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Simulation-Based Kinetic Analysis of a Packed Bed Adsorption Column using Aspen Adsorption

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ABSTRACT: Packed bed adsorption columns are commonly used for the removal of pollutants from liquid streams due to their simplicity and high efficiency. Understanding the adsorption kinetics and breakthrough behaviour is important for the proper design and operation of these systems. In this study, a simulation-based kinetic analysis of a packed bed adsorption column was carried out using Aspen Adsorption software. A dynamic model of the adsorption column was developed by defining the column geometry, adsorbent properties, and operating conditions. The Freundlich isotherm model was used to describe adsorption equilibrium, while the Linear Driving Force (LDF) model was applied to represent adsorption kinetics. Breakthrough curves were generated to study the variation of outlet concentration with time and to evaluate column performance. The simulation results showed that adsorption efficiency is strongly affected by operating parameters. An increase in flow rate led to earlier breakthrough due to reduced contact time, whereas increasing bed height delayed breakthrough and improved adsorption capacity. The outlet concentration of the target contaminant was reduced to very low ppm levels, indicating effective removal by the adsorbent. The system operated under stable temperature and pressure conditions, confirming isothermal operation and negligible pressure drop. This study demonstrates that Aspen Adsorption is an effective tool for predicting adsorption behaviour and optimizing packed bed adsorption columns, reducing the need for extensive experimental work and supporting process design and scale-up for water treatment applications.

KEYWORDS: Packed bed adsorption, Aspen Adsorption, Kinetic study, Breakthrough curve, Mass transfer

I. INTRODUCTION

Water and wastewater treatment is a major challenge due to the increasing discharge of pollutants from industrial and urban activities. Contaminants such as heavy metals, dyes, and inorganic ions present in liquid streams pose serious risks to human health and the environment, even at low concentrations. Among the various separation techniques available, adsorption has emerged as one of the most effective and widely used methods for removing such pollutants because of its high removal efficiency, operational simplicity, and economic feasibility. Packed bed adsorption columns are commonly employed in industrial applications for continuous purification of liquid streams. In these systems, the adsorbent is fixed inside a column, and the contaminated fluid flows through the bed, allowing the target species to be retained on the adsorbent surface. The performance of a packed bed adsorption column is strongly influenced by adsorption kinetics, mass transfer mechanisms, and operating conditions such as flow rate, inlet concentration, and bed height. Accurate prediction of breakthrough behaviour and adsorption capacity is therefore essential for proper design, operation, and scale-up of these columns. Experimental studies provide valuable insights into adsorption behaviour; however, they are often time-consuming, costly, and limited in their ability to explore a wide range of operating conditions. To overcome these limitations, process simulation tools have become increasingly important in adsorption research. Aspen Adsorption is a specialized simulation software that allows detailed dynamic modelling of adsorption processes by incorporating adsorption isotherms, kinetic models, and transport phenomena. In the present study, a simulation-based kinetic analysis of a liquid-phase packed bed adsorption column is carried out using Aspen Adsorption software. The focus of this work is to understand the dynamic adsorption behaviour, analyse breakthrough characteristics, and evaluate the effect of key operating parameters on column performance. The outcomes of this study

demonstrate the usefulness of simulation-based approaches for predicting adsorption behaviour, optimizing operating conditions, and supporting the design and scale-up of packed bed adsorption systems for water treatment applications.

