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Research Article

Optimization of Bohart-Adams Model of the Fixed-Bed Adsorption Column for Treating Gas from Basra Gas Treating Unit

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ABSTRACT

Natural gas is an essential energy source that requires purification before transportation and use. At the Basrah Natural Gas Liquification (BNGL) plant, the gas dehydration unit (GDU) is tasked with minimizing water content to avert hydrate formation, corrosion, and related complications. An adsorption process using molecular sieves is necessary for separation from water vapor.An enhancement on the adsorption stage of the GDU was implemented by fitting Bohart-Adams model over 6 months using both genetic algorithm (GA) for optimization and parametersand gas concentration which include the gas velocity.Via Bohart-Adams model outlook for breakthrough behavior and investigation of the efficiency of adsorbing processThe critical parameters are optimized with a genetic algorithm in Bohart-Adams model -- e.g., adsorption rate constant (K) and saturation concentration (N_0). Optimization greatly reduced the discrepancy between theory and experimental data, improving the model's predictive ability for adsorption behavior.Also, with the aid of GA we were able to find the optimum parameter values that raised the dehydration unit's overall efficiency.The results show that the combined effect of flow rate and water vapor concentration of the breakthrough curve is large. Where the best performance was achieved Water vapor concentrations at 450 to 500 ppmV within a gas stream rate of 100 to 110 million standard cubic feet per day (MMSCFD) did not require any reactivation as occurred during avery successful test having these settings Reactivation was unnecessary under these conditions because it had completely honest behavior.

Keywords: Gas dehydration, Bohart-Adams model, Molecular sieve adsorption, Genetic algorithm optimization

1. INTRODUCTION

Natural gas is a crucial energy source that requires purification before transportation and use. Water, an impurity in natural gas, causes corrosion, hydrate formation, and obstruction of transmission lines. At the Basrah Natural Gas Liquification (BNGL) plant, dehydration is performed using three-bed molecular sieve vessels and switching valve arrangements. These vessels are filled with a water-adsorbing media bed along with associated floating mesh and support bed arrangements. In regeneration mode, the saturated adsorbent is regenerated using hot regeneration gas provided by the regeneration gas heater and circulated by a regeneration gas compressor [1]. The objective of gas dehydration is to achieve a dried gas concentration of less than 3 ppm. The regeneration gas heater was designed to deliver heated gas to regenerate the adsorber at a temperature of 290° C. The dehydration absorbers operate for a total cycle time of 15 h, with a 10 h adsorption cycle and a 5 h regeneration cycle. The regeneration cycle was further divided into three hours for heating, one hour and 15 min for cooling, and 45 min for standby time, resulting in a total cycle time of 15 h for all three beds. Optimization of the Bohart-Adams model is critical for industrial gas dehydration, as it sets out the theoretical approach to performance of the adsorption bed. In this sense, it is akin to sailing closely into operational parameters and promises a highly controlled system.Despite the wide use of molecular sieves, current models often do not take dynamic changes in the rate of adsorption adsorption stage, flow-quarter conditions and mass transfer (concentration) limitations to account for effects by including a genetic algorithm (GA)

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with the Bohart-Adams model, this study hopes to improve predictive accuracy in adsorption modeling and thus help reduce costs, save energy as well as prolong molecular sieve life.In several studies on molecular sieves Van Ness (1961) used adsorption thermodynamics to improve molecular sieve performance and predict capacity under different conditions [1]. Adamson (1982) developed surface adsorption models for molecular sieves and optimized some molecular sieve designs to achieve higher dehydration efficiency [2]. Ruthven (1984) devised finite-rate mass-transfer models for adsorption processes with the aim of lowering solvent requirements[3]. Bohart and Adams (1920) introduced a breakthrough model to predict the adsorption bed performance and optimize the design parameters [4-7]. Grace (1997) applied fluidized bed models to improve the efficiency of high-flow adsorption systems [8]. Sircar (2002) combined kinetic and equilibrium models to develop tailored solutions for energy usage reduction and enhanced adsorption processes [9 ,10]. Although these studies have laid the foundation for adsorption modeling, few have explored the integration of genetic algorithms to optimize adsorption conditions in industrial gas dehydration. This study aims to bridge this gap by applying a genetic algorithm to the Bohart-Adams model, further optimizing key parameters such as adsorption rate constants and saturation concentrations under real operating conditions. Consequently, this research provides a novel approach that improves molecular sieve activation, enhances unit performance, and ensures more efficient gas dehydration at BNGL.

2. MATERIALS & METHODS

The dehydration absorbers each had a capacity of 47.8 m^3 with the mechanical and process parameters listed in Table 1. Figs. 1(a) and (b) show the three-dimensional model for BNGL Fig. 2 shows the UNISIM model for the BNGL dehydration unit used in this study.

Table 1. Dehydration adsorber mechanical and process parameters [20].

Type	**Vertical**
Diameter (mm)	2438 ID
Length (mm)	8100T/T
Design Pressure (barg)	75.8
Design Temperature (°C)	313
MDMT (°C) @ Pressure (barg) / MMT	-29 @ 75.8 / -13.4
Operating Temperature (°C)	36.8 to 55.4
Operating Pressure (barg)	65.4

Table 2. Feed stream composition.

