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Dynamic Modelling, Simulation, and Sensitive Analysis of Lead Removal in a Fixed-Bed Adsorption Column using Waste-Based Materials

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Abstract. This study focuses on dynamic modelling and numerical simulation of lead removal from contaminated water using a fixed-bed adsorption column packed with waste-based adsorbents. The pressing need for efficient and sustainable water treatment methods, particularly for heavy metal removal, underscores the significance of this research. Lead contamination in water sources poses severe health risks, necessitating the development of effective removal strategies. The present investigation centres on a comprehensive mathematical model that considers critical parameters, including the column's physical dimensions, flow rate, initial lead concentration, adsorption rate constant, and adsorbent density. This model is expressed as a partial differential equation (PDE) describing the temporal and spatial evolution of lead concentration along the fixed-bed column. To solve the PDE, the method of lines, a powerful numerical technique that discretises the spatial domain and handles the resulting system of ordinary differential equations (ODEs) using an adaptive solver, is employed. Following that, the effect factors of the simulation process are evaluated by sensitive analysis approach. Simulations are conducted to elucidate the intricate dynamics of lead removal over time and column height. The numerical approach enables the prediction of lead concentration profiles within the column at various time intervals, providing crucial insights into the behavior of the adsorption process.

1. Introduction

Lead is a highly toxic heavy metal known for its carcinogenic effects on human health. Exposure to lead, primarily through contaminated drinking water, poses a significant risk, particularly to children and pregnant women. The presence of lead in water resources often stems from deteriorating infrastructure, such as aging lead pipes and plumbing fixtures, which can leach this hazardous element into the water supply. Chronic exposure to even low levels of lead can lead to a range of health problems, including developmental delays in children, neurological disorders, and an increased risk of cancer [1-3]. Thus, the control and mitigation of lead emissions into water resources remain critical for safeguarding public health and preventing the associated carcinogenic risks. The death rate from lead exposure is mentioned in Figure 1 in three countries including Afghanistan (as third-world country), Czech Republic (as European country), and Australia (as a developed country). The scheme demonstrated that in Afghanistan as a country with low level of environmental cares, the rate of death based on lead exposure is higher than others. Therefore, implementation of low-cost highly efficient technologies can be useful due to increase the level of health in developed and developing countries [4-6].

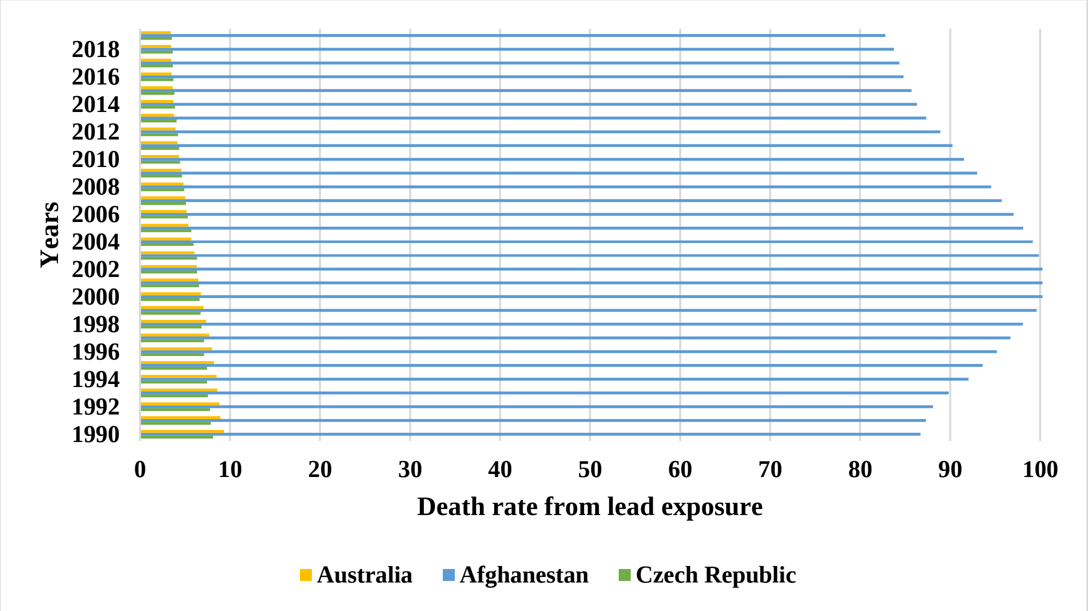

Figure 1. The dataset of lead exposure death rate in Afghanistan, Czech Republic, and Australia [6].

