Analysis of the Adsorption Capacity of Modified Materials Using a Mathematical Model

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Abstract

To determine the empirical connection between the input and output variables, data-based mathematical simulations were built for this study. Through the use of a computer-generated model, the operation and performance of a system, both in practice and in theory, can be investigated through a process known as simulation. One way to learn about a system's current quirks is to run a simulation. Adsorption system performance can be optimised or predictions about an actual system can be made through the use of simulation. The removal of manganese ions from synthetic waste-water using chemically modified adsorbents was the focus of adsorption investigations conducted at a constant temperature of 25 ± 1 ºC. In the current study, a combination of Resorcinol and Filtrasorb-400 (F-400) granular activated carbon at pH 5 was employed to effectively remove volatile organic compounds (VOCs). The experimental results were utilized to build a mathematical model based on Buckingham's theorem and state-of-the-art mathematical techniques, which were then used to forecast the optimal performance of the system.

DOI Number: 10.48047/NQ.2023.21.4.NQ23016 NeuroQuantology 2023; 21(4): 160-165

Introduction

One promising method for removing trace organic and inorganic contaminants from wastewater is adsorption using porous carbon [1-3]. The adsorbent used in this investigation was granular activated carbon (GAC) due to its high surface area, high porosity, and lack of toxicity throughout a wide range of operating conditions (temperature, pressure, and pH) [4-6]. The parameters needed to optimize GAC's removal efficiency can be predicted with relative ease using mathematical modelling. Multiple mathematical models have been developed to describe and predict the adsorption isotherm of GAC with various hazardous metals [7-10]. This link between adsorbate concentration and pH 5 and 25 +1 ºC temperature was determined using experimental data. In the current investigation, the Buckingham pi-theorem was used to create pi-terms without dimensions, allowing for a more efficient reduction of input parameters. Various design parameters, including adsorption capacity and isotherm constants, were determined using an adsorption isotherm model. This research showed that coal-based GAC combined with an organic ligand like resorcinol was effective at removing manganese ions from synthetic wastewater. Resorcinol is a benzene derivative with two hydroxyl (OH) groups, and this greatly affects the removal process by forming a coordinating bond with the metal ion during adsorption.

Experimental

Mathematical modelling: Using adsorption isotherm, a mathematical relationship

between the amount of adsorbate collected on the surface of the adsorbent and the temperature and pH of the system can be obtained. This hypothesis has been applied primarily to the investigation of multicomponent interference effects during the adsorption of metal content on GAC [11,12]. Many researchers [13-17] reported using the adsorption isotherm model for a wide range of purposes.

Bituminous coal based granular activated carbon namely Filtrasorb 400 (F-400) was used as adsorbents. The partials of approximately equal sized were obtained and the particles retained between 1400 micron and 1600 micron were used in the present study. The GACs particles were considered fit for use when the distilled water obtained after washing was visibly clear and then dried in an oven at 100-110 °C for one hour and stored in $CaCl_2$ desiccator until use. All chemicals used were of AR grade. A stock solution of Mn^{2+} ions was prepared by dissolving required quantity of Manganese Sulphate (E-Merck) in freshly prepared distilled water. The series of solutions of known concentration of Mn^{2+} ions were prepared from the stock solution in 50 mL volumetric flask. Spectrophometrically, standard calibration curve was established for Mn^{2+} [18]. The standard procedure was used to recrystallize resorcinol, whose the melting point was used as a purity test for the sample (Lit. m.p. 110 °C) [19]. All the experimental systems were carried out in batches of five units at a time. For surface modification of GAC, 0.5 g of the carbon and 200 mL of 0.001 M resorcinol solution were taken in each clean reagent bottle. The solution was stirred for about three hours in a constant temperature bath at around 500 rpm. The solution was then filtered off and the carbon was washed thoroughly with distilled water.

The dried carbon particles were then transferred to a clean shaking bottle of wide mouth and 200 ml of manganese solution of pH = 5 was added carefully. The pH of all experimental solution was adjusted to 5 using nitric acid, sodium hydroxide and buffer solutions. All the systems were then stirred for five hours completely with the same speed at constant temperature 25 ± 0.5 °C. The initial and final concentrations of the Mn^{2+} were then determined spectrophotometrically at a wavelength of 527 nm.

