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Dynamic Study Of Adsorption Performance For Removing Arsenic (v) Through Polyacrylonitrile (pan) Fiber Using Aspen Adsorption

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Abstract

Arsenic is known to be one of the most significant and severe inorganic pollutants in drinkable water globally. Many important techniques have been read for better results, such as ion-exchange, flocculation, precipitation, coagulation, adsorptions and other membrane technologies , when complying with the MCL (maximum contaminant level), Arsenic(V) around 10 ìg / l in drinkable water) developed worldwide by the major World Health Organization, These available water treatment technologies are applicable; adsorption has proven to be a favorable and efficient technology for the removal of Arsenic from any form of water with dissimilar concentrations. In this analysis, Arsenic (As (V)) removal from water that studied by the packed bed column by modeling and simulation using iron ore adsorbent in the ASPEN ADSIM V11 software. The various effects on the efficiency of the adsorption column, such as bed height, feed-flow rate and the initial Arsenic concentrations of different operating parameters, were studied theoretically. Experiments were performed in specific cases to verify the results. Bed-depth greater then more Arsenic (v) are adsorbed and the Arsenic removal was achieved 100 % at a bed-height of 29.0 cm for simulation. The percentage of Arsenic removal, as well as the total adsorption of Arsenic increase with the decrease in flow rate, it is observed that when the bed height is increased the service time of adsorption bed also increases. The results showed that the design parameters such as adsorbent bed depth and column diameter, together with operating parameters such as Arsenic inlet concentration, have great effects on the overall column efficiency.

***Keywords**: Arsenic Removal, Modified PAN Fiber, Adsorption Column*

1. Introduction:

The world health organization has presented many alarming contaminations including fluorides, arsenic compounds, and nitrate etc., which has caused several health problems for living beings around the globe (Organization, 2008). . Drinking water quality is affected by toxic metal contamination of As^{+3} and As^{+5}. It is reported that arsenic is a deadly factor in more than 70 countries, which causes serious health problems worldwide. Higher arsenic concentrations, as recommended by the WHO, above 10 ppb can cause various diseases such as cancer and skin problems (Bhatti et al., 2020). Groundwater contamination by these pollutants specifically with arsenic is becoming an unavoidable challenge for the research community(Amini et al., 2008). Arsenic content in our ecological system has been observed dominantly

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among all the contaminants (Abe et al., 2004). The response surface analyses and analysis of variance reveals an excellent fit of experimental data into the quadratic model, and the interactive effect of pH and initial concentration was highly significant on arsenate removal capacity(Sawood et al., 2021) In the major part of the world groundwater is been considered most frequent and easy source for drinking water which is been consistently reported with heavy metal contaminations specifically with arsenic natural contamination by leaching rock state,. if Fe(III)-AO PAN and hydrogen peroxide are used for removing As(III), we can not only oxidize As(III) to As(V) through the Fenton-like reaction, but also simultaneously remove As(V) by using the excellent adsorption performance of Fe(III)-AO PAN (Gao et al., 2020) .Arsenic is one of the most toxic contaminants which is a serious problem all over the globe. Many of developed and developing countries suffering from this issue. The acceptable limit set by WHO World Health Organization is 10ppb for drinking water, but due to increase in natural and anthropogenic activities it exceeds to suggested level. In some areas of Punjab and Sindh province of Pakistan arsenic level is above 50ppb which results in different diseases. Although previous study suggests that around 60 million people all over the globe are exposed to elevated level of arsenic containing drinking water. The current study focuses mainly on exceeded arsenic contamination and health risk around the globe, with special consideration to the condition of Pakistan. Among many methods for remediation of Arsenic contamination, adsorption is found to be most economical and effective approach. Research till date suggested numerous adsorbents, recently attention is being paid to graphene-based adsorbents as novel adsorbent to remove arsenic due to its amazing properties. Through Aspen ADSIM the operation parameters for arsenic adsorption over modified Poly Acrylonitrile fiber were optimized and performance evaluation of adsorption column was carried out with various simulations.