Various methods are employed for the decontamination of lead from water resources, but adsorption processes stand out for their efficiency and versatility. Adsorption involves the attachment of lead ions to the surface of a solid adsorbent material, such as activated carbon or ion-exchange resins [7,8]. This method offers several advantages, including high removal efficiency, ease of operation, and adaptability to different water sources. Adsorption processes can effectively remove lead from both point-of-use and point-of-entry systems, making them suitable for households and municipal treatment facilities. Moreover, they are cost-effective, environmentally friendly, and capable of treating a wide range of water conditions. The reversible nature of adsorption also allows for regeneration and reuse of the adsorbent materials, reducing waste and enhancing sustainability in lead decontamination efforts [9].

Continuous flow decontamination of lead using waste-based adsorption columns plays a pivotal role in various industrial applications. These columns are designed to consistently remove lead from wastewater or process streams as they pass through the adsorbent material, ensuring a continuous and efficient treatment process. In industries like metallurgy, battery manufacturing, and electronics, where lead contamination is a significant concern, these columns offer a reliable solution for meeting stringent environmental regulations. Additionally, continuous flow adsorption systems are widely employed in water treatment plants to purify drinking water and industrial effluents, safeguarding public health, and preventing lead pollution [10]. Their ability to handle large volumes of water while maintaining high removal efficiencies makes them indispensable in these settings, providing a sustainable and cost-effective means of mitigating lead contamination [11].

Waste-based adsorbents utilised in column systems offer a sustainable and environmentally friendly approach to wastewater treatment and pollutant removal. These adsorbents are typically derived from discarded materials such as agricultural residues, industrial byproducts, or even certain types of waste biomass [12]. Their advantages lie in their cost-effectiveness, as they repurpose waste materials that would otherwise be disposed of reducing both economic and environmental burdens. Furthermore, waste-based adsorbents often exhibit high adsorption capacities and can effectively remove various contaminants, including heavy metals, organic pollutants, and dyes, from aqueous solutions. This eco-friendly approach not only mitigates pollution but also promotes resource conservation and a circular economy, making waste-based adsorbents a promising solution for sustainable water treatment processes in fixed-bed column systems [13,14].

There are lots of research items in the field of simulation of lead decontamination by adsorption process in column as continues flow which are summarised in Table 1.

Table 1. The summarised literature review in this study

Goals	Tools	Achievements	Ref.
1. Uptake Optimisation: Determine the optimal conditions for lead uptake using ecofriendly biosorbents, specifically red marine algae Jania ruben, with varying pretreatment methods (CaCl2 and formaldehyde). 2. Isotherm and Kinetics Modelling: Identify and compare the best-fit isotherm models (Freundlich, Langmuir, Temkin, Redlich–Peterson, Elovich) and kinetic models (Pseudo-first order and Pseudo-second-order) for lead adsorption. 3. Column Adsorption Modelling: Evaluate different column adsorption models (Thomas, Yoon-Nelson, Yan, Clark) to describe lead removal in column experiments. 4. Regeneration Assessment: Determine the regeneration potential of the biosorbent material, aiming for high regeneration efficiency to enable multiple operational cycles. 5. Characterisation: Confirm the presence of adsorbed lead in the algae material through thermal analysis.	1. Batch Experiments: Laboratory setup for batch experiments, including beakers, shakers, and analytical equipment for lead concentration measurements. 2. Column Experiments: Specialised columns for lead adsorption experiments, along with a continuous flow system for column testing. 3. Pretreatment Agents: Calcium chloride (CaCl2) and formaldehyde used as pretreatment agents for the algae material. 4. Statistical Analysis: Statistical software for identifying the best-fit isotherm and kinetic models, as well as regression analysis for column models. 5. Thermal Analysis Equipment: Thermal analysis instruments (e.g., DSC or TGA) to confirm the presence of adsorbed lead in the algae material.	1. Optimal Lead Uptake: The highest adsorption capacity of 774 mg/g was achieved using Jania algae pretreated with formaldehyde, demonstrating the effectiveness of this pretreatment method. 2. Model Identification: Identified the most suitable isotherm models (Freundlich, Langmuir) and kinetic models (Pseudo-first order and Pseudo-second-order) to describe lead adsorption on the biosorbent material. 3. Column Modelling: Determined that the Thomas column model provided the best fit with a capacity of qTh = 1092.4 mg/g for lead removal from the breakthrough curve area analysis. 4. Regeneration Success: Achieved a remarkable 98.5% regeneration of the column, indicating the feasibility of using algae materials in multiple operational cycles, making the process more sustainable. 5. Confirmation of Adsorption: Confirmed the presence of adsorbed lead in the algae material through thermal analysis, providing evidence of successful lead uptake.	[1]
1. Simulate: Simulate lead (II) adsorption on activated carbons in a packed-bed column. 2. Compare: Compare the performance of tire-derived activated carbon (TAC) and	1. Aspen Adsorption®: Used Aspen Adsorption® V11 flowsheet simulator for column simulation. 2. Experimental Setup: Utilised a packed-bed	1. Optimal Conditions: Identified the optimum conditions for lead (II) adsorption (500 mg/L concentration, 0.6 m bed height, and 9.88×10^{-4} m3/s flow rate).	[2]