Design FEED STREAM

	Components	Composition (Mol. Frac) Summer Case	Winter Case			Composition (Mol. Frac) Summer	Winter
1	H_2S	0.0000013	0.00000143	18	M-Mercaptan	0.0000	0.0000
2	CO_2	0.0000014	0.00000139	19	E-Mercaptan	0.0000	0.0000
3	Nitrogen	0.0079	0.0077	20	nPMercaptan	0.0000	0.0000
4	Methane	0.6105	0.6568	21	nBMercaptan	0.0000	0.0000
5	Ethane	0.1911	0.1949	22	Benzene	0.0002	0.0001
6	Propane	0.1032	0.0890	23	Toluene	0.0001	0.0001
7	i-Butane	0.0177	0.0117	24	E-Benzene	0.0000	0.0000
8	n-Butane	0.0442	0.0267	25	p-Xylene	0.0000	0.0000
9	i-Pentane	0.0100	0.0052	26	o-Xylene	0.0000	0.0000
10	n-Pentane	0.0109	0.0057	27	n-BBenzene	0.0000	0.0000
11	n-Hexane	0.0010	0.0007	28	m-Xylene	0.0000	0.0000
12	n-Heptane	0.0003	0.0003				
13	n-Octane	0.0000	0.0000		**Total**	**1.00**	**1.00**
14	n-Nonane	0.0000	0.0000				
15	n-Decane	0.0000	0.0000				
16	H_2O	0.0029	0.0012				

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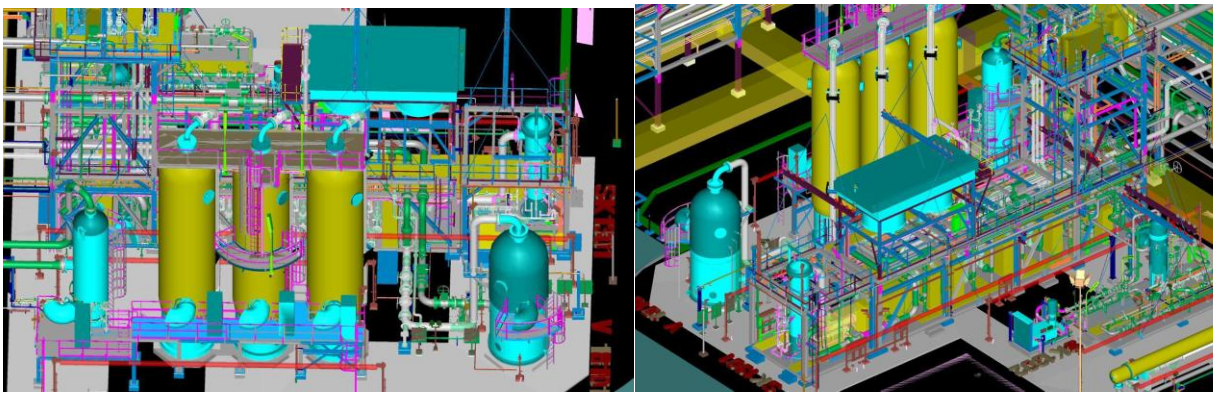

(a) (b)

Fig. 1. (a) (b) Three-dimensional model for BNGL dehydration unit.

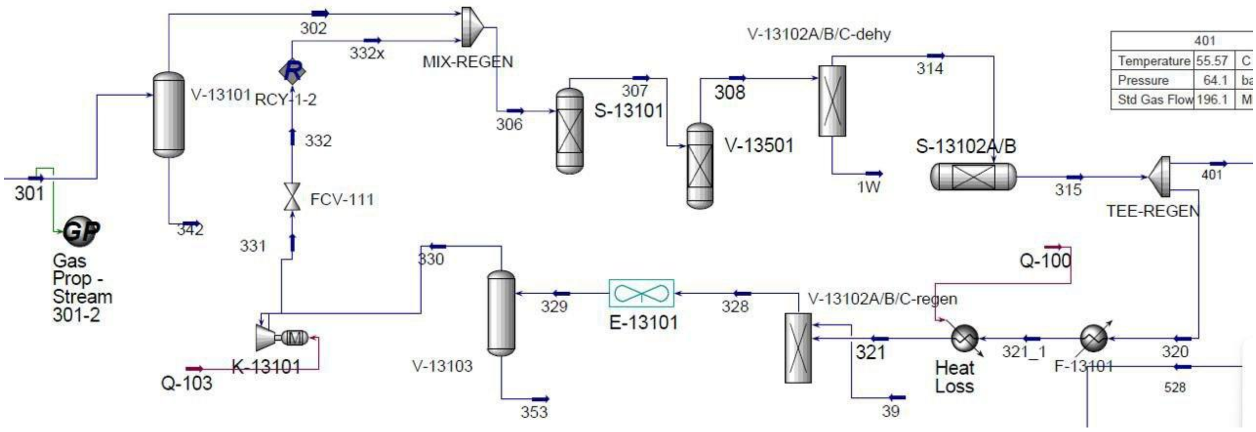

Fig. 2. UNISIM R480 model for BNGL dehydration unit

3. MATHEMATICAL MODELING

The model assumed that radial and axial dispersions were absent in the mass balance equation, and radial dispersion was also absent in the energy balance equation. The gas flow was presumed to move downward in the adsorption and cooling beds and upward in the heating bed [11] [12].