II. LITERATURE REVIEW

Packed bed adsorption is a widely used separation technique for the removal of pollutants from liquid and gas streams due to its simplicity, high efficiency, and continuous operation. Numerous studies over the past decades have focused on understanding the dynamic behaviour of packed bed adsorption columns, particularly adsorption kinetics, mass transfer mechanisms, and breakthrough characteristics. One of the earliest studies was reported by Bohart and Adams (1920), who established a relationship between bed depth and service time, demonstrating the strong influence of bed height on adsorption performance. This model laid the foundation for fixed-bed adsorption design, although it assumed simplified kinetic behaviour. Later, Thomas (1944) developed a kinetic model for adsorption in flowing systems, which has been extensively used to predict breakthrough curves and estimate adsorption capacity in packed bed columns. Despite its wide application, the Thomas model assumes plug flow conditions and neglects axial dispersion effects. To simplify breakthrough prediction, Yoon and Nelson (1984) proposed a model that describes outlet concentration behaviour using only two parameters. Although easy to apply, this model does not explicitly account for mass transfer resistance or intraparticle diffusion, limiting its applicability for detailed kinetic analysis. A comprehensive theoretical understanding of adsorption processes was provided by introduced the intraparticle diffusion model and demonstrated that adsorption often occurs in multiple stages. Further studies by Han et al. (2001) confirmed that both external film resistance and internal pore diffusion significantly influence adsorption kinetics, especially in liquid-phase systems where diffusivity is relatively low.

Ruthven (1984), who emphasized the role of equilibrium relationships, kinetic rate expressions, and mass transfer phenomena such as film diffusion and pore diffusion in packed bed systems. The importance of diffusion-controlled adsorption was highlighted by Weber and Morris (1963), who introduced the intraparticle diffusion model and demonstrated that adsorption often occurs in multiple stages. Further studies by Han et al. (2001) confirmed that both external film resistance and internal pore diffusion significantly influence adsorption kinetics, especially in liquid-phase systems where diffusivity is relatively low.

III. METHODOLOGY

A. Simulation Tool

The packed bed adsorption column was simulated using Aspen Adsorption software to analyse the dynamic adsorption behaviour of the system.

B. Column Model

A cylindrical packed bed adsorption column operating under plug flow conditions was considered. A contaminated liquid stream with a constant inlet concentration was fed continuously into the column at a fixed flow rate.

C. Adsorption Models

The Freundlich isotherm model was used to describe adsorption equilibrium, while the Linear Driving Force (LDF) model was applied to represent adsorption kinetics and mass transfer effects.

D. Operating Conditions

The simulation was carried out under isothermal conditions with negligible pressure drop across the adsorption bed.

E. Breakthrough Analysis

Breakthrough curves were obtained by plotting the ratio of outlet concentration to inlet concentration (C/C_0) as a function of time.

F. Parametric Study

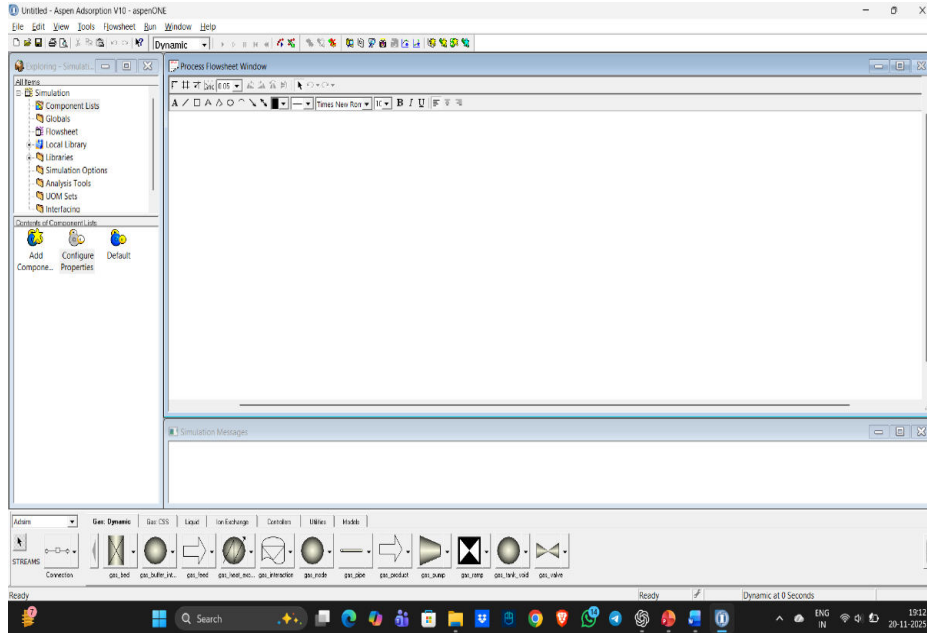
Key operating parameters such as flow rate and bed height were varied to evaluate their effect on adsorption performance and breakthrough behaviour.