commercial activated carbon (CAC) in lead (II) adsorption. 3. Optimise: Determine the optimum operating conditions for lead (II) adsorption. 4. Evaluate: Evaluate breakthrough times and adsorption capacities for TAC and CAC. 5. Assess: Assess the potential of TAC for lead (II) adsorption.	column for experimental simulations. 3. Parameter Variation: Adjusted initial lead (II) ion concentrations, bed heights, and flow rates as experimental parameters. 4. Temperature and Pressure Control: Maintained constant temperature (25 °C) and pressure (3 bar) during simulations. Data Recording: Recorded breakthrough times, adsorption capacities, and other relevant data during the experiments.	2. Breakthrough Times: Recorded breakthrough times of 488 s for TAC and 23 s for CAC under optimal conditions. 3. Adsorption Capacity: Measured an adsorption capacity of 114.26 mg/g for TAC and 7.72 mg/g for CAC at t0.5. 4. Performance Comparison: Demonstrated the superior performance of TAC compared to CAC in lead (II) adsorption. 5. Simulation Validation: Validated the potential of TAC through simulation results.	
1. Test GAC: Evaluate the potential of granular activated carbon (GAC) for heavy metals removal, specifically cadmium (Cd) and lead (Pb). 2. Continuous Adsorption: Simulate real-world adsorption conditions through a fixed bed column test. 3. Flow Rate Effects: Assess the impact of different flow rates on the performance of the adsorption column. 4. Breakthrough Curve Prediction: Use the Adam-Bohart equation to predict and understand the breakthrough curves during adsorption. 5. Heavy Metals Removal: Determine the effectiveness of GAC in successfully removing cadmium and lead from solution.	1. Granular Activated Carbon (GAC): Used GAC as the adsorbent material for heavy metals removal. 2. Fixed Bed Column: Employed a fixed bed column to simulate continuous adsorption processes. 3. Prepared Solutions: Created solutions containing cadmium and lead for testing. 4. Flow Rate Control: Varied flow rates to investigate their impact on column performance. 5. Adam-Bohart Equation: Utilised the Adam-Bohart breakthrough curve equation for prediction and analysis of adsorption capacity and breakthrough curves.	1. Effective Removal: Demonstrated that GAC is capable of successfully removing cadmium and lead from prepared solutions through adsorption. 2. Column Simulation: Conducted a fixed bed column test to closely mimic continuous adsorption processes. 3. Flow Rate Impact: Evaluated the effects of different flow rates on the column's performance, yielding different breakthrough curves. 4. Accurate Prediction: The Adam-Bohart equation accurately predicted and explained the breakthrough curves based on the experimental data. 5. Environmental Benefit: Highlighted the potential of GAC as an effective method for mitigating the release of heavy metals into the environment.	[3]
1. Model Adsorption: Develop a surface complexation model to describe the adsorption of lead (Pb) and protons onto a natural porous medium (red pozzolan). 2. Surface Heterogeneity: Determine the minimum number of surface sites required to account for the surface heterogeneity of red pozzolan. 3. Model Parameterisation: Determine adjustable parameters (site concentrations and apparent formation constants) through	1. Red Pozzolan: Used red pozzolan as the natural porous medium for adsorption experiments. 2. Acid−Base Titration: Conducted acid−base titration experiments to determine surface heterogeneity. 3. Lead Adsorption Tests: Performed lead adsorption tests at various pH levels and total lead concentrations to complete the model structure.	1. Surface Complexation Model: Developed a surface complexation model capable of describing the adsorption of Pb and protons on red pozzolan. 2. Surface Site Identification: Identified two amphoteric sites (SOH and TOH) and a monoprotic site (MOH) to represent the surface heterogeneity. 3. Parameter Determination: Successfully determined the adjustable parameters for the model through regression of experimental data. 4. Experimental Representation: Achieved a good representation of the	[4]