2. Methodology:

The systems of ordinary and partial differential equations (ODEs, and PDEs) along with appropriate algebraic equations with suitable initial boundary conditions were used in Aspen ADSIM, to simulate the adsorption process in ion-exchange column. All the simulations work was carried out through official ADSIM Ver. 11 platform of Aspen-tech for commercial Microsoft windows system. The recent data from literature work performed on removal of arsenic through kaolin was considered to run the simulation, where and adsorbent bad was developed and arsenic contaminated water with known concentration was passed to examine the removal efficiency. The developed simulation scheme is well described in Fig. 1, where initial feed in entered from the top of the column. ideal initial flow is assumed in the column due to which uniform motion of water and arsenic molecules occur, therefore, adsorption will only be a function of convective force.

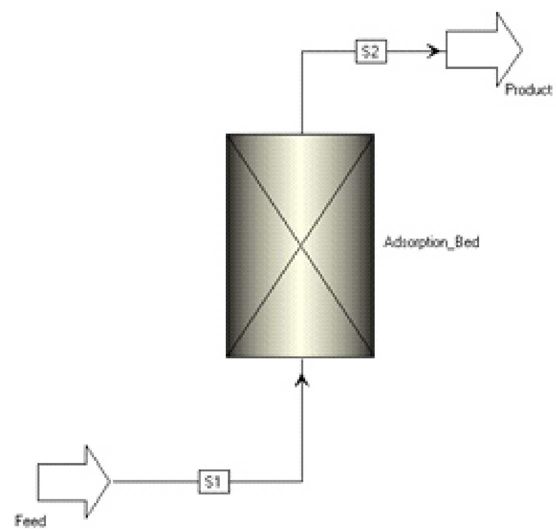

Figure 1: Schematic Presentation of Fixed Bed Adsorption Column for Simulations in AdsimV11.

The simulations were performed by taking into account the default isotherms i.e. Langmuir and mass transfer coefficient values present in the model, with considering constant temperature of 25°C. Bi upward difference scheme (BUDS) method was used to compute the simulation with 50 nodes numbers, however the geometry of the cylindrical column with 2cm of diameter and 10cm in hight was considered in the simulations.

2.1 Adsorbent Simulation and Characteristic Data:

Kaolin is a suitable solution to remove arsenic from groundwater. There is significant research has been documented on the perspectives and applications of Kaolin by conducting parametrical studies on the chemical and physical properties of Kaolin. The initial and boundary condition and some literature data (Rafique et al., 2008) considered in the current study are listed in Table

Table 1: PAN Fiber Simulation and Characteristic Data

Sr. No.	Operational/Physical Parameter	Value
1	Porosity (Intra Particle)	0.412 m^3 void/m^3 bed
2	Porosity (Intra Particle)	0.4 m^3 void/m^3 bed
3	Density of Material	2.65 gm/cm^3
4	Coefficient for Mass Transfer	0.23 sec^{-1}
5	IP1 (Langmuir Isotherm)	0.021
6	IP2 (Langmuir Isotherm)	0.7231

2.2 Parametric Simulations:

Parametric simulations were carried out for optimization of different operating and physical parameters to investigate impact on the absorption column performance. The important parameters such as bed height, flowrate of feed, and concentration of fluoride while entering into the column. Data of each case considered in the study are tabulated in Table 2.

Table 2: Case Data Information for Simulation

Case No	Initial-Concentration	Feed-Flow	Bed -Height
	Mol/lit	Lit/min	cm
1	3.4×10^{-5}	0.050	10
2	3.4×10^{-5}	0.050	20
3	3.4×10^{-5}	0.050	30
4	3.4×10^{-5}	0.075	10
5	3.4×10^{-5}	0.075	20
6	3.4×10^{-5}	0.075	30
7	3.4×10^{-5}	0.100	10
8	3.4×10^{-5}	0.100	20
9	3.4×10^{-5}	0.100	30
10	6.8×10^{-5}	0.050	10
11	6.8×10^{-5}	0.050	20
12	6.8×10^{-5}	0.050	30
13	6.8×10^{-5}	0.075	10
14	6.8×10^{-5}	0.075	20
15	6.8×10^{-5}	0.075	30
16	6.8×10^{-5}	0.100	10
17	6.8×10^{-5}	0.100	20
18	6.8×10^{-5}	0.100	30
19	10.2×10^{-5}	0.050	10

