

SHORT COMMUNICATION

ADSORPTION EQUILIBRIUM OF CARBON DIOXIDE
ON ZEOLITE 13X AT HIGH PRESSURES

Kamila Zabielska, Tomasz Aleksandrak*, Elżbieta Gabruś

West Pomeranian University of Technology, Szczecin, Faculty of Chemical Technology
and Engineering, Institute of Chemical Engineering and Environmental Protection Processes,
al. Piastów 42, 71-065 Szczecin, Poland

Carbon dioxide (CO₂) is a compound responsible for the greenhouse effect. One of the methods of CO₂ capture from the gas stream is adsorption process. In this paper, the adsorption equilibrium isotherms of CO₂ on zeolite 13X were measured at different temperatures (293.15 K, 303.15 K, 313.15 K, 323.15 K, 333.15 K, 348.15 K, 373.15 K, 393.15 K) and under pressures up to 2 MPa. These data were obtained using an Intelligent Gravimetric Analyzer (IGA-002, Hiden Isochema, UK). Selected multitemperature adsorption isotherm equations, namely Toth, Langmuir–Freundlich, and Langmuir were correlated with experimental data.

Keywords: carbon dioxide, zeolite 13X, adsorption equilibrium, adsorption isotherm

1. INTRODUCTION

The greenhouse effect is caused by the emission of compounds such as water vapor, carbon dioxide, methane, ozone, and freon into the atmosphere. These gases can originate in both natural sources and human activity. Carbon dioxide is the main greenhouse gas that contributes to global warming. It is emitted into the atmosphere in the processes of electricity and heat generation based on fuel combustion (Kotowicz and Janusz, 2007; Lin et al., 2003).

According to the Kyoto Protocol from 1997 the greenhouse gas emission was intended to be reduced in 2008–2012 by 5% in relation to the level in 1990. The protocol imposed a requirement to monitor greenhouse gas emission and prepare annual reports. The energy and climate package consists of four legal acts. One of them is a commitment signed by the European Union Member States of about 20% reduction of greenhouse gas emissions to the atmosphere by 2020. To achieve this goal the development of clean coal technology should take place simultaneously with the development of CO₂ capture and storage technologies (CCS) (Kyoto Protocol, 1998; Miłek, 2009; Nowak et al., 2014; Stewart and Hessami, 2005).

There are five main technologies of carbon dioxide capture: pre-combustion capture, post-combustion capture, oxy-fuel combustion, combustion with flue gas recirculation of O₂/CO₂ and chemical looping combustion. In each of the capture methods, separation processes such as absorption, adsorption, membrane filtration and cryogenic techniques can be used (Kidnay and Parrish, 2006; Nowak et al., 2014).

* Corresponding author, e-mail: tomasz.aleksandrak@zut.edu.pl
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The absorption methods allow obtaining a high purity product. The process can be carried out due to chemical or physical absorption. During the chemical absorption the flue gas is passed through the absorption column, where it reacts with a liquid capturing CO₂. This process is used when high degree of component removal is required. Typically, amines such as monoethanolamine (MEA), diethanolamine (DEA) as well as aqueous ammonia solution are used as a solvent. In the physical absorption process, CO₂ can be absorbed by the solvent according to Henry's law and regenerated by pressure reduction at increased temperature (Creamer et al., 2015; Kidnay and Parrish, 2006; Nowak et al., 2014; Yang et al., 2008).

Membrane separation of gases is based on the difference in physical or chemical interaction between components present in a gas mixture with the membrane material. Membranes can be used to separate gas mixture or to absorb a gas component when concerning carbon dioxide capture (Creamer et al., 2015; Yang et al., 2008). CO₂ removed by the cryogenic method must be compressed and cooled to the temperature at which it can be separated in a liquid form.

This paper is focused on adsorption process of gas mixture separation. It is commonly used in industry for gas stream purifying and component recovery (Creamer et al., 2015; Nowak et al., 2014). Physical adsorption takes place as a result of adhesion of molecules, atoms or ions on the surface or boundary of physical phases, causing local concentration changes on surface of solid adsorbent. Adsorption is more effective at low temperature and high pressure (Nastaj, 2013; Paderewski, 1999; Sarbak, 2000).