IV. EXPERIMENTAL PROCEDURE

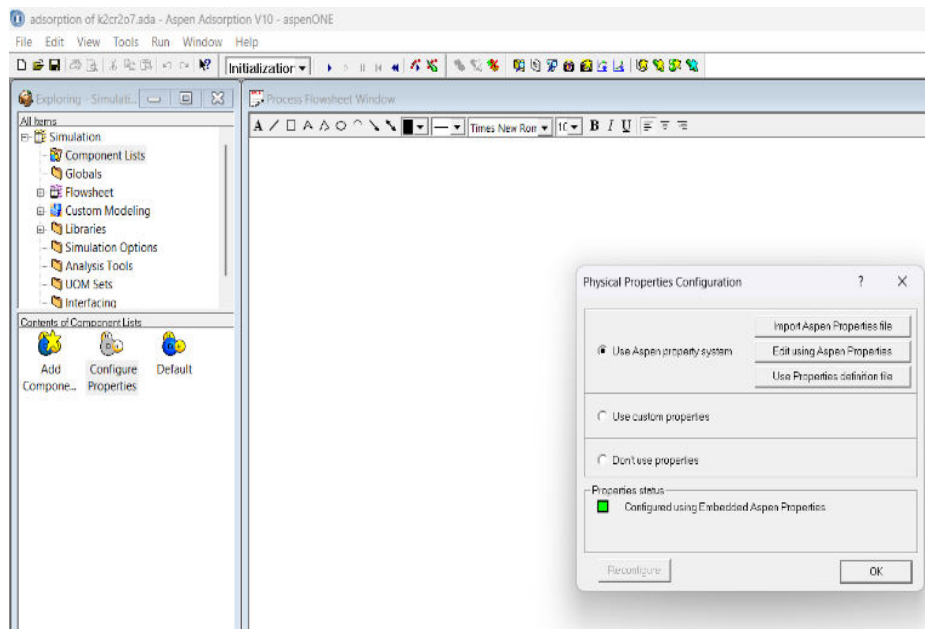
The experimental procedure was carried out using Aspen Adsorption software by developing a virtual packed bed adsorption column by Removing $K_2Cr_2O_7$ From Industrial Wastewater. The simulation setup, including flowsheet configuration, column specifications, and operating conditions, is shown through screenshots. Dynamic simulations were performed to obtain breakthrough curves and analyse adsorption performance.

1. Open Aspen Adsorption software

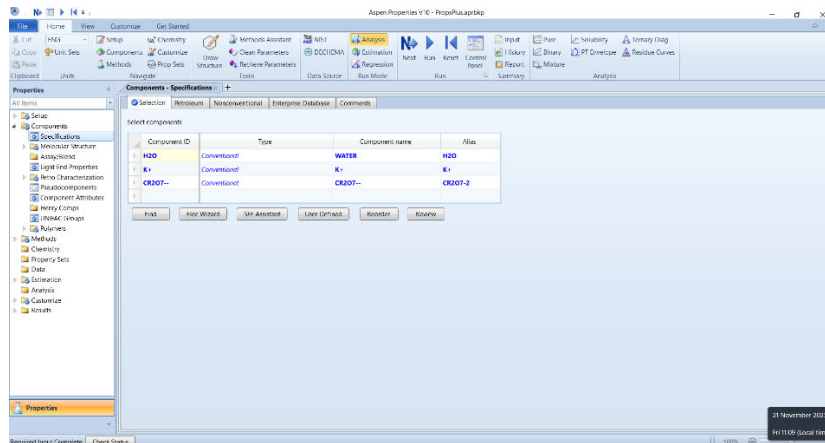
Double click on aspen adsorption software icon or search ‘aspen adsorption’ in windows search bar