20	10.2×10^{-5}	0.050	20
21	10.2×10^{-5}	0.050	30
22	10.2×10^{-5}	0.075	10
23	10.2×10^{-5}	0.075	20
24	10.2×10^{-5}	0.075	30
25	10.2×10^{-5}	0.100	10
26	10.2×10^{-5}	0.100	20
27	10.2×10^{-5}	0.100	30

3. Results And Discussion:

Removal efficiency of arsenic form contaminated water is briefly investigated through different simulations via Aspen Adsorption platform and results are discussed in hereunder.

3.1 Arsenic Removal as a function of Bed Height:

Simulation results are presented in Figure 2, 3, and 4 for arsenic concentration remained in treated water after passing through different bed heights of Kaolin i.e. 10cm, 20cm, and 30cm with a flowrate variation in feed flow such as 0.050, 0.075 and 0.100 L/min, while varying the concentration of arsenic in the water i.e. (3.4×10^{-5}, 6.8×10^{-5}, and 10.2×10^{-5} mol/L). The efficiency of adsorbent bed is evaluated and plotted in the figure 2, by considering the initial and final concentration i.e. (Co/Ci) of arsenic found in the contaminated and treated water.

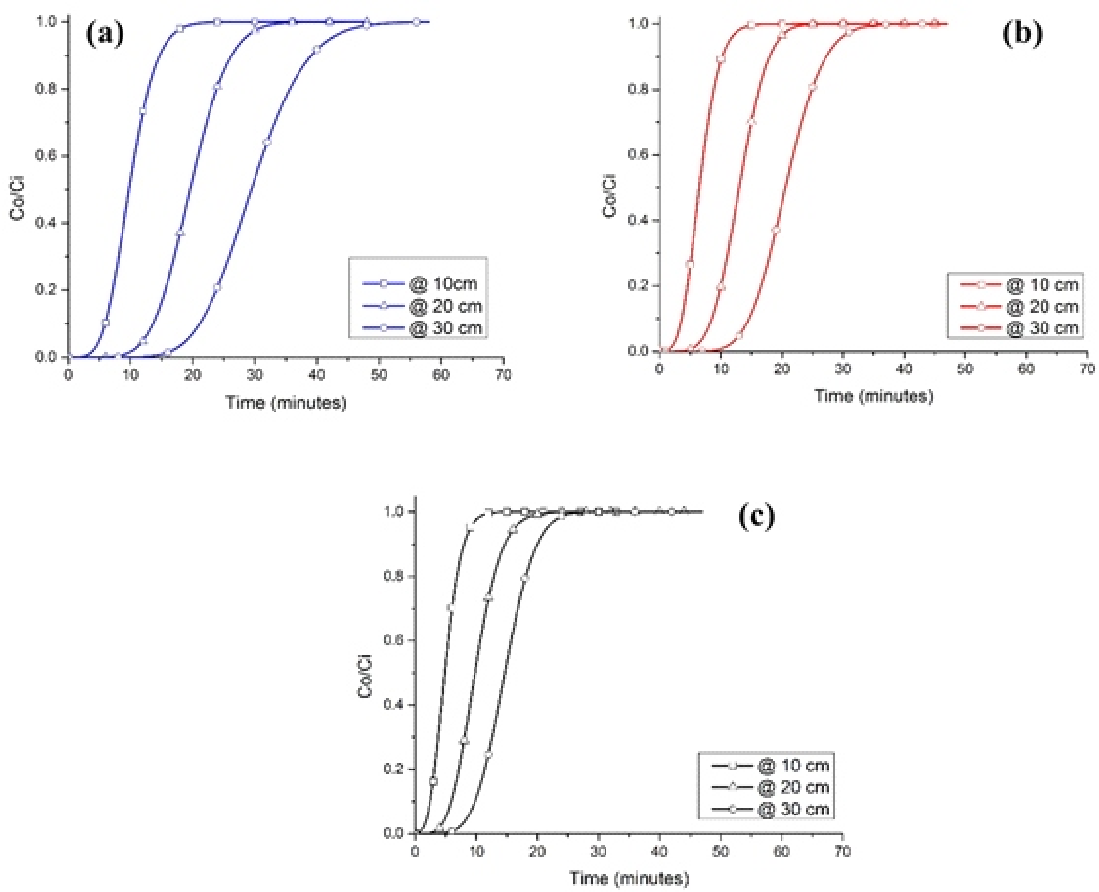

Figure 2: Breakthrough curves for studying the effects of bed height and feed flowrate with constant inlet concentration (3.4×10^{-5} mol/Lit): **a)** Feed flowrate =0.050 Lit/min; **b)** Feed flowrate =0.075 Lit/min; **c)** Feed flowrate =0.100 Lit/min

It was observed that by increasing the bed height volume of breakthrough was also increased which resulted more binding surface area for adsorption, however service time increase resulted in the diffusion of intra-particle for inner pores. These findings depicted that bed height has a larger impact on arsenic removal through the current methodology where 100% removal efficiency found with a height of 30cm.

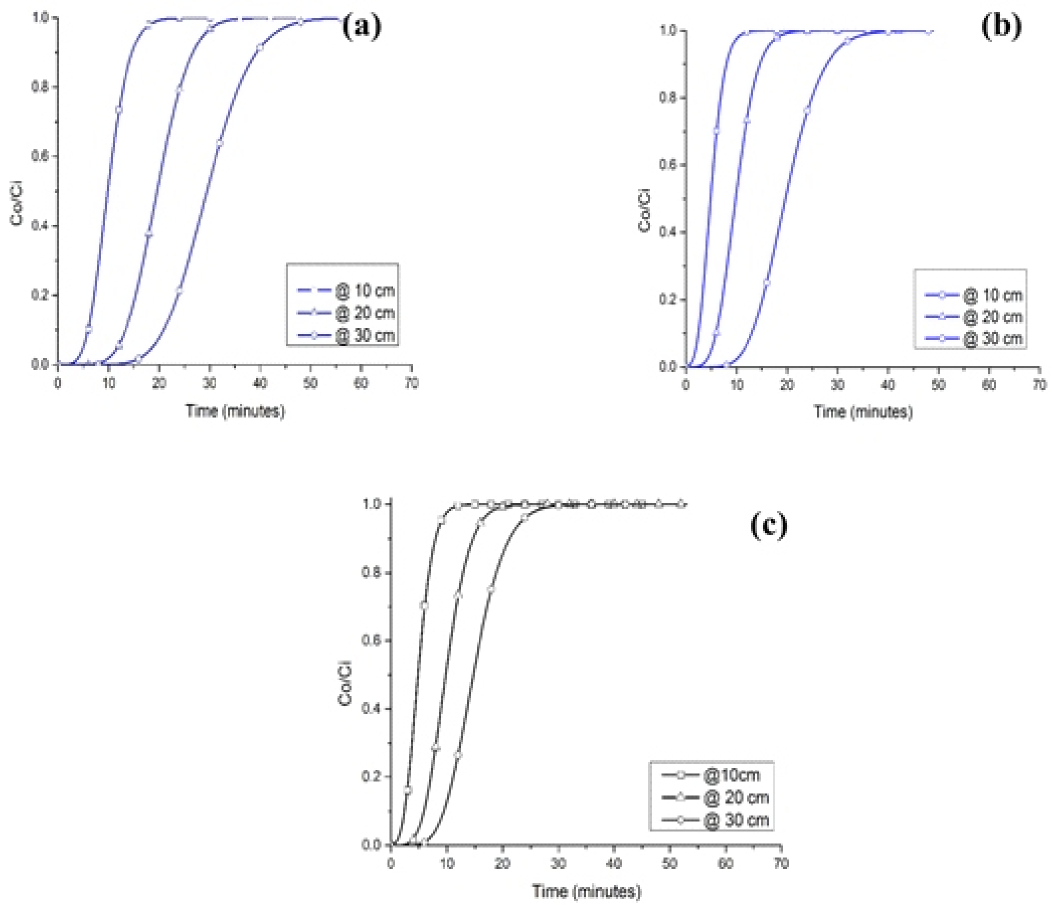

Figure 3: Breakthrough curves for studying the effects of bed height and feed flowrate with constant inlet concentration (6.8×10^{-5} mol/Lit): a) Feed flowrate =0.050 Lit/min; b) Feed flowrate =0.075 Lit/min; c) Feed flowrate = 0.100 Lit/min

