



Modeling and Comparison of Optimized Isotherm Models for H₂, N₂, CO, CH₄ and CO₂ Adsorption Using Cuckoo Search Optimization Algorithm

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ABSTRACT

In this study, modeling of hydrogen, nitrogen, carbon monoxide, methane and carbon dioxide sorption on UTSA-16 framework extrudates in the pressure swing adsorption process was carried out. The pure gas adsorption of these gases at the pressure range (0 to 80) bars at (298, 313, and 338) K have also been measured in a fixed bed. Langmuir, Toth, Sips, UNILAN, Virial and Dubinin-Astakhov adsorption models were tested on adsorption data to estimate the sorption capacity, intensity and energy. Cuckoo search optimization algorithm was used for solving the problem to estimate the parameters of adsorption models. The results show that Langmuir isotherm provided the best fit to the equilibrium data with a square of residuals (Fobj) of 0.022, 0.2670, 0.4840, 0.1813 and 1.9619 for hydrogen, nitrogen, carbon monoxide, methane and carbon dioxide respectively. There was a good agreement between the predicted theoretical breakthrough curves and the experimental results with Langmuir, Dubinin-Astakhov, Sips, Toth and UNILAN, respectively.

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1. INTRODUCTION¹

Depending on the source and geographical situation, natural gas is a blend that includes about 95% methane, carbon dioxide, nitrogen, and small amounts of higher molecular weight hydrocarbons, i.e. ethane, propane and butane [1]. It is necessary to develop new technologies that will allow using fossil fuels while reducing the emissions of greenhouse gases. The last few decades have seen a considerable increase in the applications of adsorptive gas separation technologies, such as pressure swing adsorption (PSA). The pressure swing adsorption (PSA) process is a mature technology for gas separation or purification [2]. PSA is an adsorption-based separation process where an adsorbent preferentially adsorbs one of the main components in the gas feed mixture [3]. PSA is a mature technology for gas drying

and purification of dilute mixtures; this technology is widely used in petroleum refining industry for solvent vapor recovery, air fractionation, production of hydrogen from steam-methane reformer (SMR) and petroleum refinery off-gases. The advent of commercial PSA processes started with the early patents on this subject granted to Skarstrom [4] and Guerin de Montgareuil and Domine [5]. Recently, a novel microporous metal-organic framework, entitled to UTSA-16, has been presented for capturing carbon dioxide from gas mixtures by PSA in view of its high carbon dioxide adsorption capacity and selectivity at ambient conditions [6]. This material has small cages of about 0.45 nm and 0.33×5.4 nm² in diameter and pore openings, respectively and exhibits a gas (such as carbon dioxide) sorption capacity which is one of the highest among MOF materials [6]. The high capacity of MOF materials with the zeolite-like density makes it a suitable candidate for H₂ purification from SMR off-gases [7]. In recent years, optimization is considered as an efficient theoretical tool to solve various complex

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industrial and engineering problems in theory and practice. The global optimization algorithm is widely used to estimate the minimization or maximization solutions to the problems. A series of optimization algorithms have been developed over the past few decades to solve different problems, including structure optimization, engineering design and other applied sciences. Cuckoo search (CS) algorithm is a population-based heuristic optimization algorithm proposed by Yang and Deb [8], which is used to simulate the fascinating breeding behavior such as brood parasitism of certain species of cuckoos. Compared with other optimization algorithm, the significant advantage of CS algorithm is that the Levy flight approach employed to characterize the foraging behavior of cuckoo. Specifically, the Levy flight is made up of the local random walks and characteristics of a sequence of sudden jumps, and thus CS algorithm is suitable for solving optimization problems when the parameter settings are proper. Research shows performance of CS is better than most existing algorithms such as genetic algorithm (GA) and particle swarm optimization (PSO) [9]. In this research, modeling of hydrogen, nitrogen, carbon monoxide and methane adsorption onto UTSA-16 framework in pressure swing adsorption process was carried out using Cuckoo search optimization methods for solving the problem of estimating the parameters of adsorption models. Langmuir, Toth, UNILAN, Virial and Dubinin-Astakhov adsorption isotherm models were tested for sorption data.