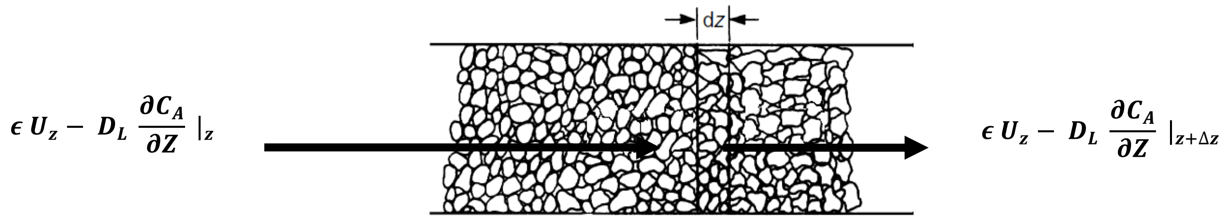

Fig. 3. Fixed bed adsorber column.

$$\epsilon S\left[-D_L \frac{\partial C_A}{\partial z} + C_A U_z\right]_{z,t} - \epsilon S\left[-D_L \frac{\partial C_A}{\partial z} + C_A U_z\right]_{z+\Delta z,t} = \left[S\Delta Z\epsilon \frac{\partial C_A}{\partial t}\right]_z + \left[S\Delta Z(1-\epsilon)\frac{\partial C_{As}}{\partial t}\right]_z \quad (1)$$

This equation represents the mass balance of a differential control volume in an adsorption column, accounting for axial dispersion, convective transport, and accumulation in both gas phases.

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Rearranging the equation above and dividing both sides by $\epsilon\ S\ \Delta Z$ gives:

$$\frac{D_L \frac{\partial C_A}{\partial Z}|_{z+\Delta z,t} - D_L \frac{\partial C_A}{\partial Z}|_{z,t}}{\Delta Z} - \frac{C_A U_z|_{z+\Delta z,t} - C_A U_z|_{z,t}}{\Delta Z} = \frac{\partial C_A}{\partial t}|_z + \frac{1-\epsilon}{\epsilon}\frac{\partial C_{As}}{\partial t}|_z \tag{2}$$

By applying a limiting process to ΔZ and assuming that the axial diffusion coefficient and velocity are constant, Eq. (2) can be expressed as follows:

$$\left(D_L \frac{\partial^2 C_A}{\partial Z^2}\right)_t - \left(U_z \frac{\partial C_A}{\partial Z}\right)_t = \left(\frac{\partial C_A}{\partial t}\right)_z + \left(\frac{1-\epsilon}{\epsilon}\frac{\partial C_{As}}{\partial t}\right)_z \tag{3}$$

The Bohart–Adams model describes the adsorption of a single component. The dispersion axial term and mass transfer zone exert no influence on the fluid velocity; hence, the velocity was considered constant in this model, characterizing it as plug flow in a trace system. Considering the flow to be unidirectional, the fundamental mass-balance equation is:

$$\left(U_z \frac{\partial C_A}{\partial Z}\right)_t + \left(\frac{\partial C_A}{\partial t}\right)_z + \left(\frac{1-\epsilon}{\epsilon}\frac{\partial q}{\partial t}\right)_z = 0 \tag{4}$$

Letting

$$\left(\frac{\partial q}{\partial t}\right)_z = K_{AB} C(q_\circ - q) \tag{5}$$

The Chu (2020) and Bohart-Adams models are mathematically equivalent. The following logistic equation represents the response of the model. The Bohart-Adams model parameters are outlined in Table 3.

$$ln\left(\frac{C_o}{C} - 1\right)_t = a - bt \tag{6}$$

Table 3. Bohart-Adams model parameters.

Model	Bohart-Adams
A	$K_{BA}N_oZ/u$
B	$K_{BA}C_O$

Therefore,

$$\left(\frac{C_o}{C}\right)_z = 1/(1 + \exp\ \langle K_{BA} C_0 \left[\frac{N_o Z}{C_o U} - t\right]\rangle \tag{7}$$

with **e**ach symbol in the equation described below:

Symbols	*Description*	*Unit*
C_o	initial concentration	ppmV
C	Case concentration	ppmV
N_o	saturation capacity from BA model	mg/L.cm
K_{AB}	Rate constant in BA model	L/mg.s
Q	Volumetric flow rate	MMSCFD
Z	Bed depth of the column	Cm
T	Time required for 50% adsorbate breakthrough from BA Model	Sec
q_0	sorption capacity	mg/L
Uz	The superficial velocity of the gas phase in the z-direction	m/s
DL	Axial dispersion coefficient	m^2/s
ϵ	Void fraction (porosity) of the packed bed	Dimensionless
S	The cross-sectional area of the packed bed	m^2
ΔZ	Small differential length along the the z-direction	m

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4. EXPERIMENTS

The work on the gas dehydration unit (GDU) at BNGL was conducted over a six-month period to identify the parameters directly influencing the process and to provide input data for the Bohart-Adams model implemented in MATLAB 2024a. The gas dehydration unit optimization was conducted using GA because compared to conventional optimization approaches, GAs are better at handling complicated, nonlinear, and multi-objective issues. Adsorption rate, bed saturation, and flow rate are three operational parameters in molecular sieve dehydration that are intricately related to one another. In contrast to the GA population-based search techniques, which guarantee a more thorough exploration of the solution space, traditional gradient-based approaches frequently converge to local optima and struggle with nonlinearities [13].

Unlike traditional optimization methods, GA does not rely on mathematical formulations or explicit derivative information, thereby offering a great deal of flexibility when dealing with experimental and empirical data [14]. In addition, GA can easily manage both continuous (temperature and flow rate) and discrete (cycle duration and switching time) variables in the optimization of the dehydration process [15]. Because GA is based on mutation and crossover procedures, it increases the likelihood of discovering a global optimum and helps avoid premature convergence, in contrast to approaches based on Newton or gradient descent, which can get trapped in local minima [16]. These benefits prompted us to select GA as the best optimization strategy for boosting the efficiency of the BNGL gas dehydration unit.