3.2 Arsenic Removal As A Function Of Feed Flowrate:

The flowrate of inlet feed was varied to investigate the optimized condition, and separate simulation was carried by keeping inlet concentration as constant (3.4×10^{-5} mol/Lit, 6.8×10^{-5} mol/L, and 10.2×10^{-5} mol/L on each value respectively) for a range of bed heights i.e. (10, 20, and 30cm) considered in current study, and detailed results are plotted in Figure 2, 3 and 4.

The breakthrough volume of the packed bed was decreased by increasing the feed flowrates, which seems that this increase resulted decrease in the residence/contact time of contaminated water with adsorbent bed, ultimately reduced the service time for adsorption, however the decrease in feed flowered resulted a marginal increase in arsenic removal efficiency of adsorbent bed on replicate conditions. Which clearly argued that this decrease actually increased penetration time for contaminated water into the pores of adsorbent bed, therefore these results depicted that intra-particle diffusion has a significant importance in the process of adsorption.

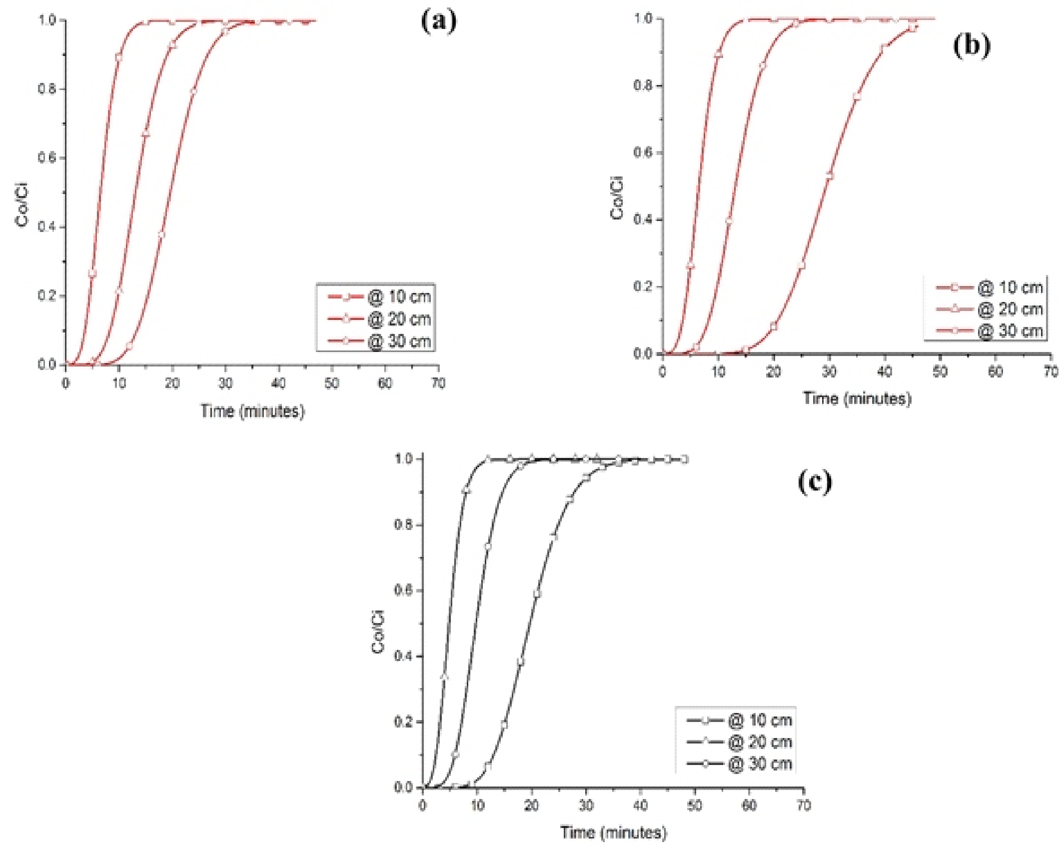