2. MATERIALS AND METHODS

2. 1. Experimental Data

UTSA-16 was provided according to the method reported in the literature [6, 10]. Prepared UTSA-16 was extrudate to use for measurement of the pure adsorption equilibrium isotherms of the cited gases at different temperatures (298, 313 and 338 K), reaching pressures of 80 bars for hydrogen, 50 bars for nitrogen and 50 bars for methane, 5 bars for carbon monoxide, and 40 bars for carbon dioxide. A chromatographic method (diffusion measurements) has been used to measure the pure gas adsorption Henry's law constants and the reciprocal diffusion time constants from pulse responses. Pulse experiments were carried out in a column packed with UTSA-16 extrudates, where the adsorbent bed is placed inside a stainless-steel column (i.d. =0.92 cm, 2.22 cm long), placed inside the temperature controlled oven of a gas chromatograph (Agilent 6890) coupled with a thermal conductivity detector (TCD). In each pulse experiment, a small loop volume (20 μ l loop) placed in a rotary valve is filled with the studied gas, which is swept by the carrier gas, crossing the adsorbent bed, and the pulse response is analyzed by the TCD detector of the chromatograph. To measure the rest of hydrogen,

nitrogen, methane, carbon monoxide and carbon dioxide, helium was used as the carrier gas. Pulses of helium (considered as a nonadsorbing gas, with nitrogen as carrier gas) were also recorded to measure the void volume and the global dispersion in the installation. Prior to the pulse experiments, the UTSA-16 was regenerated at 373 K overnight under helium flow [7]. Thermodynamic modeling of hydrogen, nitrogen, carbon monoxide, methane and carbon dioxide sorption onto UTSA-16 framework extrudate by different isotherms using Cuckoo search optimization methods was done by using Vicente I. Agueda et.al [7] experimental data are illustrated in Figure 1.

2. 2. Cuckoo Search (CS) Algorithm

Cuckoo search (CS) is an emerging biologically inspired optimization algorithm, which is inspired by the breeding parasitism behavior of the Cuckoo bird, and Cuckoos engage the obligate brood parasitism by laying their eggs in the nests of other host birds (often different species) [11]. In CS algorithm, the search starts with a given number of nests each contain a candidate solution to form an initial generation of solution. Thereafter, the best nests with high-quality eggs will be carried over to the next generations, and it means that the nest with lower quality egg would be replaced. Furthermore, CS depends on Levy flight mechanism as the local random walks and occasional long jumps used to generate a new solution (Cuckoos) from a current solution according to the following equation:

$$x_i^{t+1} = x_i^t + \alpha \oplus \text{levy}(\lambda) \quad (1)$$

where x_i^{t+1} and x_i^t represent the new solution and current location unit, respectively. α is the step size factor that should be associated with the scales of the problem at hand. The notation \oplus represents means entry-wise multiplications. $\text{levy}(\lambda)$ is the transition probability, and it carries out a random walk drawn from a Levy distribution for large steps, which is given by Equation (2) :

$$L(\lambda) \sim u = t^{-\lambda} \quad (1 < \lambda < 3) \quad (2)$$

The next task in CS algorithm is the generation of the new solutions by using the similarity between the existing eggs/solutions and the host eggs/solutions with a discovery rate p_a . The number of available host nests is fixed, and the egg laid by a Cuckoo can be discovered by the host bird and it would be abandoned from the nest, the event may occur based on the probability p_a . Thence, the p_a can be regarded as the probability of an individual to be retained. The new solution is expressed as follows:

$$x_i^{t+1} = \begin{cases} x_i^t + \gamma(x_i^t + x_k^t) & \text{rand} > p_a \\ x_i^t & \text{otherwise} \end{cases} \quad (3)$$