The effective adsorbent should have a high specific surface area and high adsorption capacity of carbon dioxide. The following adsorbents are mainly used: activated carbons, carbon and zeolite molecular sieves, and silica gels. The 13X zeolite was selected in this study because of its unique structure, resistance to high temperatures and its high regeneration degree.

Zeolites are crystalline aluminosilicates of alkali metals and divalent metals. They are composed of elementary tetrahedrons of SiO₄/AlO₄ connected with other oxygen ions. The combined tetrahedrons form polyhedrons. Various molecular sieves can be obtained by different arrangement and connection of polyhedrons. These adsorbents have homogeneous pores and the shape and size of pores determine which molecules are able to enter a pore and be adsorbed on its surface. Zeolites can be divided into three types: A, X and Y (Małeckki and Rajewski, 2008; Paderewski, 1999; Sarbak, 2000; Thomas and Crittenden, 1998).

Mostly, an adsorbent is placed in a column with the form of a fixed bed, which operates in cycles. The cyclic adsorption process consists of two main stages: adsorption and regeneration of an adsorbent. In the adsorption stage a gas stream flows through a column with a packed adsorbent bed. As a result of the adsorption process CO₂ is removed from gas stream by an adsorbent. When the adsorbent is saturated the regeneration stage can occur. Various cyclic adsorption processes can be used for separation of carbon dioxide:

- Pressure Swing Adsorption (PSA) where the adsorption step takes place at increased pressure;
- Temperature Swing Adsorption (TSA) in which the adsorbent is regenerated by raising its temperature;
- Electrothermal Swing Adsorption (ETSA) in which the adsorbent is regenerated by passing through it a low-voltage electric current;
- Vacuum Pressure Swing Adsorption (VSA) in which the adsorbent is regenerated by vacuum (Keller and Staudt, 2005; Nastaj, 2013).

Most papers concerning adsorption equilibrium isotherms of CO₂ on zeolite 13X determined them (i.e. isotherms) under pressures below 2 MPa (Cavenati et al., 2004; Costa et al., 1991; Delgado et al., 2014; Hefti et al., 2015; Hyun and Danner, 1982; Lee et al., 2002; Li et al., 2008; Ling et al., 2014; Maring and Webley, 2013; Merel et al., 2008; Wang and LeVan, 2009). Cavenati et al. (2004) measured the equilibrium using gravimetric method at temperatures of 298.15 K, 303.15 K, 323.15 K and under pressures up to

3.4 MPa for about 20 pressure measurement points. Siriwardane et al. (2005) used the same method for temperatures of 303.15 K and 393.15 K and pressures up to 2.5 MPa for 12 pressure measurement points.

In this paper, the adsorption equilibrium isotherms of CO₂ on zeolite 13X were determined at temperatures of 293.15 K, 303.15 K, 313.15 K, 323.15 K, 333.15 K, 348.15 K, 373.15 K, 393.15 K and under pressures up to 2 MPa. The experiments were performed for 33 pressure measurement points allowing to determine the multitemperature adsorption isotherm of the studied system with high accuracy.

2. MATERIALS AND METHODS

2.1. Characteristics of adsorbent and adsorbate

Experimental research concerned adsorption equilibrium of carbon dioxide onto zeolite 13X, which was manufactured by Polskie Odczynniki Chemiczne S.A. (Gliwice, Poland). Basic physical properties of the adsorbent (Fig. 1) are presented in Table 1.



Fig. 1. Molecular sieves 13X

Table 1. Physical properties of zeolite 13X (Nastaj, 2013)

Property	Value
BET surface area, m ² /g	726
bulk density, kg/m ³	689
density, kg/m ³	1100
bed porosity	0.374
pellet porosity	0.247
pellet diameter, m	0.0036
pore radius, nm	23

2.2. Description of experimental apparatus and measurement

Studies of adsorption equilibrium were performed using an Intelligent Gravimetric Analyzer (IGA-002, Hiden Isochema, United Kingdom) (Fig. 2). The main element of the IGA system is a precision balance with weighing resolution of 0.1 μg (Nastaj and Aleksandrak, 2003).