2. Add Components

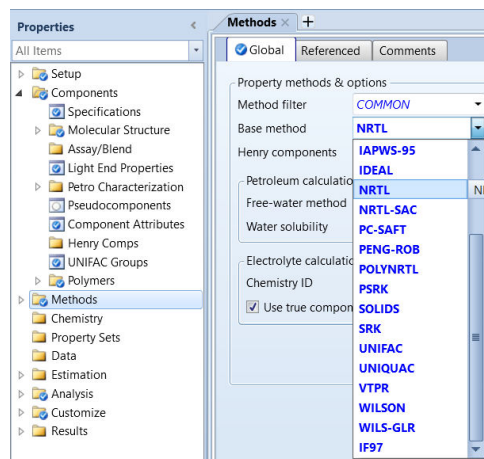


Click on ‘configure properties’ option from ‘component lists’ tab in explorer window, then click edit using aspen properties’

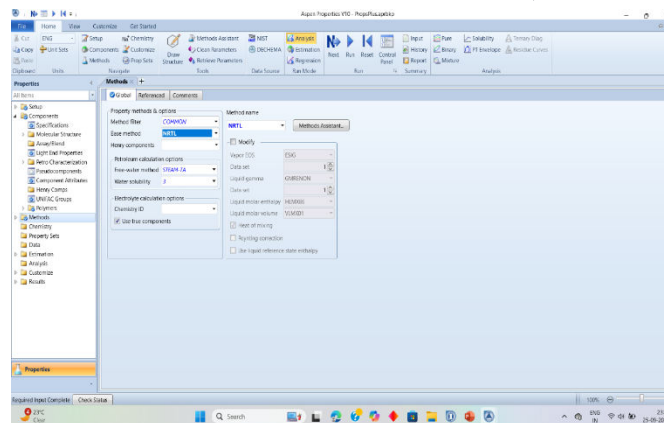


The required components (H₂O, K⁺, Cr₂O₇²⁻) were added in Aspen by selecting them from the built-in component database.

3. Add Property Method



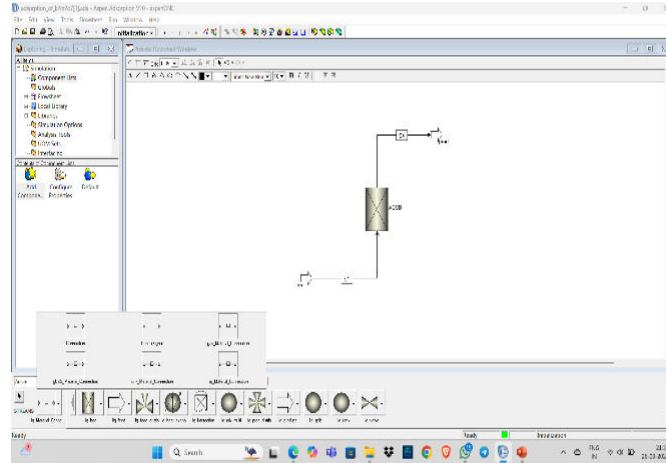
A suitable thermodynamic property method ‘NRTL’ was selected as base method



Save and exit aspen properties window, and return to aspen adsorption software window