nonlinear multivariate regression using titration and adsorption data. 4. Experimental Representation: Create a model that accurately represents the acid−base and adsorption properties of red pozzolan over a specified pH and lead concentration range. 5. Validation: Independently validate the model by simulating breakthrough experiments for Pb and pH in chromatographic columns.	4. Nonlinear Multivariate Regression: Employed regression analysis to determine adjustable model parameters using titration and adsorption data. 5. Simulation Software: Utilised simulation software, such as IMPACT, to validate the model through the simulation of Pb and pH breakthrough experiments in chromatographic columns.	acid−base and adsorption behavior of red pozzolan over the specified experimental range. 5. Model Validation: Independently validated the model's accuracy by simulating Pb and pH breakthrough experiments in chromatographic columns without requiring parameter adjustments.	

Table 1 presents four distinct research endeavours, each with specific objectives, accomplishments, and instrumental methods. The first research item seeks to enhance lead uptake using eco-friendly biosorbents and deploys a suite of tools, such as batch and column experiments, pretreatment agents, statistical analysis software, and thermal analysis equipment. It successfully identifies optimal adsorption models, achieves efficient column regeneration, and confirms lead adsorption in algae materials [1]. The second research item focuses on simulating lead (II) adsorption on activated carbons, employing tools like Aspen Adsorption® and experimental setups to optimise conditions, record breakthrough data, and validate simulations [2]. The third item evaluates granular activated carbon for heavy metals removal, utilising GAC, fixed bed columns, and the Adam-Bohart equation, resulting in effective heavy metals removal and accurate breakthrough predictions [3]. Lastly, the fourth research item aims to develop a surface complexation model for lead and proton adsorption, relying on tools like red pozzolan and nonlinear regression, leading to the creation of a precise model validated through simulations. Collectively, these research endeavours showcase a diverse range of experimental and modelling approaches in the context of adsorption and environmental remediation [4].

Therefore, based on the literature review, the application of computational approaches due to column adsorptive of lead is a rare issue which is not considered by previous research items. Therefore, the viewpoints of the present study will fill this research gap with concentration on sensitive analysis. The present study aims to:

- Simulate the waste-based adsorption in column with the application of a partial differential equation (PDE) describing.
- Evaluation of lead distribution during the column as per time and height.
- Sensitive analysis of the most important features during the simulation process with concentration on water flow rate and dispersion coefficient.

In the following, the methodology, results/discussions, and conclusion of this research are mentioned in Sections 3,4, and 5, respectively.

2. Methodology

The research roadmap of the present study is mentioned in Fig 2. The research roadmap demonstrated that in the first step of this research, the equations of PDE are extended in the case study and then the profiles of column height and time are illustrated. Finally, with the application of MATLAB programming, the sensitive analysis will be done based on water flow and diffusion coefficient features.

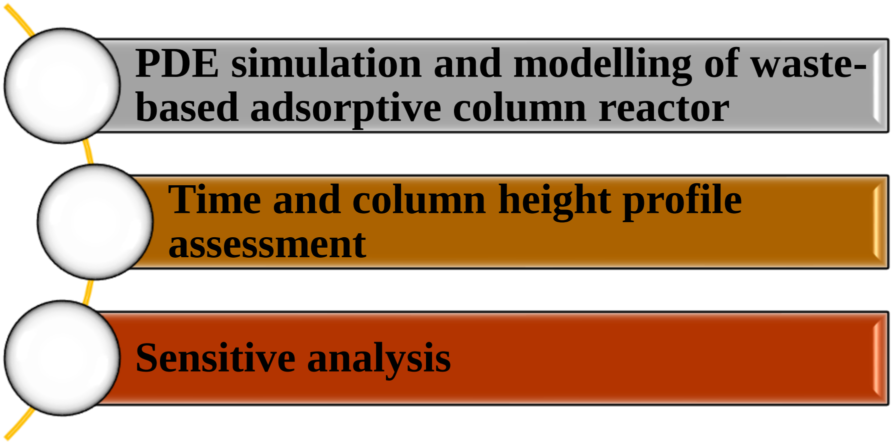

Figure 2. The research roadmap of the present study.