where x_i , x_j and x_k are three different solutions that are

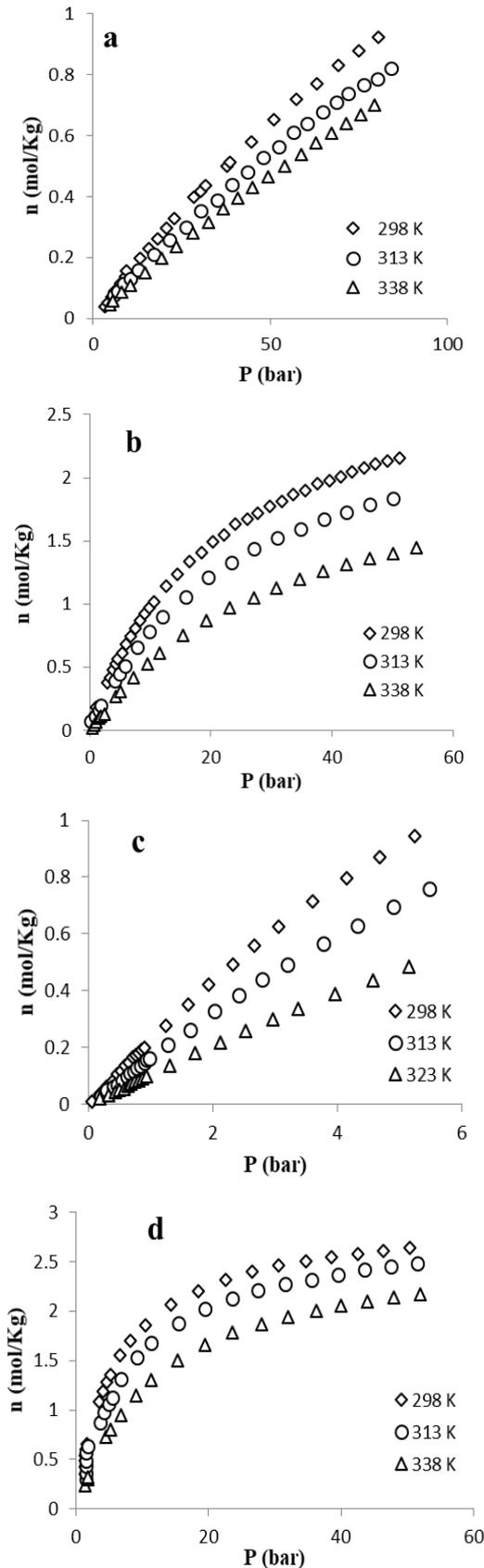


Figure 1. Experimental adsorption data of (a) hydrogen, (b) nitrogen, (c) carbon monoxide, (d) methane and (e) carbon dioxide onto UTSA-16 extrudates at different temperatures [10].

chosen at random, $Rand$ and γ are random numbers drawn from a uniform distribution in $[0, 1]$. Additionally, in CS algorithm, the initial location of the host nest was obtained as follows:

$$x_i = Lb + rand \times (Ub - Lb) \tag{4}$$

where the Ub and Lb are the upper and lower bounds of the search space, respectively. Table 1 indicates the parameter settings of the cuckoo search optimization method in this work for all experiments. To solve the problem of the parameter estimation, the best fitting parameters were found by minimizing the objective function, the square of residuals F_{obj} [12].

$$F_{obj} = \sum_{T=1}^3 \sum_{P=0}^{P_{max}} \sum_{S=1}^n (q_{exp} - q_{calc})^2 \tag{5}$$

where T_i and P_{max} are the three different temperatures (298, 313 and 338 K) and the maximum pressure of

TABLE 1. Parameter settings for Cuckoo search algorithm

| Parameter | Value |
|--|-------|
| number of optimization variables | 3 |
| Lower and Upper bounds for Parameter | [0-1] |
| number of the initial population | 50 |
| minimum number of eggs for each cuckoo | 2 |
| maximum number of eggs for each cuckoo | 4 |
| maximum iterations of the Cuckoo Algorithm | 100 |
| number of clusters that we want to make | 2 |
| maximum number of cuckoos that can live at the same time | 50 |
| Control parameter of egg laying | 0.5 |
| population variance that cuts the optimization | 1e-10 |

each isotherm respectively. S is the number of the point per isotherm per gas. The optimization algorithms used in this paper are programmed in MATLAB.