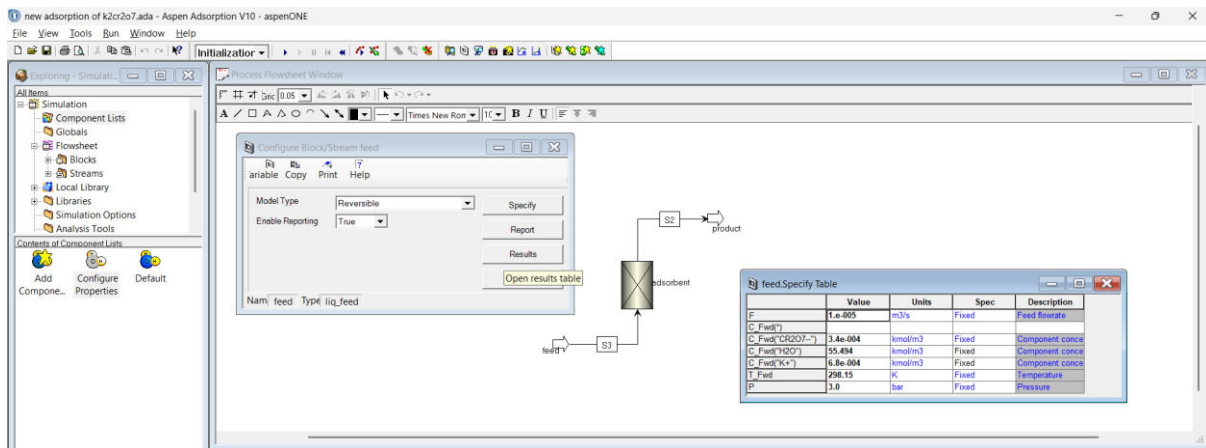
4. Flowsheet Preparation

insert the adsorber unit – ‘Liquid bed’ from model library and Connect inlet and outlet material streams



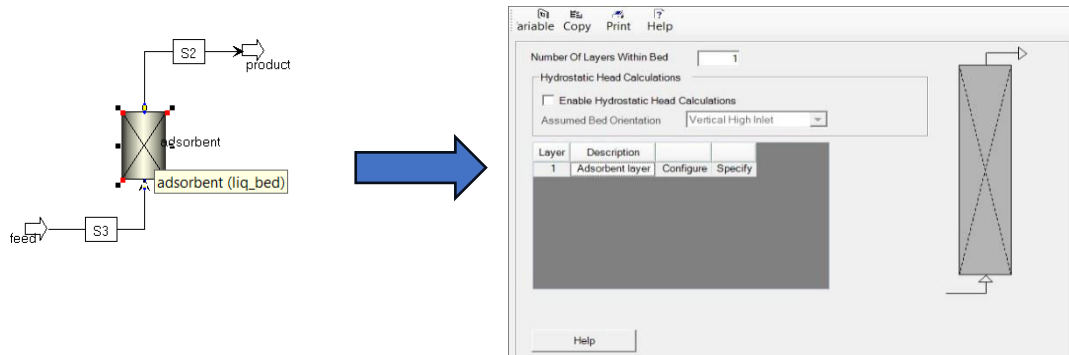
5. Input feed parameters

Input feed specifications like flowrate, feed composition, Temperature, Pressure by double clicking on the liquid feed block



6. Adsorption column inputs

Double click on adsorbent bed to open configure block window



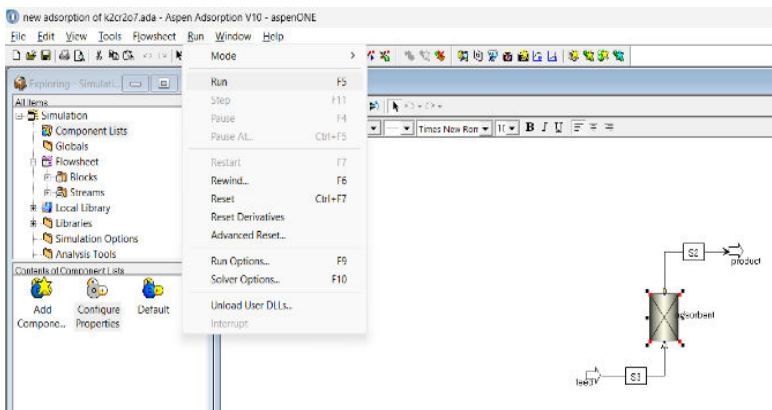
7. Adsorbent bed inputs

Specify adsorbent bed parameters like height of adsorbent layer, internal diameter of adsorbent layer, Inter-particle void age, solid density, Constant Mass transfer coefficient, Isotherm Parameter etc.