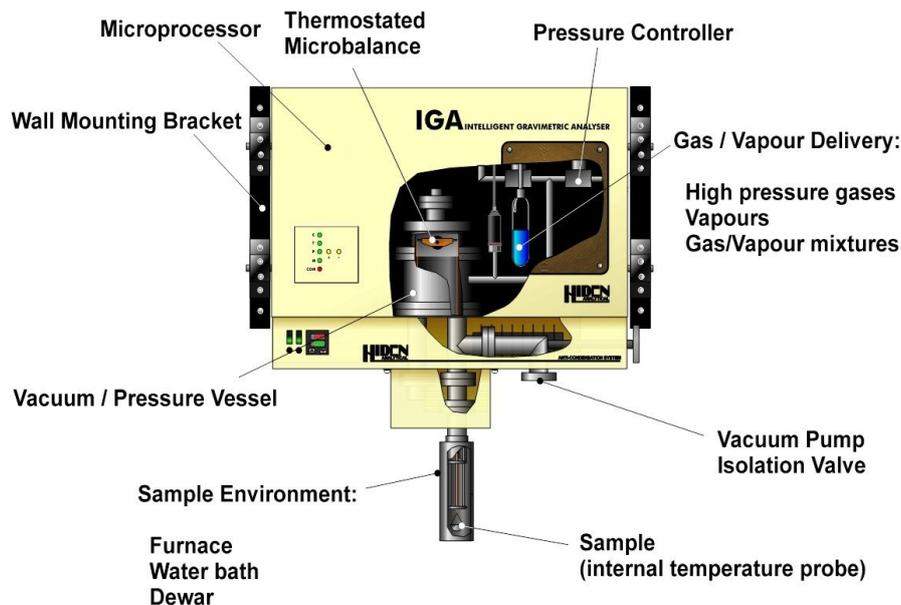


Fig. 2. Intelligent Gravimetric Analyzer IGA-002 (Nastaj and Aleksandrak, 2003)

A sample of the adsorbent (about 82 mg) was placed on a stainless steel sieve which was suspended on the balance inside the metal reactor using a gold chain and a tungsten wire. At the condition of ultra-high vacuum the reactor was thermostated using a circulation water bath GR 150 (Grant Instruments, United Kingdom) or heated with electric furnace Cryofurnace (Hiden Isochema, United Kingdom). The sample temperature measured using a Pt 100 sensor was regulated by the PID controller the accuracy of ± 0.05 °C for the water bath and ± 0.1 °C for the furnace. The reactor pressure was measured using a manometer with the resolution of ± 0.625 Pa. Before each measurement, the sample was degassed “in situ” for 2 hours at the temperature of 200 °C and vacuum of 10^{-6} Pa. Such a low pressure was obtained by the system of two vacuum pumps: the MD 1 membrane pump (Vacuumbrand, Germany) and the TMU 071 P turbomolecular pump (Pfeiffer Vacuum Technology, Germany) (Nastaj and Aleksandrak, 2003).

After degassing the sample, the adsorption equilibrium measurement was made for set values of temperature and pressure. The source of CO₂ was the gas cylinder (purity of CO₂ was 99.995%). IGA controlled pressure inside the chamber, in which a sample was located, by adjusting automatically the input and output valves of the reactor. For each measuring point (set pressure and temperature values) real time processor (RTP), which was responsible for recording sample weight changes, predicted an asymptotic value of mass sample. After reaching 99.9% of the predicted weight value, the IGA system continued the measurement for the next isotherm point (next set point pressure). When all pressure setpoints were examined the sample was degassed and the measurement was performed for the next temperature value (Nastaj and Aleksandrak, 2003).

2.3. Types of adsorption equilibria

As a result of gas phase contact with the solid surface, part of the gas phase molecules is adsorbed on the surface of the solid. The amount of adsorbed substance per unit of adsorbent weight is called adsorption capacity. Adsorption is a surface phenomenon that occurs at any pressure and temperature (Keller and Staudt, 2005; Paderewski, 1999; Thomas and Crittenden, 1998).

Number of molecules adsorbed in equilibrium conditions on the surface of the adsorbent q^* depends on the process temperature T and the partial pressure of the adsorbed substance p :

$$q^* = f(T, p) \quad (1)$$

As there are three parameters in Equation (1), the equilibrium may be described in three ways:

- at constant temperature T – adsorption isotherm:

$$q^* = f(p)_T \quad (2)$$

- at constant vapor pressure p – adsorption isobar:

$$q^* = f(T)_p \quad (3)$$

- at constant concentration of adsorbed component on the solid phase q – adsorption isostere:

$$p = f(T)_q \quad (4)$$

The adsorption equilibrium is considered mostly as an adsorption isotherm which can be classified according to the recommendation of the International Union of Pure and Applied Chemistry classification (IUPAC) as one of 6 different types (Keller and Staudt, 2005; Paderewski, 1999; Thomas and Crittenden, 1998).