3. RESULTS AND DISCUSSION

The experimental adsorption isotherms data were fitted adequately with Langmuir, Toth, UNILAN, Virial and Dubinin-Astakhov adsorption isotherm models at different temperatures (298, 313 and 338 K) in the studied pressure range using Cuckoo search optimization algorithm.

3. 1. Langmuir Equation

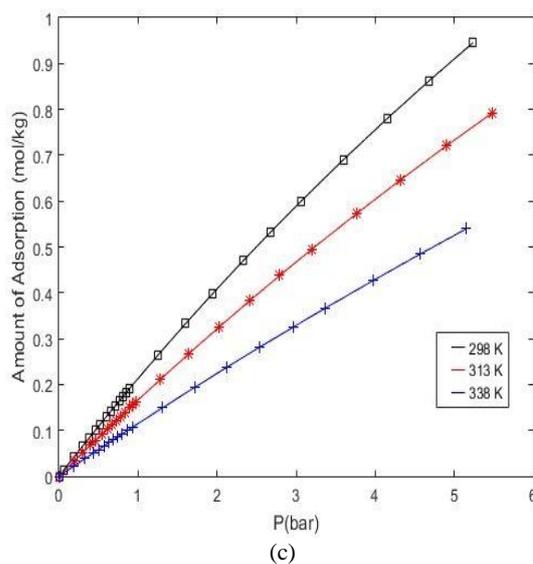
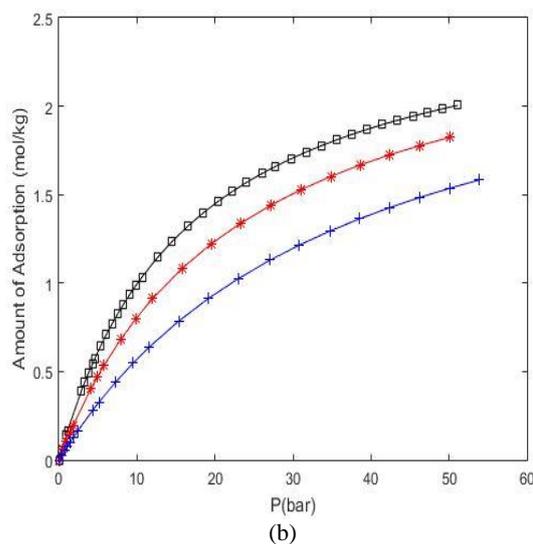
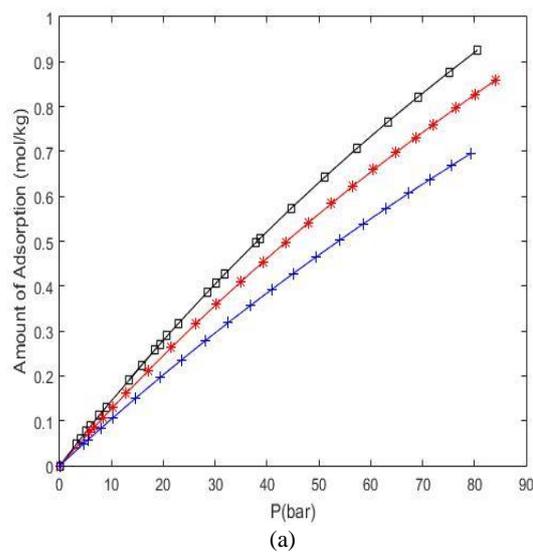
Langmuir isotherm model is based on the four assumptions: (a) there exists a fixed number of sites for adsorption process, (b) identical sites, (c) each site only accommodates one adsorbate molecule, and (d) adsorbate molecules do not interact with each other. The experimental data were compared with the theoretically predicted curves based on single gas isotherms by using Langmuir isotherm equation, which is defined as the following equation [13]:

$$\frac{q_i}{q_{mi}} = \frac{KP}{KP + 1} \tag{6}$$

where K is the equilibrium constant between the gas and adsorbed phases and q_{max} is the monolayer maximum adsorption capacity of the adsorbent material. The calculated constants for Langmuir isotherm model equations along with the objective function, square of residuals F_{obj} is presented in Table 2. The table shows that Langmuir equation correlates the experimental data with the square of residuals F_{obj} of 0.022, 0.2670, 0.4840 and 0.1813 for hydrogen, nitrogen, carbon monoxide, methane and carbon dioxide, respectively. Figure 2 shows the fitting using Langmuir equation for all pure gases at pressure range (0 to 80) bars at (298, 313, and 338) K. Results indicate that there is a good agreement between the experimental and predicted values (with minimum objective function). In this study,

TABLE 2. Langmuir isotherm parameters and error functions for different gases adsorption onto UTSA-16

| | q_{mi} (mol/kg ⁻¹) | n | ΔH_{st} (kJ/mol ⁻¹) | K_L (Mpa ⁻¹) | F_{obj} |
|-----------------|-------------------------------------|---|--|-------------------------------|-----------|
| Hydrogen | 3.9123 | - | 7.2041 | 0.0002 | 0.022 |
| Nitrogen | 2.6614 | - | 16.4198 | 0.0001 | 0.2670 |
| Carbon monoxide | 5.1540 | - | 15.1160 | 0.0001 | 0.4840 |
| Methane | 2.8447 | - | 18.7976 | 0.0001 | 0.1813 |
| Carbon dioxide | 4.6679 | - | 26.4516 | 0.0001 | 1.9619 |



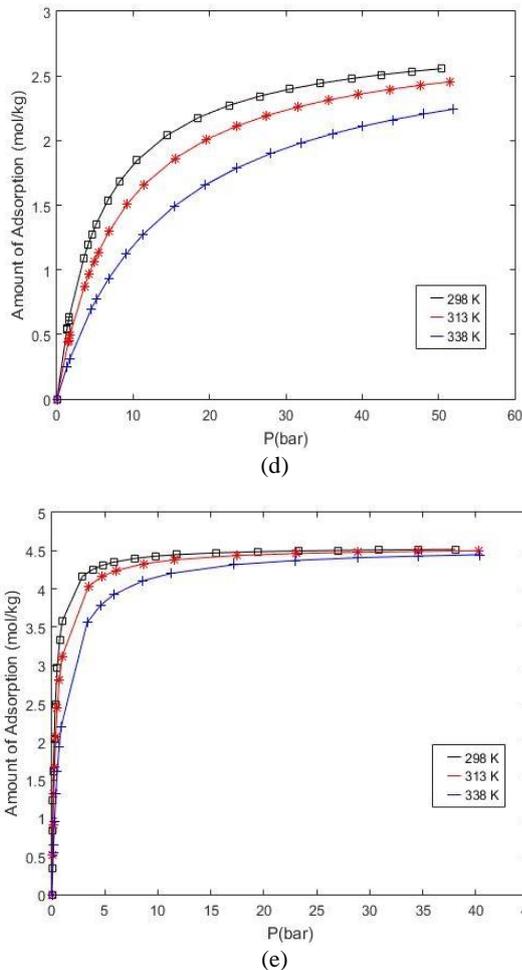


Figure 2. Gases adsorption equilibrium (a) hydrogen, (b) nitrogen, (c) carbon monoxide, (d) methane, and (e) carbon dioxide) onto UTSA-16 extrudates. \diamond) 298 K; \circ) 313 K; \triangle) 338K; using Langmuir isotherm model

Langmuir isotherm model can be more useful for describing the adsorption process of different gases by UTSA-16. In this temperature range, physical interaction between the different gases and UTSA-16 is probably larger due to the existence of a higher number of exposed adsorption sites. So, because of the many active sites the adsorption feature of the experimental system might be caused by the monolayer adsorption in the experimental conditions.

