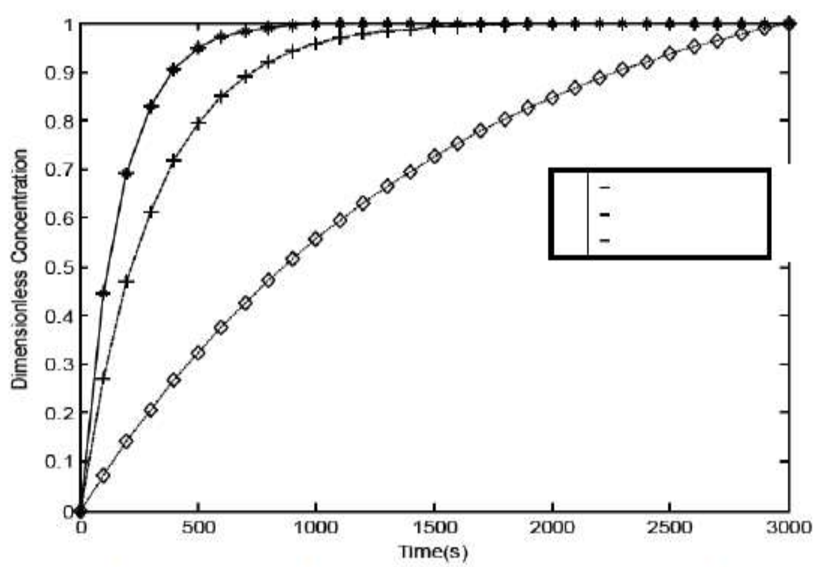

Fig. 3: Effect of Particle Diameter on Simulated Breakthrough Curve

The breakthrough curve becomes less steep as the particle radius increases, as seen in Figure 3. This implies that, especially at high linear velocities, smaller particles have a higher breakthrough capacity because they attain kinetic equilibrium more quickly. Larger particles, on the other hand, lengthen the internal diffusion path within the pores and form a thicker stationary film around each particle, which slows overall adsorption kinetics since it takes longer for adsorbate molecules to reach active sites.

For example, the breakthrough time along the bed is 1325 seconds (a 17% change) when the particle radius is 3.1×10^{-2} m. The percentage changes in breakthrough time increase to 22% and 29%, respectively, for particle radii of 4.1×10^{-1} m and 6.1×10^{-1} m. These findings demonstrate that the impact of velocity fluctuations on the breakthrough curve grows with particle size.

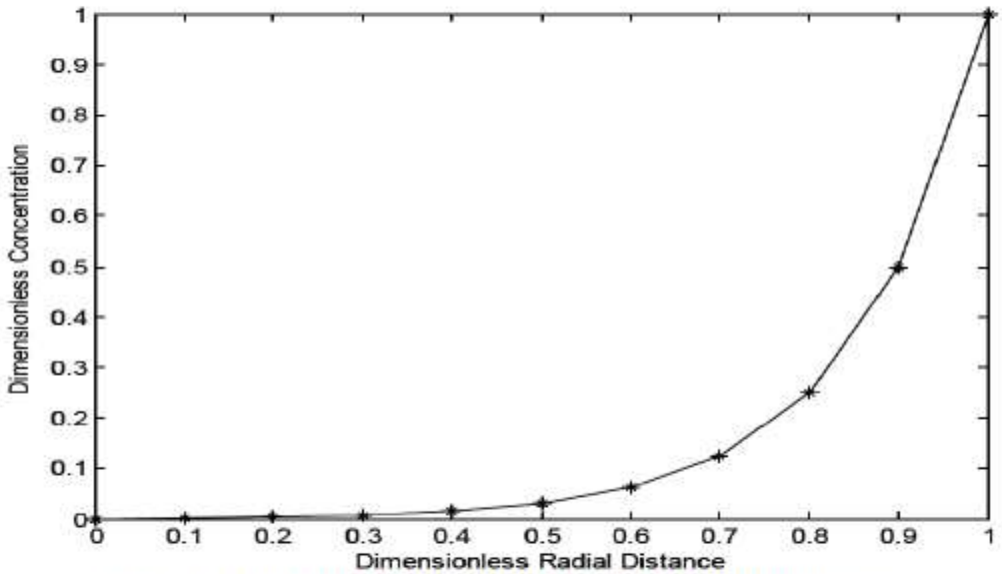

Fig. 4: Concentration Profile of Metal Contaminants

The model's capacity to forecast the outflow adsorbate concentration at different radial points within the bed is demonstrated in Figure 4. The plot, which is based on simulation data and shows dimensionless concentration against dimensionless radial distance, shows that the solute concentration inside the pores increases as the adsorption process progresses. This behavior shows how well the model captures the adsorbate's internal distribution and movement along the column while it is operating.

CONCLUSIONS

This study showed that a consistent and unified formulation of equations across different breakthrough curve models is made possible by the inclusion of dimensionless variables. The development and evolution of the concentration front were successfully examined before reaching steady state by numerically solving the associated systems of partial differential equations in MATLAB. These results provide important information for evaluating breakthrough curves when employing activated carbon-based filters to remove metal ion pollutants.

Using MATLAB R2012a, a mathematical model of a fixed-bed adsorption column was created and numerically solved using the implicit backward Euler finite-difference approach. According to parametric analysis, smaller particle sizes result in shorter breakthrough durations, while decreasing bed porosity shortens the solute residence time and increases the adsorption rate. On the other hand, raising the flow rate causes the adsorbate concentration at the column output to rise more quickly. These findings support earlier research, demonstrating the validity and suitability of the suggested methodology for assessing fixed-bed adsorption performance in isothermal settings. Furthermore, the model can be expanded in further studies to investigate non-adiabatic and non-isothermal systems.

The design and operation of fixed-bed adsorption columns for the removal of contaminants from industrial wastewater were also covered in this work, which provided a useful method for creating breakthrough curves. The following are some ways that the findings advance knowledge:

1. A steeper breakthrough curve indicates improved removal efficiency when the bed porosity is lowered, while a higher porosity results in decreased efficiency.
2. The amount of removal and total adsorption efficiency are decreased when the influent flow rate is increased because the adsorbate leaves the column before equilibrium is reached.
3. As illustrated in Figure 4, the study showed a strong relationship between dimensionless concentration and dimensionless radial distance, providing important information about the solute distribution inside the adsorption bed.

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