2.1. PDE computations

The objective of this study is to simulate the lead adsorption process in a fixed-bed column, considering the effects of dispersion, adsorbent density, flow rate, initial lead concentration, and the reduction in adsorption performance with height and time. This study defines various parameters and initial conditions for the simulation:

Length of the fixed-bed column, L (m)
End time for simulation, T_{end} *(seconds)*
Number of spatial discretisation points, N_x
Number of time steps, N_t
Dispersion coefficient, D (m^2/s)
Adsorbent density, ρ_{ads} (kg/m^3)
Flow rate, Q (m^3/s)
Initial lead concentration in the influent, C_0 *(mg/L)*

The present research considers two profiles that describe the reduction in adsorption performance with height and time. Adsorption performance reduction with height and time is mentioned in Equations 1 and 2. The computation of this section is related to adsorption performance profiles evaluation of the case study reactor [15].

$$\text{Adsorption\_height\_profile}\ (x) = \exp(-x/L) \tag{1}$$

$$\text{Adsorption\_time\_profile}\ (t) = \exp(-t/T_{end}) \tag{2}$$

In the next step, the discretisation section is divided into spatial domain discretisation and temporal domain discretisation. The spatial domain is discretised using Nx points, and the spatial step size, Δx, is calculated as Equation 3. The temporal domain is also discretised using Nt time steps, and the time step size, Δt, is computed as Equation 4.

$$\Delta x = L/N_x \tag{3}$$

$$\Delta t = T_{end}/N_t \tag{4}$$

The method of lines is employed to numerically solve the PDE describing lead adsorption in the fixed-bed column. The time-stepping loop is used to update the concentration profile at each time step [16].

For each time step *n*, the spatial derivatives of concentration are approximated numerically using the finite difference method. Specifically, the second spatial derivative, d^2C/dx^2, is calculated at each spatial grid point *i* as Equation 5.

$$d^2C/dx^2= [C(i+1, n)-2C(i,n)+C(i-1,n)]/\Delta x^2 \quad (5)$$

The governing equation for lead adsorption in the column is given by Equation 6.

$$dC/dt=D(d^2C/dx^2)-Q(C-C_0) \cdot \text{adsorption\_height\_profile}(x) \quad (6)$$

where:
dC/dt is the rate of change of concentration with respect to time.
D is the dispersion coefficient.
Q is the flow rate.
C is the concentration of lead.
$C_0$is the initial lead concentration.
Adsorption_height_profile (x) accounts for the reduction in adsorption performance with height.

The concentrations are updated using an implicit time-stepping scheme, ensuring stability and accuracy of the numerical solution. The adsorption performance reduction with time is incorporated at each time step. All programming of this study was carried out in MATLAB 2019b.

2.2. Time and height fluctuations

The steps of time and height profile programming in this study are mentioned in Table 2.

Table 2. The steps of time/height profile programming in waste-based adsorptive column in interaction of lead ions.

Step	Description
Step 1	Implement a time-stepping loop that iterates through each time step (n) to solve the PDE for lead adsorption.
Step 2	Inside the loop, calculate spatial derivatives of concentration using a finite difference approximation.
Step 3	Update concentrations at each spatial point and time step using an implicit time-stepping scheme. Incorporate the reduction in adsorption performance with height and time into the concentration update.

2.3. Sensitive analysis

Different stages of the PDE computations in this study are demonstrated in Table 3. The two first steps of the programming are related to sensitive analysis setup and two other steps are linked to sensitive analysis loop implementations.

Table 3. The stages of sensitive analysis in this research.

Step	Description
Step 1	Define a range of values for the dispersion coefficient (D) and flow rate (Q) to conduct a sensitivity analysis. These parameter values are stored in arrays such as D_values and Q_values.
Step 2	Create a 4D matrix (heatmap) to store concentration profiles for different combinations of D and Q. The dimensions of this matrix represent spatial points, time points, D values, and Q values.

Step 3	Nested loops iterate through different combinations of D and Q values to analyse the sensitivity of the system to these parameters.
Step 4	For each parameter combination, the PDE solution is computed, and the resulting concentration profiles are stored in the heatmap matrix.

3. Results and discussion

The results of residual lead (II) concentration in different heights (or vertical length) of the simulated column are demonstrated based on Figure 3. The computations are done based on 1m column height and both water flow and initial concentration are considered equal to 0.1 m^3s^{-1} and 10 mgL^{-1}. Likewise, adsorbent density is considered equal to 500 kg/m^3. The computations demonstrated that in up-flow reactors, with increasing length of column, the performance of reaction is reduced.