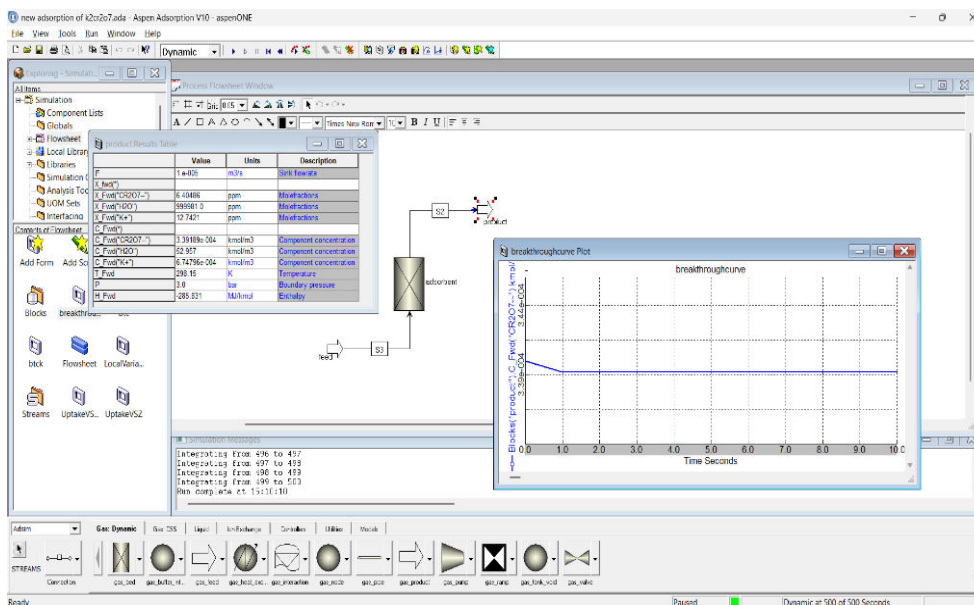
	Value	Units	Description
Hb	5.0	cm	Height of adsorbent layer
Db	1.0	cm	Internal diameter of adsorbent layer
Ei	0.4	m ³ void/m ³ bed	Inter-particle voidage
RHOs	1800.0	kg/m ³	Solid density
Ez(")			
Ez("CR2O7--")	1.e-005	m ² /s	Constant Dispersion Coefficient
Ez("H2O")	1.e-005	m ² /s	Constant Dispersion Coefficient
Ez("K+")	1.e-005	m ² /s	Constant Dispersion Coefficient
MTC(")			
MTC("CR2O7--")	1.0	1/s	Constant mass transfer coefficients
MTC("H2O")	1.0	1/s	Constant mass transfer coefficients
MTC("K+")	1.0	1/s	Constant mass transfer coefficients
IP(")			
IP(1,"CR2O7--")	0.2	n/a	Isotherm parameter
IP(1,"H2O")	1.0	n/a	Isotherm parameter
IP(1,"K+")	0.1	n/a	Isotherm parameter
IP(2,"CR2O7--")	0.25	n/a	Isotherm parameter
IP(2,"H2O")	1.0	n/a	Isotherm parameter
IP(2,"K+")	0.33	n/a	Isotherm parameter
Direction	0.0	n/a	Specified flow direction

8. Running the simulation

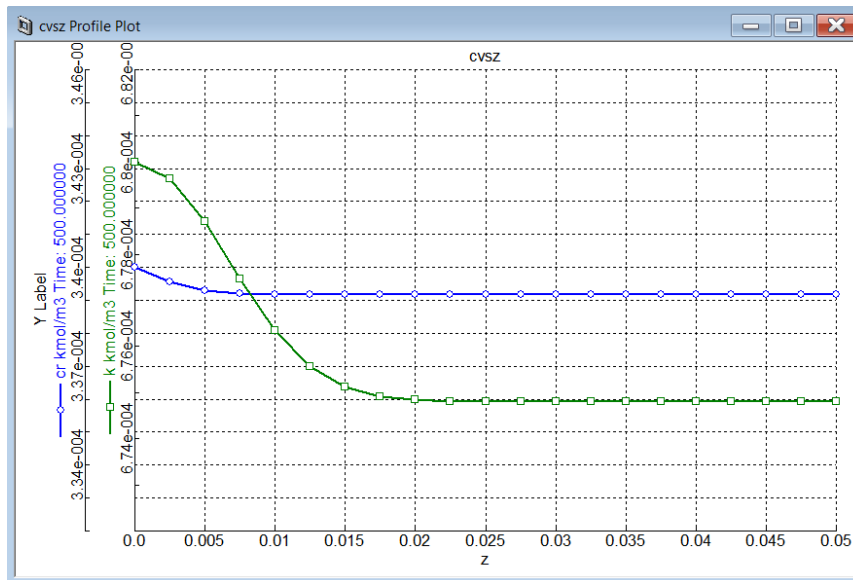
Select 'Initialization' as run mode and then 'Run' the simulation from Run tab as shown below