2.4. Adsorption isotherm models

Practical application of measured adsorption isotherms at various temperatures requires presenting them in the form of mathematical equations. To correlate equilibrium models with the experimental data, the multitemperature adsorption isotherm equations of Toth, Langmuir–Freundlich and Langmuir were selected (Do, 1998).

2.5. Langmuir equation

Isotherm model developed by Langmuir in 1916–1918 describes the adsorbed component – the adsorbent system in which the surface is coated by the adsorbed component and confined to the monomolecular layer (Langmuir, 1918). The equation was formulated on the basis of dynamic equilibrium between the adsorbed phase and the gas (vapour) phase. It was found that the rate at which the gas molecules of the adsorbed component hit the surface of the adsorbent is proportional to the partial pressure p and the size of the adsorbent surface, which has not been covered by the adsorbed substance and are available as an adsorption place. Langmuir supposed that the rate of desorption from the adsorbent surface is directly proportional to the surface occupied by the adsorbed substance. The Langmuir isotherm equation can be written as (Do, 1998; Keller and Staudt, 2005; Langmuir, 1918; Thomas and Crittenden, 1998):

$$q = q_m \frac{b(T) \cdot p}{1 + b(T)p} \quad (5)$$

The mathematical form of multitemperature Langmuir adsorption isotherm is:

$$q = q_m \cdot \exp\left(\frac{a_{1L}}{T}\right) \frac{b_{1L} \exp\left(\frac{c_{1L}}{T}\right) p}{1 + b_{1L} \exp\left(\frac{c_{1L}}{T}\right) p} \quad (6)$$

where q_m , b are characteristic coefficients for the adsorbed substance – adsorbent system.

Langmuir made several simplifying assumptions while deriving his equation: heat of adsorption is constant and independent of the degree of adsorbent coverage (as a consequence, there is no interaction between molecules); each adsorbed molecule can occupy only one active center; adsorption is located (the molecule stays in place until the desorption process occurs) (Keller and Staudt, 2005; Langmuir, 1998; Thomas and Crittenden, 1998).

2.6. Langmuir–Freundlich equation

In order to achieve greater flexibility, the equation of the Langmuir and Freundlich isotherms was combined into the form of an empirical relation which can be presented as (Paderewski, 1999, Thomas and Crittenden, 1998):

$$q = q_m(T) \frac{b(T) \cdot p^{n(T)}}{1 + b(T) \cdot p^{n(T)}} \quad (7)$$

In Equation (7) q_m , b and n are characteristic coefficients for adsorbed component – adsorbent system and depend on the temperature T according to the relations:

$$q_m(T) = a_{0LF} + \frac{a_{1LF}}{T} + \frac{a_{2LF}}{T^2} \quad (8)$$

$$b(T) = \exp\left(b_{0LF} + \frac{b_{1LF}}{T} + \frac{b_{2LF}}{T^2}\right) \quad (9)$$

$$n(T) = n_{0LF} + \frac{n_{1LF}}{T} \quad (10)$$

After substituting Eqs. (8)–(10) into Eq. (7) the mathematical form of multitemperature Langmuir–Freundlich adsorption isotherm is obtained (Paderewski, 1999, Sarbak, 2000; Thomas and Crittenden, 1998):

$$q = \left(a_{0LF} + \frac{a_{1LF}}{T} + \frac{a_{2LF}}{T^2}\right) \frac{\left(\exp\left(b_{0LF} + \frac{b_{1LF}}{T} + \frac{b_{2LF}}{T^2}\right)\right) p^{\left(n_{0LF} + \frac{n_{1LF}}{T}\right)}}{1 + \left(\exp\left(b_{0LF} + \frac{b_{1LF}}{T} + \frac{b_{2LF}}{T^2}\right)\right) p^{\left(n_{0LF} + \frac{n_{1LF}}{T}\right)}} \quad (11)$$