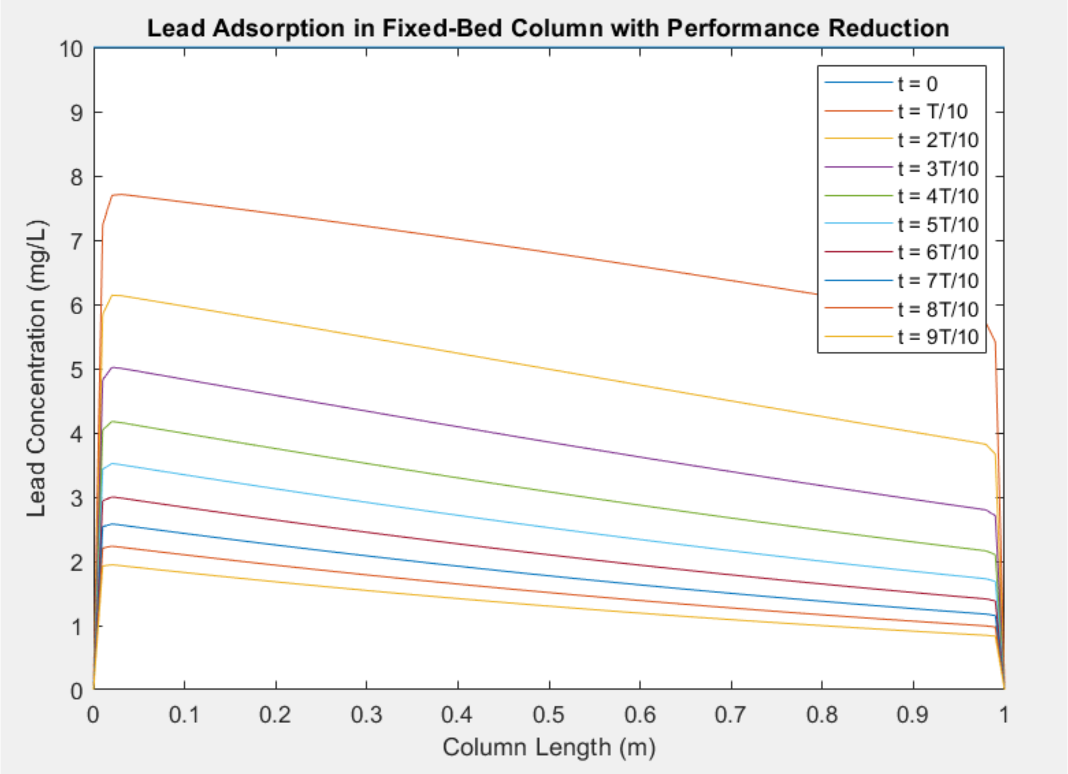

Figure 3. The height profile of remained lead (II) in the adsorption column.

In the research conducted by Makarem et al. (2023) [17], they found that the NiCo-LDHs-rGO composite efficiently removes up to 99.7% of Pb2+ ions, highlighting the significance of optimising factors such as pH and adsorbent dosage. Their findings on the composite's mesoporous structure, with a notable surface area, inform potential enhancements to the adsorbent density settings in our simulations.

Based on the insights derived from Figure 4, a key observation emerges: the efficiency of the adsorption process exhibits a noticeable decline after approximately 100 seconds of operation. This critical temporal threshold marks a pivotal point in the performance of the system.
It becomes evident that when operating under a constant flow rate of $Q=0.1\ m^3/s$, the system reaches a significant milestone after treating 10 m^3 of water contaminated with lead (II) ions. At this juncture, the system ceases to function optimally, signalling the necessity for a crucial intervention: the regeneration of the adsorbent materials.

The need for regeneration arises as the adsorbent materials, while highly effective, become saturated with adsorbed lead (II) ions over time. This saturation leads to a decrease in their adsorption capacity, rendering them less efficient in removing further ions from the contaminated water. The regeneration process involves restoring the adsorbent materials to their initial state, allowing them to resume their adsorption capabilities effectively. This essential step ensures the continued functionality and longevity of the system for the treatment of lead (II) ion-contaminated water.

