

## Adsorbate-adsorbent interaction potential: Water - Zeolite 13X

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**Abstract:** The law proposed in this paper to the adsorbate-adsorbent interaction potential, as a function of the dimensions of the pores, based on a simple and obvious hypothesis: the amount of material adsorbed per unit time is proportional to the variation of the potential. This law is purely experimental. The experimental study of the flux allowed us to determine the expression of the variation of the potential, and by integration, to specify the expression of the latter. Experience shows that the adsorption potential is constant and highest for micropores and that it decreases linearly in the case of mesopores and macropores, finally it is low for side surface interactions of the adsorbent when saturation is almost reached. The tangent intersects the curve in the part relating to the adsorption of mesopores and macropores, which implies a change in the type of adsorbate-adsorbent interaction forces. This physically implies the existence of two types of interaction forces: one type of force is active in the case of adsorption in micropores and mesopores and the other is active during adsorption in macropores and on the lateral surface of Zeolite 13X. These findings justify the existence of the two most commonly used models, Dubinin-Astakov and BET.

**Keywords:** Adsorption; Flow; Interaction potential; Microporous solids; Zeolite 13X

### 1. Introduction

The mechanism of physical adsorption in microporous solids consists mainly of pore filling, in which the adsorbate molecules are captured by the available sites of the adsorbent. At the fluid / solid interface, and adsorbed molecule has relatively high kinetic energy which is related to its gas phase velocity. This molecule will lose kinetic energy and will be extremely less mobile when approaching the surface of a solid by the presence of interaction forces exerted by the surface itself, but also by other adsorbed molecules. Interactions between molecules in the system can be classified into two categories: van der Waals forces and electrostatic forces (Tagliabue *et al.*, 2009). The first are intermolecular forces due to a weak electrical interaction between two molecules, resulting from three different physical effects: orientation effect (Keesom force), induction effect (Debye forces), and dispersion effect (forces of London). The second includes the forces between the electric field of the solid and the dipole and quadrupole moments of molecules. The polarization of the molecules adsorbed in the electric field of the surface of the adsorbent produces a very important interaction potential. This potential depends on the intensity of the electric field at the surface of the adsorbent and on the

polarizability of the gas molecules. Adsorbents capable of promoting electrostatic interactions are generally qualified as hydrophilic. They can adsorb small polar molecules (like water) much stronger than one would expect from van der Waals forces alone. Common hydrophilic adsorbents are zeolites, alumina, and silica. Conversely, adsorbents working exclusively with van der Waals forces (e.g. most activated carbons) are called hydrophobic.

In the scientific literature, these forces of interaction between the molecules of the adsorbent and those of the adsorbed substance are often too complex to be described by a simple potential model. Some researchers use the Lennard-Jones potential as a basis to study adsorption potential. The potential of Lennard-Jones (also called potential LJ, potential 6-12 or potential 12-6): it results from the combination of an attractive global term ( $1/r^6$ ), dominant at a great distance, bears the name of the interaction of Van der Waals and a dominant short-range repellent term ( $1/r^{12}$ ) (Maghfiroh *et al.*, 2020). This potential is a mathematical model that approximates the interaction between a pair of neutral atoms or molecules. For example, Patrick Bonnaud uses the potential PN-TrAZ (Pellenq Nicholson-Transferable Adsorption in Zeolites) in the Monte Carlo Grand Canonical simulation for an oxygen atom of a water molecule in interaction with the substrate of hydroxylated silica (P. bonnaud, 2010). In addition, Eddy Bernard uses Density Functional Theory (DFT) to study the physisorption interaction of a hydrogen molecule with a metallic surface (E. Bernard, 2017).

Derijcke et al used as a basis in their analysis of the interactions due to the potential, the confinement parameter  $s$ , with  $s = d/L$ , where  $d$  is the mean equilibrium distance between the molecule and the pore wall and  $L$  is the mean pore diameter (Derycke *et al.*, 1991; Derouane, 2007). If the values of the parameter ( $s$ ) are less than the unit corresponding to the most stable situation (maximum interaction between the fluid molecules and the walls of the pores), This shows that whatever the value of the diameter of the molecules, the latter can penetrate the pores with smaller sizes because their effective van der Waals cross-section is reduced in a microporous environment as a result of the confinement effect.