2.7. Toth equation

The Toth model is a semi-empirical equation which describes adsorption in a monolayer. The equation is related to the heterogeneity of the surface and interactions of the adsorbed molecules. Relation developed by Toth (Toth, 2001) has the following form:

$$q = q_m \frac{p}{(b(T) + p^{n_T})^{1/n_T}} \quad (12)$$

In Eq. (12) the coefficient b depends on the temperature according to the formula:

$$b(T) = b_{0T} \cdot \exp\left(-\frac{n_T \cdot \Delta H}{R \cdot T}\right) \quad (13)$$

After substituting Eq. (13) into Eq. (12) the mathematical form of multitemperature Toth adsorption isotherm is obtained (Sarbak, 2000; Thomas and Crittenden, 1998; Toth, 2001):

$$q = q_m \frac{p}{\left(b_{0T} \cdot \exp\left(-\frac{n_T \cdot \Delta H}{R \cdot T}\right) + p^{n_T}\right)^{1/n_T}} \quad (14)$$

Values of model parameters were calculated by nonlinear regression of experimental data using Statistica 13.1 (Statsoft). The average relative error \bar{a} , which is the measure of fitting quality was calculated as follows:

$$\delta = \frac{1}{N} \sum_{i=1}^N \left| \frac{q_{exp} - q_{sim}}{q_{exp}} \right| 100\% \quad (15)$$

In addition the coefficients of determination R^2 were calculated for each isotherm model.

3. RESULTS

As a result of measurements, the adsorption isotherms for carbon dioxide–zeolite 13X system were determined at temperatures: 293.15 K, 303.15 K, 313.15 K, 323.15 K, 333.15 K, 348.15 K, 373.15 K, 393.15 K and under pressures up to 2 MPa. All isotherms are type I according to the IUPAC classification (Keller and Staudt, 2005).

The multitemperature adsorption isotherm models of Toth, Langmuir–Freundlich, and Langmuir were fitted to the experimental data. The obtained values of isotherm parameters are shown in Tables 2 through 4. Average relative errors δ and coefficients of determination R^2 for all the equilibrium models are presented in Table 5.

Table 2. Adsorption isotherm parameters for the Toth model

Parameters	Value
q_m , mol/kg	6.437
b_{0T} , Pa ⁻ⁿ	576.902
n_T , –	0.464
ΔH , J/mol	31864.04

Table 3. Adsorption isotherm parameters for Langmuir–Freundlich model

Parameters	Value
a_{0LF} , mol/kg	6.159
a_{1LF} , mol·K/kg	13.673
a_{2LF} , mol·K ² /kg	0.567
b_{0LF} , Pa ⁻ⁿ	-11.28
b_{1LF} , Pa ⁻ⁿ ·K	2912.8
b_{2LF} , Pa ⁻ⁿ ·K	17.37
n_{0LF} , –	1.03
n_{1LF} , –	-144.97

Table 4. Adsorption isotherm parameters for Langmuir model

Parameters	Value
q_m , mol/kg	1.641
a_{1L} , mol/kg·Pa	378.063
b_{1L} , Pa ⁻¹	0.0003
c_{1L} , K	1514.889

The experimental and correlated by the Toth model isotherms for the studied adsorption system at various temperatures and under pressures up to 2 MPa and up to 0.1 MPa are presented in Figs. 3 and 4, respectively.

Table 5. Average relative errors δ and coefficients of determination R^2 for the carbon dioxide-zeolite 13X system for selected of equilibrium models

Equilibrium model	δ , %	R^2 , –
Toth	8.57	0.9948
Langmuir–Freundlich	18.79	0.9961
Langmuir	22.89	0.9657

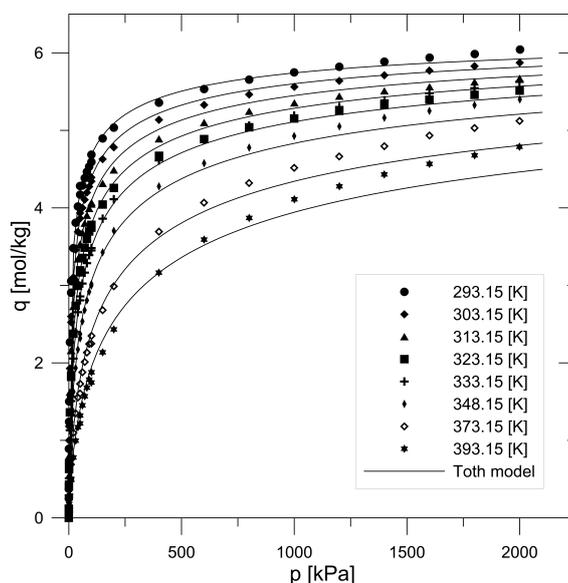


Fig. 3. Experimental and correlated (Toth equation) isotherms for carbon dioxide adsorption onto zeolite 13X at various temperatures