The continuous-flow adsorption results were recorded on the GDU at BNGL. In addition, multiple experimental conditions were tested to acquire a comprehensive understanding of the adsorption process. Gas concentrations were varied (C_1 = 300 ppmV, C_2 = 350 ppmV, ..., C_{14} = 1000 ppmV) while maintaining an internal diameter of 2438 cm and an adsorber height of 8100 cm. The gas flow rate remained constant at 60 million standard cubic feet per day (MMSCFD). In other studies, the concentration remained constant while altering the flow rate (e.g., Q_1 = 40 MMSCFD, Q_2 = 50 MMSCFD, ..., Q_{10} = 130 MMSCFD). Pressure and temperature were held constant during both tests to isolate the effects of variations in flow rate.

5. RESULTS AND DISCUSSION

The objective was to predict the breakthrough behavior in an adsorption column using the Bohart-Adams model, with an emphasis on concentration and flow rate fluctuations over time. Key model parameters, namely saturation concentration (N_0) and adsorption rate constant (K) [17], were optimized using a systematic methodology. The goal of this optimization was to minimize the discrepancy between the concentration data obtained experimentally and determined theoretically. With the help of the MATLAB code, a breakthrough curve was created, plotting concentration ratio (C/C_0) as a function of time. The efficiency and performance of the adsorption column is clearly indicated in the graph. At the point where C/C_0 = 0.5, the adsorption column starts to lose its efficacy. This point was marked and underlined as an important point. To measure how well the model predicted the outcomes, R^2 values were also computed. These values, shown in Table 4, provide a statistical measure of the alignment between the experimental data and outcomes predicted by the model, serving as a strong and trustworthy assessment of the adsorption system.

Table (4) Bohart-Adams model parameters under different phases

Phase	Concentration (ppmV)	Flow rate (MMSCAFD)	Pressure (bar)	Temperature (C^0)	K (L/mg,s)	N^0 (mg/L.cm)	R^2
I	100	100	65.3	55.7	0.0069	893.68	1.1789
	200	100	65.3	55.7	0.0072	950.189	1.1528
	300	100	65.3	55.7	0.0085	940.747	1.0642
	400	100	65.3	55.7	0.009	937.7586	1.0308
	450	100	65.3	55.7	0.0097	978.86	1.0002
	500	100	65.3	55.7	0.01	926.47	9.996
	550	100	65.3	55.7	0.012	922.305	9.982

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	600	100	65.3	55.7	0.0127	938.39	0.9741
	650	100	65.3	55.7	0.0130	973.568	0.9639
	700	100	65.3	55.7	0.0175	966.712	0.9618
	750	100	65.3	55.7	0.0184	964.54	0.9524
	800	100	65.3	55.7	0.0219	968.093	0.9477
	850	100	65.3	55.7	0.0242	945.3	0.9402
	900	100	65.3	55.7	0.0280	998.985	0.9374
	950	100	65.3	55.7	0.0374	966.57	0.9352
	1000	100	65.3	55.7	0.0459	981.5	0.9327
II	450	40	65.3	55.7	0.0061	946.32	1.2711
	450	50	65.3	55.7	0.007	902.08	1.1745
	450	60	65.3	55.7	0.008	920.87	1.0967
	450	70	65.3	55.7	0.0081	978.5881	1.0915
	450	80	65.3	55.7	0.0089	877.00	1.0470
	450	90	65.3	55.7	0.0096	932.249	1.0160
	450	100	65.3	55.7	0.0097	991.607	1.0129
	450	110	65.3	55.7	0.01	963.05	1.0003
	450	120	65.3	55.7	0.0108	998.6	0.9737
		130	65.3	55.7	0.011	960.56	0.9697

5.1. Effect of concentration on breakthrough curve

The effect of the water vapor concentration on the breakthrough curves is shown in Fig. 4. Both penetration and depletion times decrease as the initial water vapor concentration increases. The water vapor removal rate decreases when the starting water vapor concentration is increased to 600 mg/L. This is attributed to the rapid saturation of binding sites within the column. When the concentration exceeds 900 mg/L, the limitations of insufficient adsorption capacity become increasingly apparent. An optimal concentration range of 450–500 mg/L, produced positive adsorption coefficient. At higher adsorbate concentrations, with *faster breakthrough*, a higher inlet concentration of water vapor leads to faster saturation of the adsorbent material, and with *reduced bed utilization*, the rapid consumption of active sites results in earlier breakthroughs and decreased adsorption bed efficiency. At lower adsorbate concentrations, with *delayed breakthrough*, a lower inlet concentration allows the adsorbent material to operate longer before saturation occurs, and with *improved adsorption efficiency*, the mass transfer zone is more effective and the adsorbent capacity is utilized more efficiently [18]. In Fig. 5, the predicted values are higher than the experimental data, whereas in Fig. 6, this trend is reversed, indicating that the bed efficiency has been reduced, accompanied by an increase in the total cycle count.