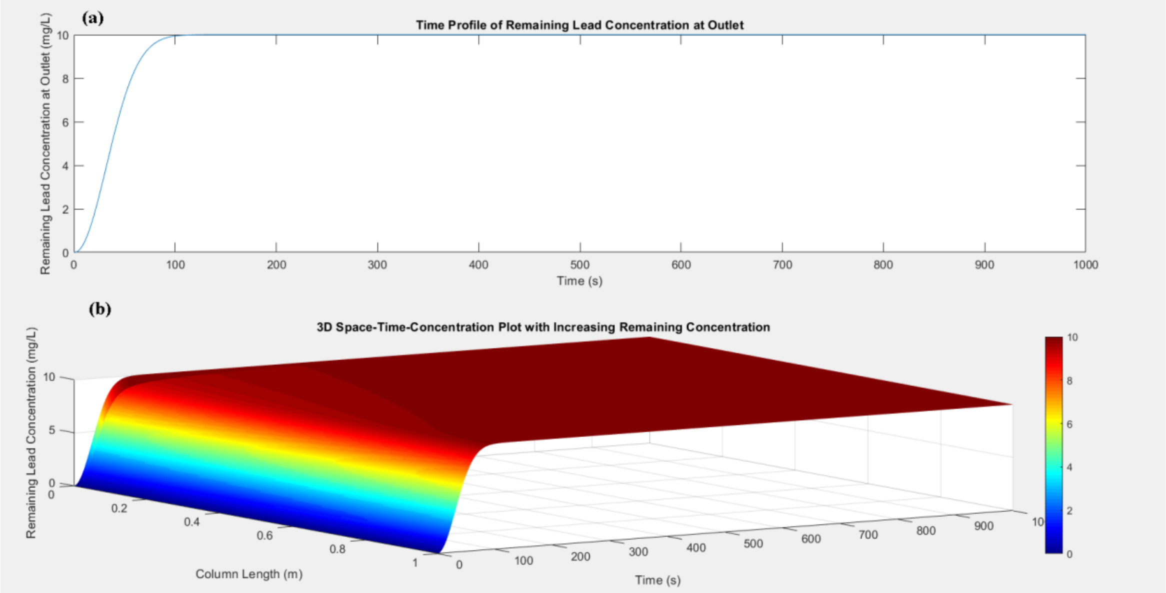

Figure 4. The time profile of lead (II) in simulated adsorption column.

The meticulous analysis of both water flow and the diffusion coefficient, as depicted in Figure 5, provides valuable insights into the behavior of the adsorption system. Notably, the findings reveal a significant trend: as the flow rate increases, the performance of the adsorption system experiences a gradual reduction. This intriguing observation prompts a closer examination of the underlying mechanisms driving this phenomenon. The primary factor contributing to the diminishing performance lies in the saturation of the adsorbent surface and the attainment of its maximum adsorption capacity. As water flows through the system at an accelerated rate, it has less contact time with the adsorbent material, limiting the extent to which lead (II) ions can be effectively captured. This saturation effect is a critical consideration in optimising the system's operational parameters.

One noteworthy aspect that merits attention is the nature of the adsorbent used in this study, which is waste based. The advantage of such materials lies in their cost-effectiveness when it comes to regeneration. The economic feasibility of regenerating waste-based adsorbents adds to the attractiveness of this approach for sustainable water treatment processes. Furthermore, the physical arrangement of materials within the system plays a pivotal role in the simulation process. Notably, an increase in particle size correlates with higher diffusivity coefficients. This, however, comes at a cost, as it inversely impacts the performance of the adsorption process, leading to reduced efficiency. Delving deeper into the sensitivity analysis under various conditions, a crucial finding emerges: the significance of water flow rate surpasses that of the diffusion coefficient when assessing the remaining lead concentration. This underscores the paramount importance of carefully controlling and optimising the water flow rate to ensure the desired level of lead (II) ion removal efficiency in the system. Furthermore, use of smart technological frameworks and data driven models such as Artificial Intelligence (AI) can be efficiently integrated to these treatment processes to provide an economic and efficient detection and removal of contaminants in water systems [18 and 19].