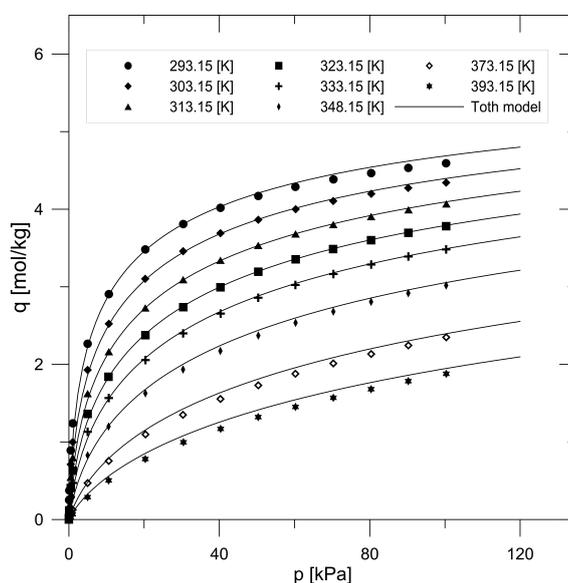


Fig. 4. Experimental and correlated (Toth equation) isotherms for carbon dioxide adsorption onto Zeolite 13X at various temperatures

All isotherms are type I according to the IUPAC classification. Type I of adsorption isotherm approaches a limiting value and is used to describe adsorption on microporous adsorbents. At the beginning, adsorption capacity increases in proportion to the pressure and this increase is slowly decreasing, then reaches a constant value. All active sites are occupied and monolayers are created (Keller and Staudt, 2005).

Adsorption capacity is high and at 293.15 K reaches 6.04 mol/kg for 2000 kPa. When the temperature increases, the adsorption capacity decreases, and at 393.15 K it is 4.79 mol/kg for 2000 kPa. It can be concluded that the zeolite 13X is a good adsorbent for carbon dioxide capture. The best fit to the experimental equilibrium data for carbon dioxide – zeolite 13X is provided by the Toth model, with a relative error of 8.57%.

In the study, three equilibrium adsorption models Toth, Langmuir–Freundlich, and Langmuir were correlated with experimental data. The Toth and Langmuir equation had four adjustable parameters and the Langmuir–Freundlich equation had eight adjustable parameters. The Toth model gave the best fit. It can provide the heat of adsorption. Langmuir–Freundlich and Langmuir models also showed a good fit for carbon dioxide – zeolite 13X.

The comparison of measured experimental isotherm equilibria for the carbon dioxide-zeolite 13X system at 293.15 K with results obtained by Costa et al. (1991), Lee et al. (2002) and Ling et al. (2014) is shown in Figs. 5 to 6. Another comparison was made for isotherm measured at 323.15 K with results obtained by

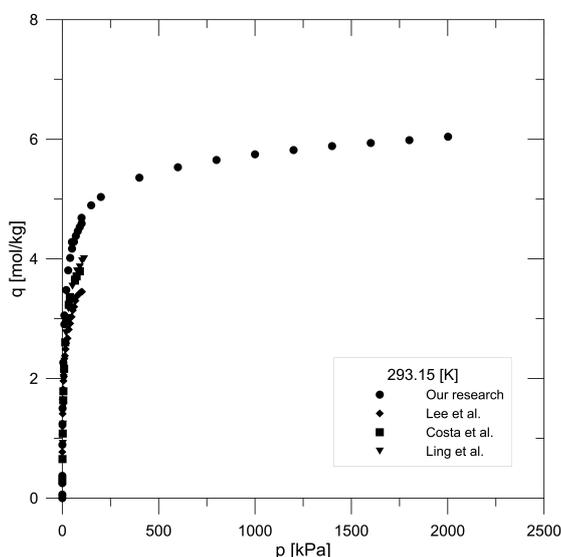


Fig. 5. Comparison of experimental isotherms for carbon dioxide adsorption onto zeolite 13X at 293.15 K in the whole range of pressure measurements