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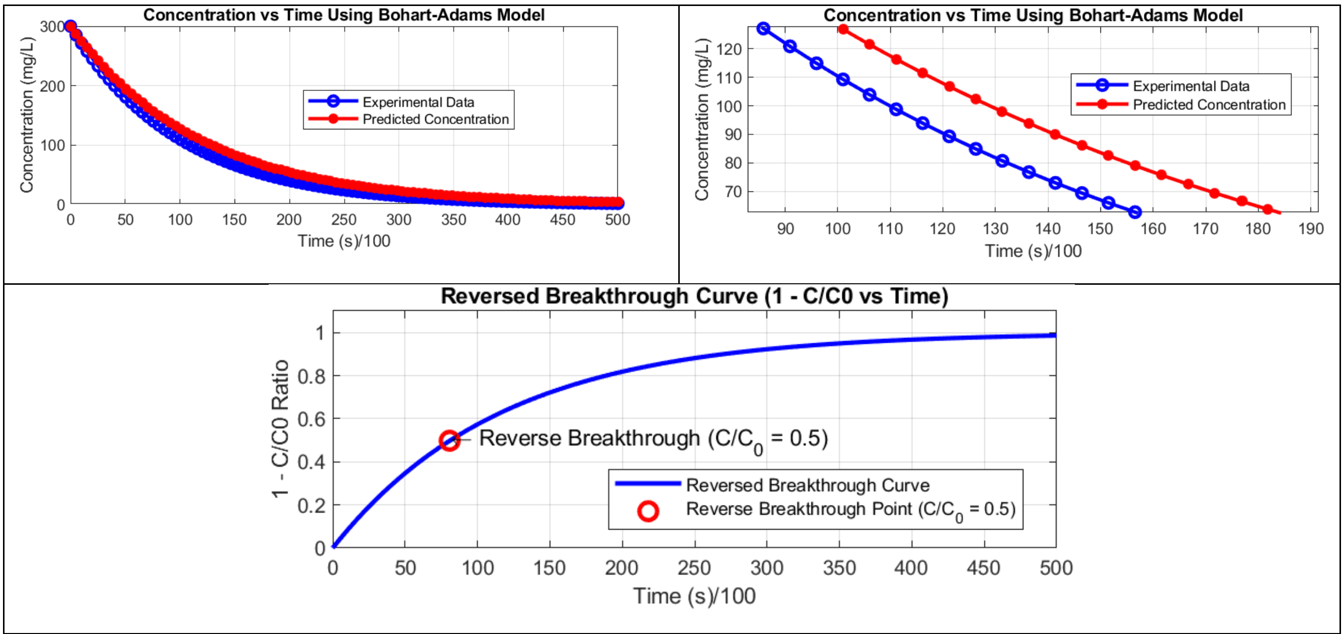

Fig. 4. Bed behavior at a concentration of 300 mg/L and flow rate of 100 MMSCFD

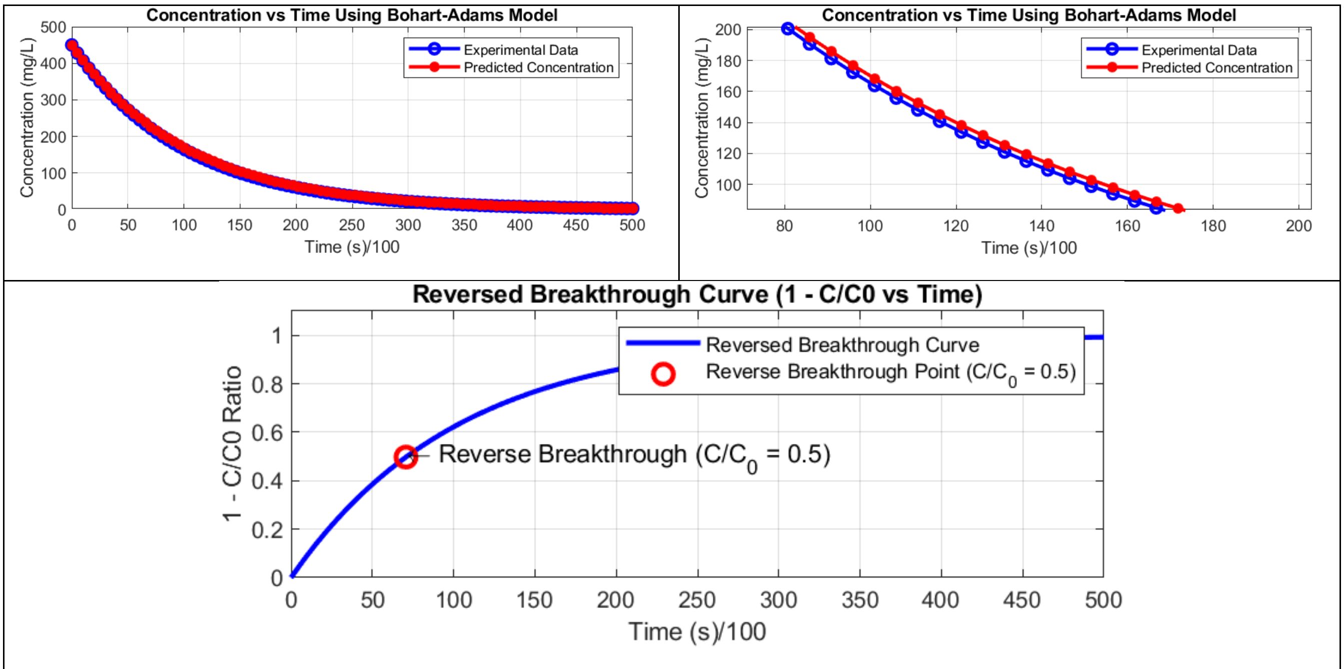

Fig. 5. Bed behavior at a concentration of 450 mg/L and a flow rate of 100 MMSCFD