3. 2. Toth Isotherm Toth isotherm is a semi-empirical expression that was extended from the Langmuir equation to consider the heterogeneity of adsorbent surfaces [14]. The three parameters Toth isotherm that assumes a quasi Gaussian energy distribution was found to be the most useful isotherm in describing the heterogeneous adsorption systems of the gases at both low and high pressure. Toth isotherm

model is often given in the form of the following equation:

$$\frac{q_i}{q_{mi}} = \frac{(K_T P)}{(1 + (K_T P)^n)^{1/n}} \quad (7)$$

where q_{mi} (mol/Kg) is the maximum adsorption capacity, K_T (Mpa^{-1}) and n are Toth isotherm constant. It is clear that when $n = 1$, the relative energies of the different adsorption sites are the same and this equation reduces to Langmuir isotherm equation. While the exact physical interpretation of n is unclear, it is believed to reflect the heterogeneity of the adsorbent, as well as the lateral interactions between adsorbed molecules [15]. The adsorption data (maximum gas sorption capacity, Toth isotherm constant, so steric heat of adsorption at zero loadings, and square of residuals F_{obj}) are presented in Table 3. Results showed that data of modeling was not nearly as good as the obtained from Langmuir and Dubinin-Astakhov models. For heterogeneous adsorbents such as activated carbon, Toth model is commonly used, because of its correct behavior at both low and high pressures and the simple form of its equation.

3. 3. Unilan Equation Unilan equation is another empirical relation obtained by assuming a patch wise heterogeneous surface and approximately continuous energy distribution of site yields, in which each patch is ideal so that the local Langmuir isotherm is applicable on each patch. This equation is limited to Henry's law, therefore it is valid at extremely low adsorbate concentrations. The distribution of energy on the surface is assumed to be uniform (the term Unilan comes from a uniform distribution and Langmuir local isotherm) and represented by [16]:

$$\frac{q_i}{q_{mi}} = \frac{1}{2n} \ln \left[\frac{1 + KP \exp(n)}{1 + KP \exp(-n)} \right] \quad (8)$$

where n and K are Unilan isotherm constant. q_{mi} (mol/Kg) is the maximum adsorption capacity. The resulting fit of experimental adsorption data with

TABLE 3. Toth isotherm parameters and error functions for different gases adsorption onto UTSA-16

| | q_{mi} (mol/kg ⁻¹) | n | ΔH_{st} (kJ/mol ⁻¹) | K_T (Mpa ⁻¹) | F_{obj} |
|-----------------|-------------------------------------|--------|--|-------------------------------|-----------|
| Hydrogen | 5.5580 | 0.9822 | 6.197 | 0.0002 | 0.0323 |
| Nitrogen | 3.4530 | 0.9943 | 14.558 | 0.0001 | 0.4049 |
| Carbon monoxide | 8.6956 | 0.8609 | 12.769 | 0.0001 | 0.5706 |
| Methane | 3.6975 | 0.6559 | 13.868 | 0.0007 | 0.4489 |
| Carbon dioxide | 4.9256 | 0.6758 | 20.00 | 0.0019 | 3.5181 |

UNILAN equation is presented in Table 4. As can be seen, there isn't a good harmony between the experimental and predicted values.