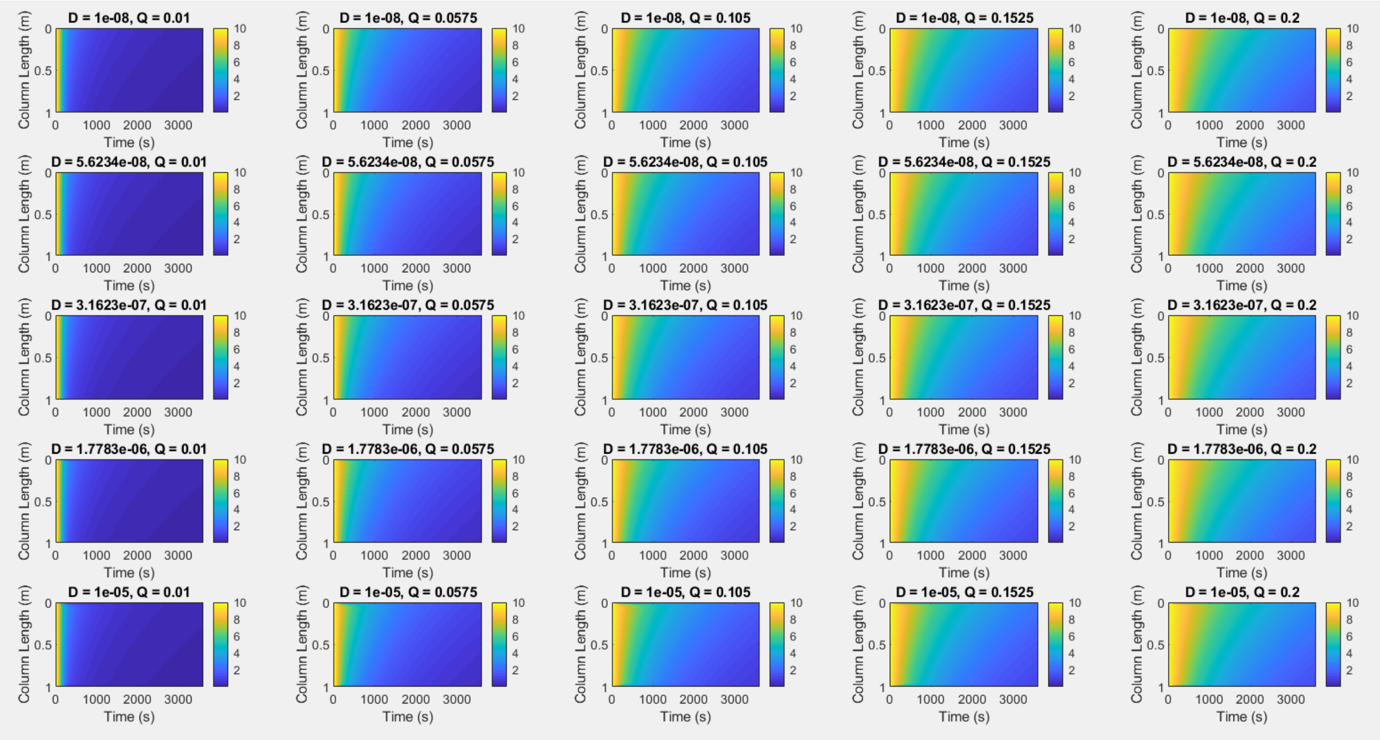
D = 1e-08, Q = 0.01
D = 1e-08, Q = 0.0575
D = 1e-08, Q = 0.105
D = 1e-08, Q = 0.1525
D = 1e-08, Q = 0.2
D = 5.6234e-08, Q = 0.01
D = 5.6234e-08, Q = 0.0575
D = 5.6234e-08, Q = 0.105
D = 5.6234e-08, Q = 0.1525
D = 5.6234e-08, Q = 0.2
D = 3.1623e-07, Q = 0.01
D = 3.1623e-07, Q = 0.0575
D = 3.1623e-07, Q = 0.105
D = 3.1623e-07, Q = 0.1525
D = 3.1623e-07, Q = 0.2
D = 1.7783e-06, Q = 0.01
D = 1.7783e-06, Q = 0.0575
D = 1.7783e-06, Q = 0.105
D = 1.7783e-06, Q = 0.1525
D = 1.7783e-06, Q = 0.2
D = 1e-05, Q = 0.01
D = 1e-05, Q = 0.0575
D = 1e-05, Q = 0.105
D = 1e-05, Q = 0.1525
D = 1e-05, Q = 0.2

Figure 5. The sensitive analysis of water flow and diffusion coefficient changes.

4. Conclusions

The present study has cantered its attention on the utilisation of PDE computations for simulating an adsorption column system employing waste-based materials, with the primary objective of purifying water resources contaminated with lead ions. Through meticulous analysis, we have explored the impact of various critical parameters using a sensitivity analysis approach. The outcomes of this modelling endeavour have yielded valuable insights. Firstly, the model's efficacy has been established, showcasing its suitability for assessing system performance across different column heights. Additionally, it has been proven instrumental in predicting the continuous adsorption process over time, a key requirement for the successful implementation of water purification systems. Perhaps the most significant revelation to emerge from the sensitivity analysis is the paramount importance of water flow rate in the adsorption process. This finding underscores the critical role that flow control plays in optimising the efficiency of lead ion removal, emphasising its significance in the design and operation of water treatment systems.

Looking ahead, this study advocates for the integration of metaheuristic algorithms as powerful Artificial Intelligence tools for the purpose of optimising the design of water treatment systems. The application of machine learning algorithms also holds promise in accurately forecasting the performance of adsorption packages, further enhancing the precision and efficiency of water purification processes. Furthermore, developing comprehensive management frameworks for water quality forecasting can also be helpful for detecting such contamination in the first place in water systems [20].

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