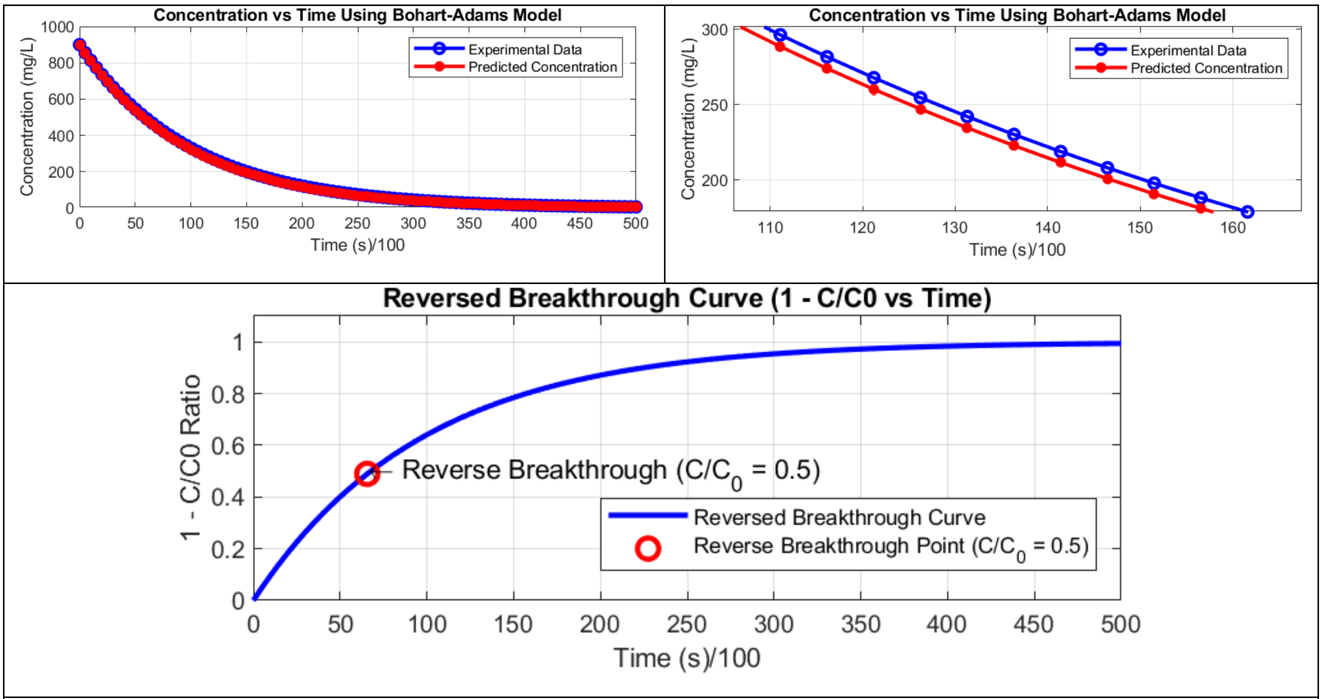

Fig. 6. Bed behavior at a concentration of 900 mg/L and flow rate of 100 MMSCFD

5.2. Effect of flow rate on breakthrough curve

The diffusion curves at different flow rates, shown in Fig. 7, indicate that dispersion occurs more swiftly at higher flow rates. The duration required for complete saturation increases as the flow rate decreases. At reduced intake flow rates, the entering gas has more time to engage with the molecular sieve, leading to enhanced elimination of water vapor molecules inside the column. The results demonstrate an inverse correlation between the flow rate and removal efficiency after the optimal condition (100 - 110 MMSCFD) is attained, whereas a direct correlation exists before this range, indicating the possibility of material inactivation due to inadequate flow in certain instances. An increased flow rate with accelerated breakthrough elevated gas flow rates, decreases the residence time of the adsorbate in the bed, thereby reducing the contact duration between gas and adsorbent. The change from total adsorption to saturation occurs more suddenly because of restricted diffusion and mass transfer . The reduced flow rate in prolonged breakthrough decreases the flow rates, facilitating an extended residence time, which improves the interaction between adsorbate and adsorbent. The mass transfer zone exhibits increased uniformity, leading to the progressive saturation of the bed. In Figs. 7 and 8, the projected values exceed the experimental data, whereas in Fig. 9, the inverse tendency exists. This indicates that under these conditions, the bed efficiency declines, resulting in an increased overall cycle count.