3. 4. Sips Equation Sips adsorption isotherm model described mainly the localized adsorption without adsorbate-adsorbate interactions. The Sips isotherm is a combined form of Langmuir and Freundlich expressions developed to predict the heterogeneous adsorption systems and circumventing the limitation of the rising adsorbate concentration associated with the Freundlich isotherm. At low adsorbate concentrations, it is converted to Freundlich isotherm. At high adsorbate concentrations, it predicts monolayer adsorption in a similar manner as Langmuir isotherm. Sips adsorption isotherm model is presented as the following equation [17]:

$$\frac{q_i}{q_{mi}} = \frac{(KP)^{1/n}}{1 + (KP)^{1/n}} \tag{9}$$

where P is the pressure, qmi (mol/Kg) is the maximum adsorption capacity, K is the adsorption affinity, and n is a dimensionless parameter that qualitatively characterizes the heterogeneity of the adsorbate-adsorbent system. The Values of fitting parameters of Sips isotherm model are given in Tables 5. Results showed that Sips isotherm had Fobj lower than Langmuir and Dubinin–Astakhov (DA) isotherm.

TABLE 4. Unilan isotherm parameters and error functions for different gases adsorption onto UTSA-16

| | q _{mi} (mol/kg ⁻¹) | n | ΔH _{st} (kJ/mol ⁻¹) | K ₀ (Mpa ⁻¹) | F _{obj} |
|-----------------|--|-------|---|--|------------------|
| Hydrogen | 5.5820 | 1.017 | 7.6120 | 0.0001 | 0.0318 |
| Nitrogen | 3.3280 | 1.013 | 11.9829 | 0.0003 | 0.5779 |
| Carbon monoxide | 3.8267 | 1.00 | 15.5637 | 0.0001 | 0.5460 |
| Methane | 3.0427 | 1.00 | 15.8024 | 0.0002 | 0.4744 |
| Carbon dioxide | 4.6400 | 1.00 | 20.00 | 0.0011 | 3.9327 |

TABLE 5. Sips isotherm parameters and error functions for different gases adsorption onto UTSA-16

| | q _{mi} (mol/kg ⁻¹) | n | ΔH _{st} (kJ/mol ⁻¹) | K (Mpa ⁻¹) | F _{obj} |
|-----------------|--|--------|---|---------------------------|------------------|
| Hydrogen | 4.9994 | 1.0000 | 8.2083 | 0.0001 | 0.0283 |
| Nitrogen | 3.0460 | 1.0004 | 15.2840 | 0.0001 | 0.3547 |
| Carbon monoxide | 3.2964 | 1.0399 | 14.0635 | 0.0003 | 0.5564 |
| Methane | 3.8714 | 1.0843 | 15.6670 | 0.0002 | 0.3409 |
| Carbon dioxide | 4.1605 | 1.1415 | 20.00 | 0.0011 | 2.6327 |

Because the heterogeneity factor (n) is close to 1, the Sips isotherm behaves similarly to the Langmuir isotherm and the surface is homogeneous. So, monolayer adsorption was carried out in the experimental conditions.

3. 5. DA-Equation Dubinin–Astakhov (DA) equation adsorption model was considered to be a semi-empirical one and was derived by energy balance, where gases are filled in the micropores of the adsorbent. But it seems that there are two main unsolved problems connected with the DA equation. The first one is the applicability of DA isotherm as a local one in general adsorption isotherm equation and the second problem is the importance of the empirical parameter n of DA equation [18]. The general equation is expressed as follows:

$$\frac{q_i}{q_{mi}} = \exp \left\{ - \left[\frac{RT}{E} \ln \left(\frac{P^{sat}}{P} \right) \right]^n \right\} \tag{10}$$

where q_{mi} is the adsorption capacity in the adsorbent. R is the gas constant. T is the temperature. E is the heat of adsorption. P_s is the saturated vapor pressure. n is the structural heterogeneity parameter. DA equation parameter also is shown in Table 6. Results show that Dubinin–Astakhov isotherm has Fobj higher than Langmuir and lower than Sips, Toth and UNILAN, respectively. The present computer modeling indicates that the adjustment of DA equation to the experimental single-gas adsorption data reflects the correlation effects between the energies of adsorbed molecules in the micropores. Namely, if the E and heterogeneity parameters n determined from DA adjustment to the single adsorption isotherms are considerably different, the model assuming lack of correlations between the energies of adsorbed molecules is more effective. The error function analysis found that Langmuir isotherm was the best fit model with the experimental data, because this model has smaller error (Fobj) than other isotherms.