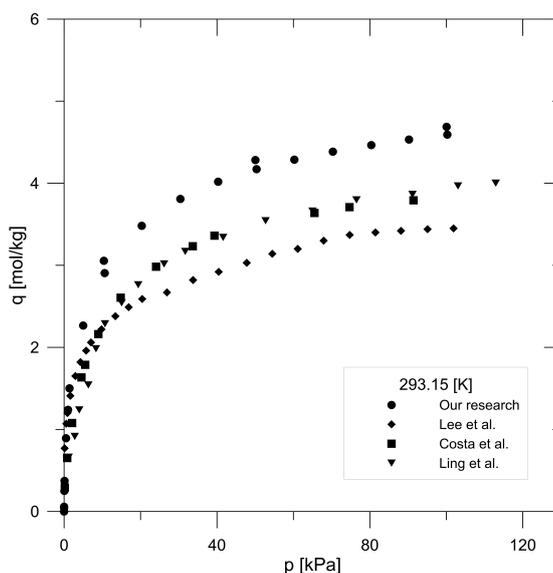


Fig. 6. Comparison of experimental isotherms for carbon dioxide adsorption onto zeolite 13X at 293.15 K

Cavenati et al. (2004), Hyun and Danner (1982), Maring and Webley (2013), Merel et al. (2008) and Wang and LeVan (2009) (Figs. 7 and 8). Our research was compared with other measurements at 293.15 and 323.15 K, because for all analyzed papers only these temperature were common. The range of pressure values used in our study presented in Figs. 6 and 8 was limited according to the range of data taken from literature sources in order to increase readability of results.

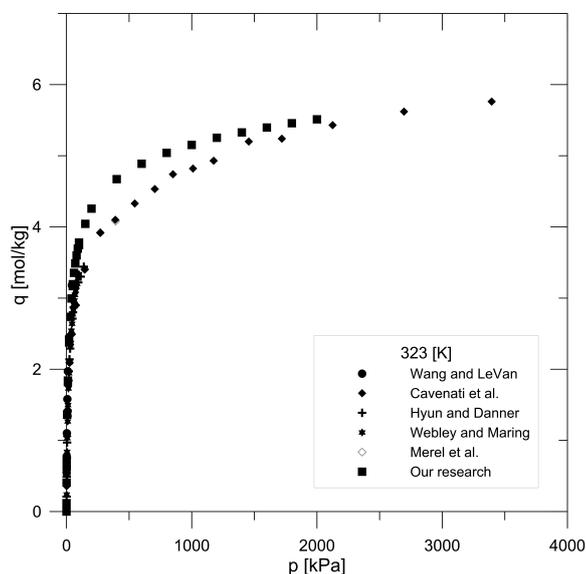


Fig. 7. Comparison of experimental isotherms for carbon dioxide adsorption onto zeolite 13X at 323.15 K in the whole range of pressure measurements

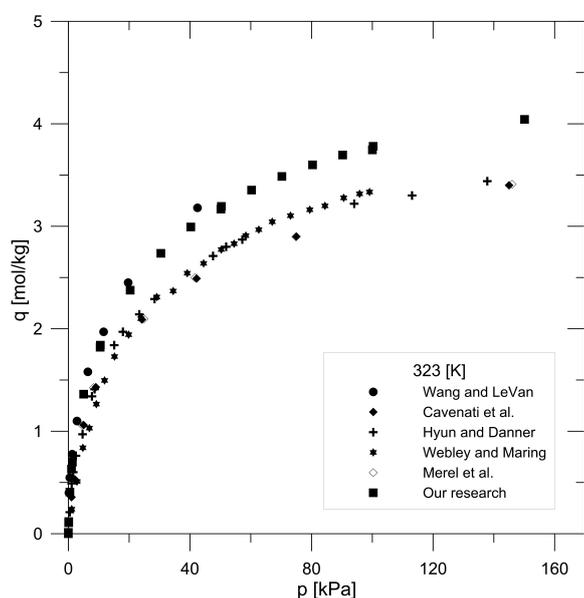


Fig. 8. Comparison of experimental isotherms for carbon dioxide adsorption onto zeolite 13X at 323.15 K

All isotherms at 293.15 K are type I according to the IUPAC classification. For this comparison our measurements gave the highest adsorption capacity of 6.04 mol/kg for 2000 kPa.