Results and Discussion

The mathematical interpretation of the adsorption isotherms for different grades of GAC was studied using mathematical model. These isotherms for different grades of granular activated carbon are shown in Fig.1. The amount of manganese on the GAC, chemically modified by ligand (resorcinol) was determined using the equation

$$q_e = (C_o - C_e) \times \frac{V}{W}$$

Where,

q_e = Concentration of Mn^{2+} on the ligand loaded GAC in mg/mill moles of ligand
C_o = Initial concentration of Mn^{2+} in solution in mg/L.
C_e = Final concentration of the Mn^{2+} in solution in mg/L.
V = Volume of solution in liters
W = Millimoles of the ligand actually present on GAC.

Formulation of Mathematical Model

Data based mathematical simulations was developed to established empirical relationship between inputs and outputs. Simulation is the process of using a model to study the behavior and performance of an actual and theoretical system. In a simulation, models can be used to study the existing characteristics of a system. Simulations allow for the evaluation of a model to optimize the system performance or to make predictions about a real system. The mathematical model is developed using experimental data and contemporary mathematical tools.

The Buckingham theorem is suitable for developing the model because it states that if the inputs and outputs can be represented as dimensionless ∏ terms by dimensional analysis, then they can be represented by

their product and the indices can be obtained by multiple regressions. Any Physical quantity that undergoes a change is called variable. If particular variable is changed without affecting other variables, it is called independent variable. Similarly if a particular variable changes in response to variation of one or more variable it is called dependent variable.

The variables are listed in below.

Sr. No.	Variables	Unit	Type
1	C_o = Initial Concentration of solution	mg/L	Independent Variable
2	R = Rotation per minute	sec^{-1}	Independent Variable
3	C_e = Final Concentration of solution	mg/L	Independent Variable
4	Vs = Volume of solution	Ml	Independent Variable
5	A_{pc} = Average particle size of carbon	cm^2	Independent Variable
6	V_B = Volume of shaking bottle	Ml	Independent Variable
7	W_c = weight of Carbon	Gm	Independent Variable
9	T = Time	Sec	Independent Variable
10	S_{ac} = Surface area of Carbon	cm^2/gm	Independent Variable
11	M = Molecular weight	gm/mole	Independent Variable
12	q_e = Manganese ion adsorbed on GAC	mg/m. mole	Dependent Variable

Buckingham's ∏ theorem was adopted to develop dimensionless ∏ terms for reduction of process parameters. Dimension analysis to reduce number of independent variables

DV2 = f(IV1, IV2, IV3, IV4, IV5…….) (a)

Where

IV = Independent Variable

DV = Dependent Variable

$\Pi_4 = k \times \Pi_1^a \times \Pi_2^b \times \Pi_3^c$ (b)

Where

Π_4 = Function of dependent variable

Π_1, Π_2, Π_3 = Functions of independent variables

a, b, c = Constants

K = Proportionality Constant

$$\Pi_1 = \frac{C_0}{C_e} \qquad \Pi_2 = \frac{W_c S_{ac}}{A_{pa}} \qquad \Pi_3 = \frac{R \times T \times V_c}{pH \times V_s} \qquad \Pi_4 = \frac{q_e}{M}$$

To solve equation (b) Taking Log on both side

$\text{Log } \Pi_4 = n \text{ Log } K + a \text{ Log } \Pi_1 + b \text{ Log } \Pi_2 + c \text{ Log } \Pi_3$ (c)

Where,

$\Pi_1' = \text{Log } \Pi_1$, $\Pi_2' = \text{Log } \Pi_2$ $K' = \text{Log } K$

$\Pi_3' = \text{Log } \Pi_3$ $\Pi_4' = \text{Log} \Pi_4$

$\Pi_4' = nK' + a\,\Pi_1' + b\,\Pi_2' + c\,\Pi_3'$ $\Pi_4' = nK' + a\,\Pi_1' + b\,\Pi_2' + c\,\Pi_3'$ (d)

$\Pi_4' \Pi_1' = nK' \times \Pi_1' + a\,\Pi_1' \times \Pi_1' + b\,\Pi_2' \times \Pi_1' + c\,\Pi_3' \times \Pi_1'$ (e)

$\Pi_4' \times \Pi_2' = nK' \times \Pi_2' + a\,\Pi_1' \times \Pi_2' + b\,\Pi_2' \times \Pi_2' + c\,\Pi_3' \times \Pi_2'$ (f)