Figure 4: Breakthrough curves for studying the effects of bed height and feed flowrate with constant inlet concentration (10.2×10^{-5} mol/Lit): a) Feed flowrate =0.050 Lit/min; b) Feed flowrate =0.075 Lit/min; c) Feed flowrate =0.100 Lit/min

3.4 Bed Service Time (BST):

Bed service time is the time taken by the bed for removing 90% of impurities (for this research Arsenic is an impurity). This time tells the overall performance of the adsorption column in terms of its saturation time. The greater the BST, the greater the performance of adsorption media. Fig. 5,6, and 7 show the BST w.r.t different bed heights and inlet feed concentrations. The BST was observed very important parameter in the study because increasing the bed height resulted the BST, and BST is directly proportional to the arsenic removal efficiency. There an increase in feed flowrate resulted decrease in BST, which demonstrated that the arsenic removal by using adsorbent bed technique will be efficient on feed flowrates. The maximum BST was observed 22 minutes at 30 cm bed height and 0.00018 mol/L feed flowrate.

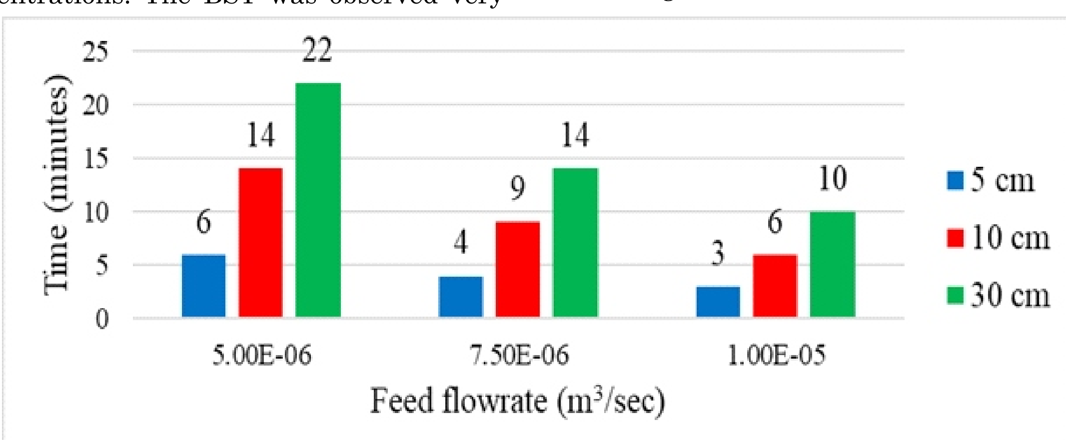

Figure 5: Time computation up to 90% removal of arsenic with initial concentration of 0.00018 mol/L