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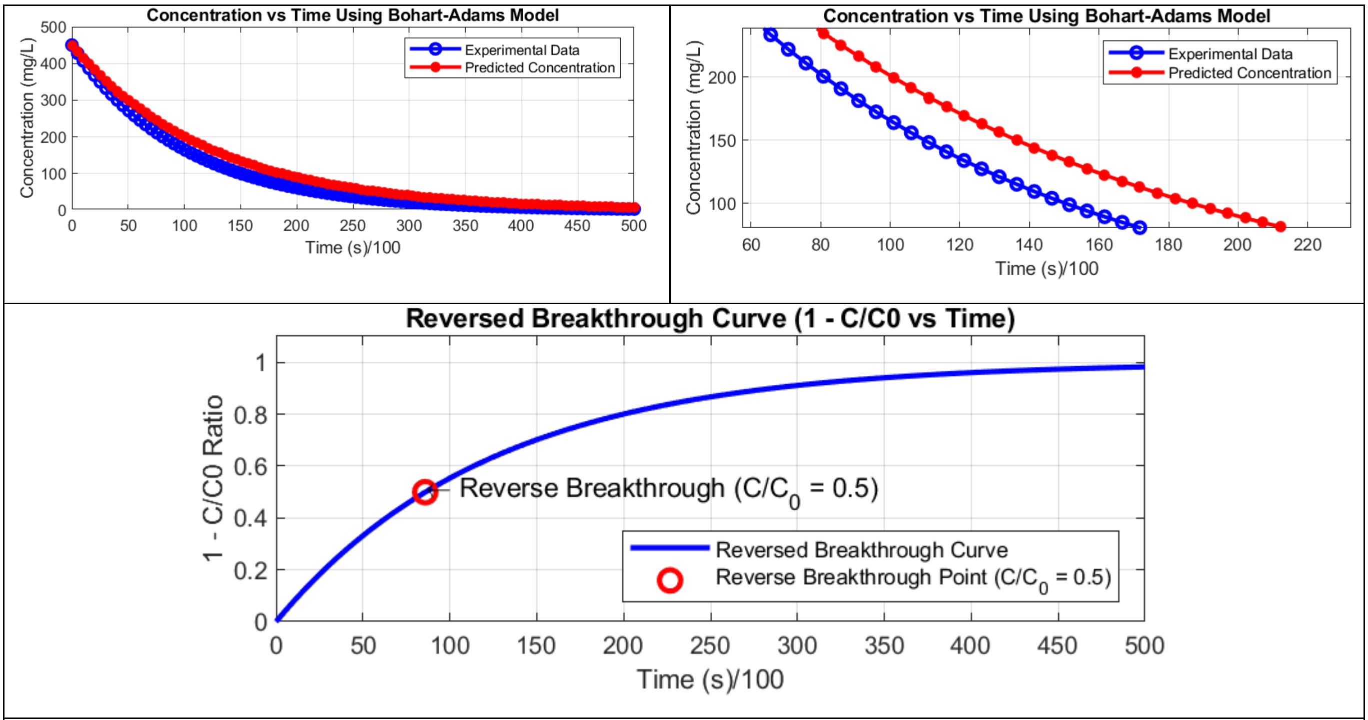