In other measurements the values of highest adsorption capacity of 3.45 mol/kg for 102 kPa, 3.79 mol/kg for 91.4 kPa, 4 mol/kg for 113 kPa were obtained by Lee et al. (2002), Costa et al. (1991) and Ling et al. (2014), respectively.

All isotherms at 323.15 K are type I according to the IUPAC classification. Our research and results obtained by Cavenati et al. (2004) gave the highest adsorption capacity of 5.51 mol/kg for 2000 kPa and 5.76 for 3395 kPa, respectively.

In other measurements the values of the highest adsorption capacity of 3.44 mol/kg for 137.8 Pa, 3.34 mol/kg for 99.1 kPa, 4.08 mol/kg for 391 kPa, 3.18 mol/kg for 42.5 kPa obtained by Hyun and Danner (1982), Maring and Webley (2013), Merel et al. (2008) and Wang and LeVan (2009), respectively were reported.

4. CONCLUSIONS

The adsorption isotherms of carbon dioxide on zeolite 13X were measured at 293.15 K, 303.15 K, 313.15 K, 323.15 K, 333.15 K, 348.15 K, 373.15 K, 393.15 K and pressures up to 2 MPa. The selected multitemperature equilibrium models of Toth, Langmuir–Freundlich and Langmuir were correlated with the experimental equilibrium data. The analysis of average relative errors δ and coefficients of determination R^2 of models fitting to experimental data showed that the best agreement was obtained for the Toth model ($\delta 8.57\%$ and $R^2 = 0.9948$). The fitting quality was the best for partial pressure range limited to 0.1 MPa (Fig. 4). In the whole studied pressure range the calculated isotherm values were underestimated in comparison with measured values obtained at temperatures of 373.15 K and 395.15 K within pressure ranged from 0.5 to 2 MPa (Fig. 3).

It was shown that zeolite 13X is characterized by high adsorption capacity and it can be used in the process of carbon dioxide capture. The highest measured adsorption capacity of 6.04 mol/kg was achieved at 293.15 K and 2 MPa.

The results of our research were compared with those obtained by other authors for two temperatures: 293.15 K and 323.15 K at 2 MPa. In most cases distinct discrepancies between them were observed (Figs. 6 and 8) except the isotherm determined experimentally by Wang and LeVan (2009) for carbon dioxide adsorption onto zeolite 13X at 323.15 K (Fig. 8). Differences in obtained results can be caused by different properties of the used adsorbent or different conditions of adsorbent regeneration.

Experimental and simulation results can be used for modeling of cyclic adsorption processes, for example temperature swing adsorption (TSA) or pressure swing adsorption (PSA). They can also be the basis for modeling multicomponent adsorption equilibrium using interpolative models.

SYMBOLS

a_{0LF}	Langmuir–Freundlich isotherm parameter, mol/kg
a_{1L}	Langmuir isotherm parameter, mol/kg·Pa
a_{1LF}	Langmuir–Freundlich isotherm parameter, mol/kg·Pa
a_{2LF}	Langmuir–Freundlich isotherm parameter, mol·K ² /kg
b_{0LF}	Langmuir–Freundlich isotherm parameter, Pa ⁻ⁿ
b_{0T}	Toth isotherm parameter, Pa ⁻ⁿ
b_{1L}	Langmuir isotherm parameter, Pa ¹
b_{1LF}	Langmuir–Freundlich isotherm parameter, Pa ⁿ ·K
b_{2LF}	Langmuir–Freundlich isotherm parameter, Pa ⁿ ·K
c_{1L}	Langmuir isotherm parameter, K
n_T	Toth isotherm parameter

n_{0LF}	Langmuir–Freundlich isotherm parameter
n_{1LF}	Langmuir–Freundlich isotherm parameter
N	number of experimental points
q	adsorption capacity, mol/kg
q_{exp}	experimental adsorption capacity, mol/kg
q_m	isotherm parameter, mol/kg
q_{sim}	calculated adsorption capacity, mol/kg
R	universal gas constant, J/mol·K
R^2	coefficient of determination
P	partial pressure of the adsorbate, Pa
T	temperature, K

Greek symbols

$\bar{\alpha}$	average relative error, %
ΔH	heat of adsorption, J/mol

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