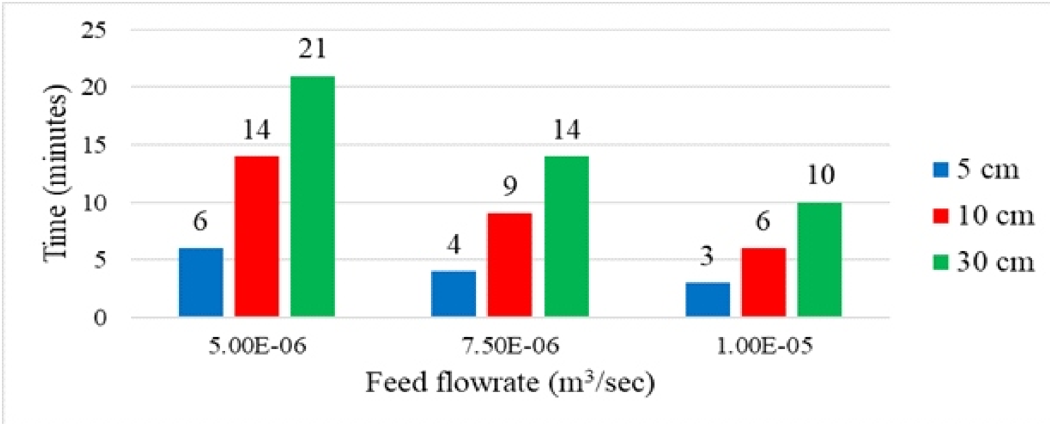

Figure 6: Time computation up to 90% removal of arsenic with initial concentration of 0.00026 mol/L

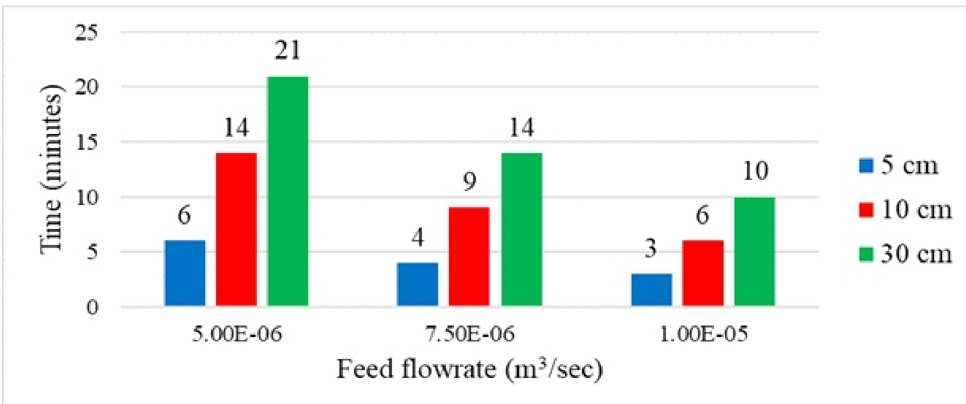

Figure 7: Time computation up to 90% removal of arsenic with initial concentration of 0.00039 mol/L

4. Comparative Study:

S. No	Technique	Adsorbent	Removal %	Reference
1	Adsorption	Aluminum-impregnated tea waste activated carbon	92%	Ghazi Mohd. Sawood etal 2021
2	Adsorption	Modified PAN Fiber	80-98%	Zulfiqar Ali Bhatti etal 2020
3	Oxidation and Adsorption	Fe(III)-Amidoximated (AO) PAN	95.2 %	Luyao Gao etal 2020

5. Conclusions:

The present research shows the effectiveness of simulations for study the arsenic removal using selected adsorbent. Adsorption of Arsenic from aqueous solution was investigated at 25°C in a continuous packed bed column of Arsenic. Polyacrylonitrile fiber (PAN) was used as adsorbent for removal of Arsenic (V) from ground water. Under the operating conditions the arsenic concentration in treated water decreased with the increase in bed height. Arsenic concentration in treated water increased with increase in feed flow rate. Adsorbent bed gave 100% efficiency up to 250 minutes with 340 Kmol/l initial arsenic concentration. It was observed that increasing the bed height increases the BST. Increasing feed flowrate decreases the BST. The maximum BST was observed 22 minutes at 30 cm bed height and 0.00018 mol/L feed flowrate.

It is suggested that arsenic treatment filters should be installed in the arsenic affected areas with MPAN and iron ore adsorbents. Modified PAN fiber prepared by chemical functionalization and iron loading procedure was observed to be an effective method because of its enhanced As^{+3} and As^{+5} removal, adsorption loading (µg/g) and simple method (Bhatti *et al.*, 2020).

Dynamic adsorption on fixed column demonstrated that As(III) in simulated groundwater could be efficiently removed from 500µg/L to <10µg/L within 130 bed volumes (BV). Furthermore, Fe(III)-AO PAN-H_2O_2 may be a promising system for removing low concentration As(III) rapidly and effectively (Gao *et al.*, 2020).

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