V. RESULTS AND DISCUSSION



The dynamic simulation of the packed bed adsorption column was successfully carried out using Aspen Adsorption V10, as shown in the process flowsheet and result windows. The simulation represents the adsorption of $K_2Cr_2O_7$ from an aqueous solution in a packed bed adsorber operating under liquid-phase conditions. The product stream results indicate a significant reduction in the concentration of the target contaminant after passing through the adsorption column. The outlet concentration of dichromate ions was reduced to a low ppm level, demonstrating effective adsorption by the packed bed. The stable values of temperature and pressure in the product stream confirm that the system operated under isothermal conditions with negligible pressure drop, which is desirable for liquid-phase adsorption process. The breakthrough curve, plotted as outlet concentration versus time, shows a rapid initial decrease followed by a nearly constant concentration profile over the simulated time period. This behaviour indicates that the adsorption bed had sufficient capacity and that the mass transfer zone was well developed within the column. The absence of a sharp breakthrough within the simulation time suggests that the bed was not fully saturated, confirming efficient utilization of the adsorbent. Overall, the simulation results are consistent with adsorption theory and previously reported studies. The generated breakthrough behaviour validates the selected kinetic and equilibrium models and confirms the suitability of Aspen Adsorption software for predicting the dynamic performance of packed bed adsorption columns. These results highlight the effectiveness of simulation-based analysis for understanding adsorption behaviour and optimizing column design without extensive experimental trials.



The CVSZ profile plot illustrates the variation of solute concentration along the axial length of the packed bed adsorption column at a simulation time of 500 seconds. The axial position (Z) represents the normalized bed length, while the concentration profiles indicate the adsorption behaviour within the column. The plot shows a significant decrease in solute concentration near the inlet region of the column, indicating strong adsorption and rapid uptake of the adsorbate by the adsorbent. This region corresponds to the active mass transfer zone, where the concentration gradient between the fluid phase and adsorbent is high. As the fluid progresses along the bed length, the concentration gradually stabilizes, suggesting reduced adsorption activity toward the outlet section. The nearly constant concentration profile beyond a certain axial distance indicates that the adsorption front has not yet reached the outlet of the column. This confirms that the packed bed possesses sufficient adsorption capacity and that the column is operating under effective mass transfer conditions. The smooth concentration gradient also suggests minimal axial dispersion and stable plug flow behaviour within the bed.

VI. CONCLUSION AND FUTURE WORK

In the present study, a simulation-based kinetic analysis of a packed bed adsorption column was successfully carried out using Aspen Adsorption software. The dynamic behaviour of the adsorption process was analysed through breakthrough curves and axial concentration profiles. The simulation results demonstrated effective removal of the target contaminant from the aqueous phase, confirming the suitability of the packed bed configuration for liquid-phase adsorption. The breakthrough analysis indicated stable column performance with delayed bed saturation, highlighting sufficient adsorption capacity and efficient mass transfer within the column. The axial concentration profiles further

confirmed proper development of the mass transfer zone along the bed length. The system operated under nearly isothermal conditions with negligible pressure drop, indicating stable hydraulic and thermal behaviour. Overall, the results validated the selected adsorption equilibrium and kinetic models and demonstrated that Aspen Adsorption is a reliable tool for predicting adsorption performance. This study shows that simulation-based approaches can effectively reduce experimental effort and support the design and optimization of packed bed adsorption columns for water treatment applications.

Future studies may focus on incorporating experimental validation to further confirm the accuracy of the simulation results. The adsorption model can be extended to study the effect of additional operating parameters such as temperature variation, particle size, and inlet concentration. Regeneration and reuse of the adsorbent can also be investigated to evaluate the economic feasibility of the process. Furthermore, the simulation approach can be applied to multi-component adsorption systems and scaled up for industrial wastewater treatment applications.

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