$\Pi_4' \times \Pi_3' = nK' \times \Pi_3' + a\,\Pi_1' \times \Pi_3' + b\,\Pi_2' \times \Pi_3' + c\,\Pi_3' \times \Pi_3'$ (g)

From Table IV and VI, putting values in equations d, e, f, g we get,

$(-21.8767) = 10\,K' + (0.8861)\,a + (-4.3573)\,b + (43.0103)\,c$ (h)

$(-1.9543) = 8.861\,K' + (0.0834)\,a + (-0.3861)\,b + (3.8111)\,c$ (i)

$(9.5323) = (-43.573)\,K' + (0.3861)\,a + (1.8986)\,b + (-18.7408)\,c$ (j)

$(-94.0925) = (430.103)\,K' + (3.8111)\,a + (-18.7408)\,b + (184.9886)\,c$ (k)

By solving equations h, i, j, k we get

$K' = 0.0000$, $a = -3.2457$, $b = -6.3998$, $c = -1.0901$

Conclusions

In present investigation experimental data based model was developed to simulate adsorption process for removal of manganese ion. The approach of mathematical formulation provides an excellent way to analyze the adsorption process to optimize the removal of metal content from aqueous phase.

The main objective of the work is not merely developing the models but set of independent parameters which optimizes the efficiency of selected adsorbent for the removal of pollutants. The mathematical data clearly showed the dependence of adsorptive capacity of carbon on surface area as well as concentration of adsorbate.

Acknowledgements

The authors are thankful to The Principal, Science College Congress Nagar, Nagpur and The Principal, Santaji College, Nagpur and for providing necessary laboratory facilities to carry out the experimental work.

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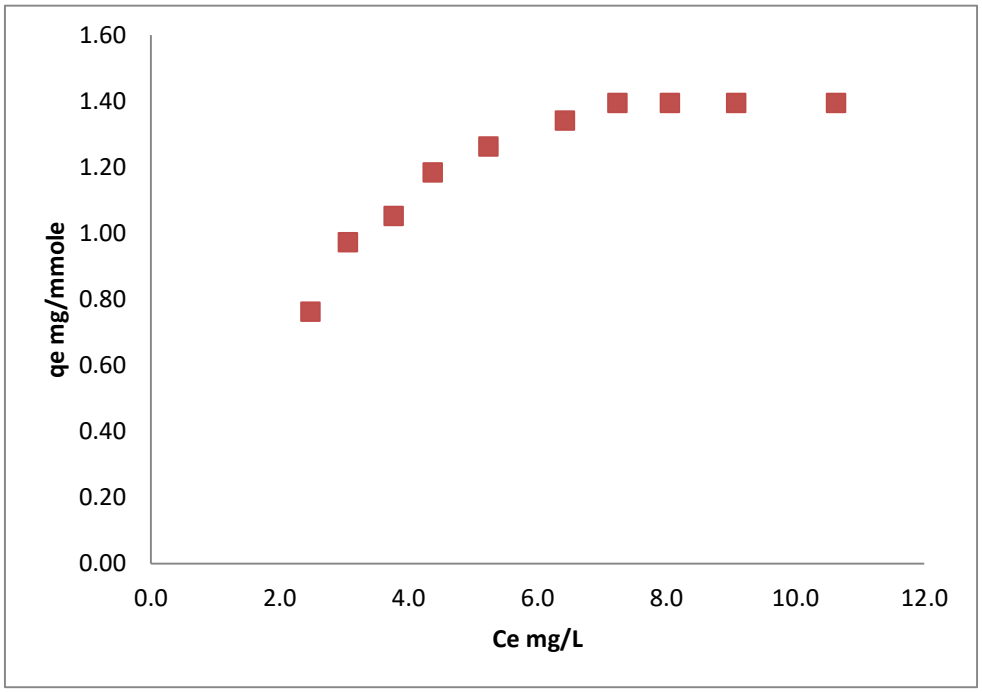