Fig. 7. Bed behavior at a concentration of 450 mg/L and flow rate of 70 MMSCFD0

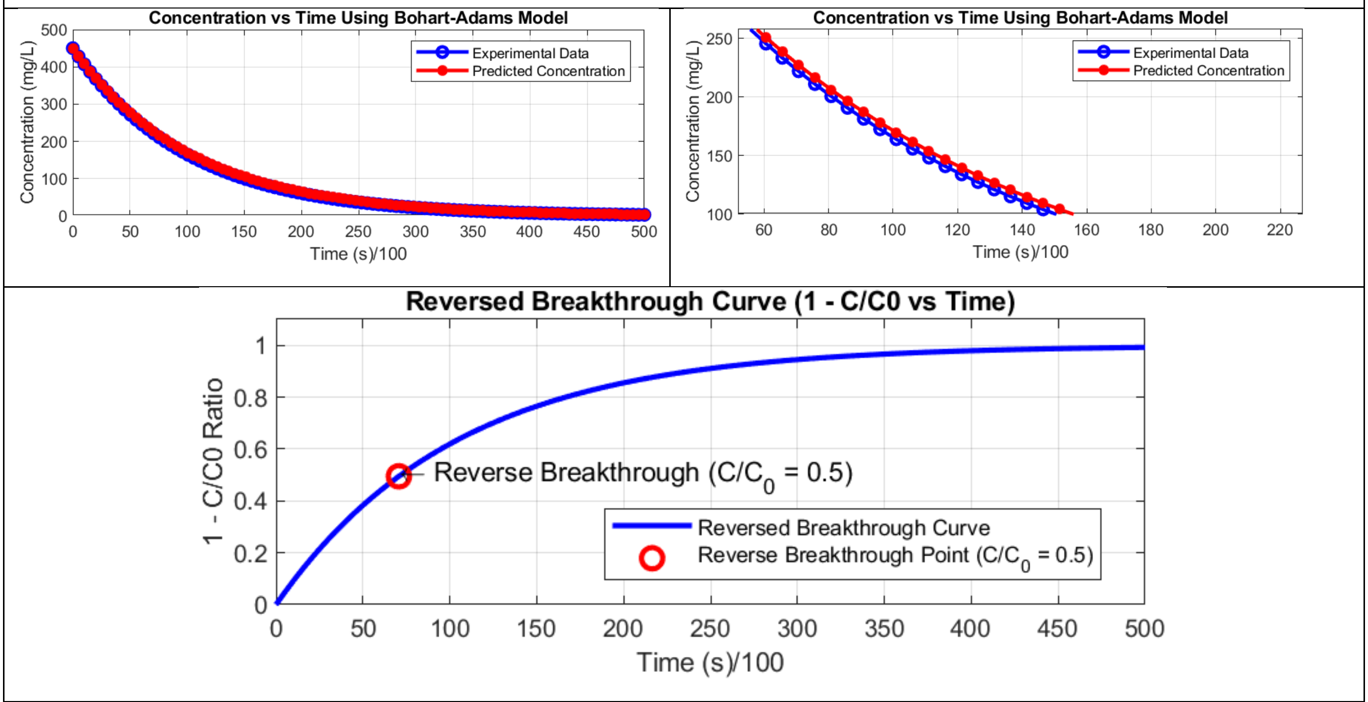

Fig. 8. Bed behavior at a concentration of 450 mg/L and flow rate of 100 MMSCFD

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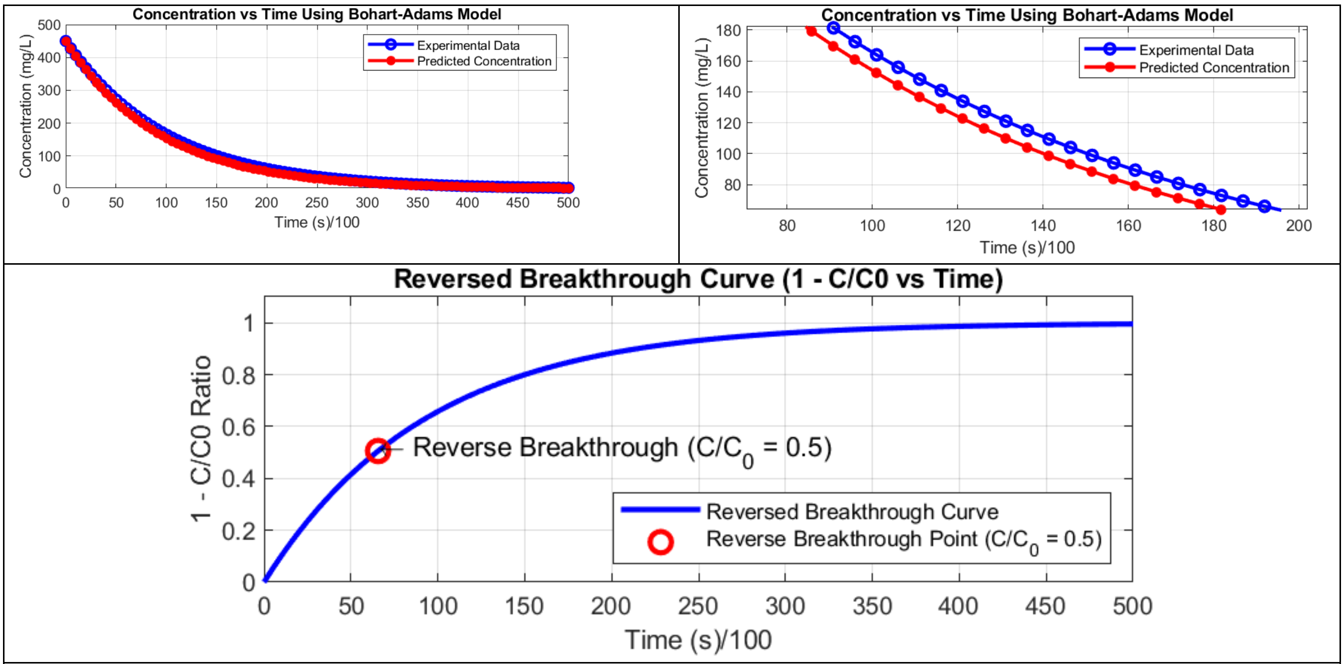

Fig. 9. Bed behavior at a concentration of 450 mg/L and flow rate of 120 MMSCFD

5.3. Combined effects of concentration and flow rate

From the previous result, it can be concluded that 450-500 ppm concentration flow rates of 100-110 MMSCFD is optimal for operating conditions. Breakthroughs are most efficiently managed when concentrations are moderate, thereby avoiding extreme saturation. The flow rates were balanced to provide a sufficient contact time without causing operational inefficiencies [19,20]. Based on these results, water vapor concentrations of 450-500 ppmV and flow rates of 100-110 MMSCFD demonstrated optimal performance in the gas dehydration units and in the mass transfer zone (MTZ), which is the region within the bed where the adsorbate concentration transitions from fully adsorbed to the breakthrough level. Higher concentrations or flow rates compress the MTZ, leading to inefficient bed capacity utilization.

6. CONCLUSION

This article uses a genetic algorithm and the Bohart-Adams model to optimize the operational performance of the gas dehydration plant at Basrah Gas Co. To this end, the main goal of this study was to evaluate the effect of adsorption over a period of six months by following closely the main system parameters such as the amounts of gas and water vapor. Using a genetic algorithm, the most important model parameters, such as saturation concentration and adsorption rate constant, are determined. The efficiency of the unit was systematically increased by optimizing conditions that allowed effective water vapor adsorption.This result shows that the concentration of water vapor and the flow velocity both have rather strong effect on the breakthrough curve. Optimal performance was observed at gas flow rates of 100–110 MMSCFD and water vapor concentrations of 450–500 ppmV, with the outer concentration remaining below 1 ppmV. Optimal adsorption occurs under these conditions, enhancing the overall performance of the dehydration unit. This paper presents a comprehensive strategy for enhancing gas dehydration systems at BNGL, aimed at optimizing water removal from natural gas and significantly increasing gas quality . The findings indicate that the integration of mathematical model approaches with optimization algorithms can result in operational excellence, which has significant implications for future advancements in gas-processing technology. Although critical adsorption parameters can be successfully optimized using GA, its search strategy does not provide complete global optimization. The efficacy of the algorithm is affected by the initial population selection, mutation rates, and convergence criteria, which may influence solution quality. Furthermore, GA does not explicitly account for the degradation of adsorbents over time, which may influence long-term efficiency forecasts. Future enhancements may use hybrid optimization methods, such as integrating genetic algorithms with machine learning models, to increase predicted precision and computing efficiency. In addition, the model can be augmented to incorporate energy consumption analysis and assess the trade-offs between adsorption efficiency and operating expenditure. This study can enhance gas dehydration technology and promote increased efficiency and sustainability in natural gas processing by addressing these areas.

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