TABLE 6. Dubinin–Astakhov (DA) isotherm parameters and error functions for different gases adsorption onto UTSA-16 extrudates

| | q _{mi} (mol/kg ⁻¹) | E (j/mol ⁻¹) | n | F _{obj} |
|-----------------|--|-----------------------------|--------|------------------|
| Hydrogen | 1.1394 | 0.0034 | 1.1960 | 0.0236 |
| Nitrogen | 3.7580 | 0.0096 | 2.0414 | 0.2789 |
| Carbon monoxide | 10.00 | 0.0032 | 1.0451 | 0.5251 |
| Methane | 2.6180 | 0.0086 | 2.1703 | 0.2518 |
| Carbon dioxide | 4.6140 | 0.0164 | 3.3610 | 2.1653 |

4. CONCLUSIONS

Cuckoo search is a suitable algorithm that can be successfully applied to find good and acceptable solutions to the problem of parameter estimation. The usage of Cuckoo search in solving the parameter estimation problem for nonlinear systems was studied. This problem typically presented difficulties to traditional parameter estimation techniques which basically depend on linearizing the system in order to apply available algorithms for linear systems. Also, as most of these traditional techniques are based on gradient descent technique, the search might be trapped at a locally optimal solution. The equilibrium results were modeled and evaluated by means of five different isotherms and error functions. On the basis of minimizing the square of residuals errors the comparison of error function was made, and the best isotherm equations were found. The results indicated that Langmuir isotherm provided the best fit to the equilibrium data with the square of residuals F_{obj} of 0.022, 0.2670, 0.4840, 0.1813 and 1.9619 for hydrogen, nitrogen, carbon monoxide, methane and carbon dioxide, respectively. There was a good agreement between the predicted theoretical breakthrough curves and the experimental results with in the following order Langmuir > Dubinin-Astakhov > Sips > Toth > UNILAN.

5. ACKNOWLEDGMENTS

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Persian Abstract

چکیده

در این مطالعه، مدل سازی جذب هیدروژن، نیتروژن، مونوکسید کربن، متان و دی اکسید کربن بر روی جاذب چارچوب UTSA-16 در فرآیند جذب فشار متغییر انجام شد. جذب گاز خالص این گازها در محدوده فشار (۰ تا ۸۰) بار در دمای (۲۹۸، ۳۱۳ و ۳۳۸) K در بستر ثابت اندازه گیری شده است. برای برآورد ظرفیت جذب، شدت و انرژی، مدل‌های جذب لانگمویر، Toth، UNILAN، Virial و Dubinin-Astakhov بر روی داده های جذب بررسی شدند. برای بدست آوردن پارامترهای مدل‌های جذب از الگوریتم بهینه سازی جستجوی فاخته استفاده شده است. نتایج نشان دادند که ایزوترم لانگمویر با داده های مربع باقیمانده (Fobj) به ترتیب ۰/۲۲۰، ۰/۲۶۷۰، ۰/۴۸۴۰، ۰/۱۸۳۳ و ۱/۹۶۱۹ برای هیدروژن، نیتروژن، مونوکسید کربن، متان و دی اکسید کربن به ترتیب مناسب ترین همپوشانی را دارد. همچنین همبستگی خوبی بین منحنیهای پیشرفت پیش بینی شده تئوری و نتایج تجربی به ترتیب با لانگمویر، Dubinin-Astakhov، Sips، Toth و UNILAN وجود داشت.