Fig. 1 : Adsorption Isotherm

System : GAC F-400- Resorcinol-Mn^{2+}

Table : I
Adsorption Isotherm
System : F-400_ Resorcinol _Mn^{2+}

Sr. No.	C_0 IV1	Ce IV2	pH IV3	A_{pc} IV4	R IV5	V_s IV6	V_B IV7	W_c IV8	T IV9	S_{ac} IV10	M IV11	q_e DVI
1	3.2368	2.4737	5	1500	500	200	300	0.5	300	1100	184.106	0.7632
2	4.0263	3.0526	5	1500	500	200	300	0.5	300	1100	184.106	0.9737
3	4.8158	3.7632	5	1500	500	200	300	0.5	300	1100	184.106	1.0526
4	5.5526	4.3684	5	1500	500	200	300	0.5	300	1100	184.106	1.1842
5	6.5000	5.2368	5	1500	500	200	300	0.5	300	1100	184.106	1.2632
6	7.7632	6.4211	5	1500	500	200	300	0.5	300	1100	184.106	1.3421
7	8.6316	7.2368	5	1500	500	200	300	0.5	300	1100	184.106	1.3947
8	9.4474	8.0526	5	1500	500	200	300	0.5	300	1100	184.106	1.3947
9	10.4737	9.0789	5	1500	500	200	300	0.5	300	1100	184.106	1.3947
10	12.0263	10.6316	5	1500	500	200	300	0.5	300	1100	184.106	1.3947

Table : II
Adsorption Isotherm Data Converted to Dimensionless Analysis
System : F-400_ Resorcinol _Mn^{2+}

Sr. No.	Π_1	Π_2	Π_3	Π_4	Log (Π_1) Π_1	Log (Π_2) Π_2	Log (Π_3) Π_3	Log (Π_4) Π_4
1	1.3085	0.3667	20000	0.0041	0.1168	-0.4357	4.3010	-2.3825
2	1.3190	0.3667	20000	0.0053	0.1202	-0.4357	4.3010	-2.2766
3	1.2797	0.3667	20000	0.0057	0.1071	-0.4357	4.3010	-2.2428
4	1.2711	0.3667	20000	0.0064	0.1042	-0.4357	4.3010	-2.1916

5	1.2412	0.3667	20000	0.0069	0.0938	-0.4357	4.3010	-2.1636
6	1.2090	0.3667	20000	0.0073	0.0824	-0.4357	4.3010	-2.1373
7	1.1927	0.3667	20000	0.0076	0.0765	-0.4357	4.3010	-2.1206
8	1.1732	0.3667	20000	0.0076	0.0694	-0.4357	4.3010	-2.1206
9	1.1536	0.3667	20000	0.0076	0.0621	-0.4357	4.3010	-2.1206
10	1.1312	0.3667	20000	0.0076	0.0535	-0.4357	4.3010	-2.1206
∑	12.2792	3.6667	200000.0000	0.0660	0.8861	-4.3573	43.0103	-21.8767

Table : III

Logarithmic Value

System : F-400_ Resorcinol _Mn^{2+}

Π_1 x Π_1	Π_1 x Π_2	Π_1 x Π_3	Π_1 x Π_4	Π_2 x Π_2	Π_2 x Π_3	Π_2 x Π_4	Π_3x Π_3	Π_3 x Π_4	Π_4 x Π_4
0.0136	-0.0509	0.5023	-0.2782	0.1899	-1.8741	1.0381	18.4989	-10.2470	5.6761
0.0145	-0.0524	0.5171	-0.2737	0.1899	-1.8741	0.9920	18.4989	-9.7919	5.1831
0.0115	-0.0467	0.4607	-0.2402	0.1899	-1.8741	0.9772	18.4989	-9.6463	5.0301
0.0109	-0.0454	0.4481	-0.2283	0.1899	-1.8741	0.9550	18.4989	-9.4263	4.8033
0.0088	-0.0409	0.4036	-0.2030	0.1899	-1.8741	0.9427	18.4989	-9.3058	4.6812
0.0068	-0.0359	0.3545	-0.1762	0.1899	-1.8741	0.9313	18.4989	-9.1925	4.5680
0.0059	-0.0334	0.3292	-0.1623	0.1899	-1.8741	0.9240	18.4989	-9.1207	4.4968
0.0048	-0.0302	0.2984	-0.1471	0.1899	-1.8741	0.9240	18.4989	-9.1207	4.4968
0.0039	-0.0270	0.2669	-0.1316	0.1899	-1.8741	0.9240	18.4989	-9.1207	4.4968
0.0029	-0.0233	0.2303	-0.1135	0.1899	-1.8741	0.9240	18.4989	-9.1207	4.4968
∑0.0834	∑-0.3861	∑3.8111	∑-1.9543	∑1.8986	∑-18.7408	∑9.5323	∑184.9886	∑-94.0925	∑47.9292