Adsorbate-adsorbent interactions play an important role in all early adsorption layers. However, the adsorption mechanism is mainly determined by the porous texture of the adsorbent (Kali *et al.*, 2022; Bouhali *et al.*, 2015). The IUPAC classification classifies pores into micropores, mesopores, and macropores based on their pore size ( $d$ , i.e. diameters of cylindrical pores or distance between sides of slit-like pores). This classification corresponds to different adsorption mechanisms, although the ratio of adsorbate molecular sizes to pore size is the effective discriminating factor. Adsorption in micropores ( $d \leq 20 \text{ \AA}$ ) occurs by volume filling of the micropores according to the Dubinin-Astakhov (DA) model (Dubinin, 1960; Dubinin and Astakhov, 1971; Hassan *et al.*, 2019). This model has been proposed as a semi-empirical relationship between the adsorbed quantity and the adsorption potential. The adsorption potential was originally proposed by Polanyi (Polanyi, 1932; Nandiyanto, 2020; Jabri *et al.* 2019) founded on a thermodynamic argument. With this approach, adsorbent-adsorbate interactions are greatly improved since gas molecules and pore size are comparable and each gas molecule experiences the force field generated by pore walls. In addition, molecular sieving can take place if one component is larger than the pore opening. Concerning the adsorption in the mesopores ( $20 \text{ \AA} < d \leq 500 \text{ \AA}$ ) than in the macropores ( $d > 500 \text{ \AA}$ ), the adsorbate molecules are organized in several layers according to the mechanistic models proposed (for example that of Brunauer–Emmett–Teller (BET) (Brunauer *et al.*, 1938)). The molecules belonging to the bed in contact with the solid surface are highly attracted while the molecules in the central region of the pore are essentially shielded from the force field. The adsorbate partial pressure inside the mesopores is higher than outside. When the partial pressure exceeds a critical value (if the adsorption temperature is lower than the critical value),

bulk adsorbate condensation occurs inside the pore. This phenomenon is called capillary condensation. Macropores ( $d > 500 \text{ \AA}$ ) act in gas adsorption like open surfaces. So, their contribution to the adsorption capacity is usually negligible and their main role is to facilitate transport inside the adsorbent particles (Lowell *et al.*, 2012).

In this paper, an approach proposed for understanding the interaction forces involved in the mechanism of adsorption of a gas by a microporous solid is based on the concept of flux: the flux of the amount of material that passes through a surface closed is proportional to the variation of the adsorbate-adsorbent interaction potential. The approach used allowed us to show that the adsorption of a gas by a microporous solid goes through two stages: adsorption in the micropores and mesopores, adsorption in the macropores, and on the lateral surface of the grains. These results justify the existence of two commonly used models, Dubinin-Astakov (in the case of microporous filling) and BET (in the case of multilayer adsorption).

## 2. Methodology

In this study, zeolite 13X and water were used as working pair. Zeolites 13X are hydrated aluminosilicates. Their structure is a three-dimensional arrangement of  $\text{SiO}_4$  and  $\text{AlO}_4$  tetrahedra linked together by oxygen atoms. Zeolites are able to adsorb organic and mineral molecules in the gas phase without any structural modification. This adsorption is due to their high specific surface, hydrophobic-hydrophilic surface effects, large pore volume, and highly developed porous structure. In addition, zeolite 13X has a high affinity for water, and the cationic sites in the structure of zeolites are effective in the adsorption properties. The high affinity of zeolite for water has a special value since preadsorbed water affects the application of zeolite as catalysis and in separation processes (Sayilgan *et al.*, 2016). The main physicochemical characteristics of zeolite 13X are presented in Table 1 below.

**Table 1.** Characterization of zeolite 13X (Mhiri, 2016)

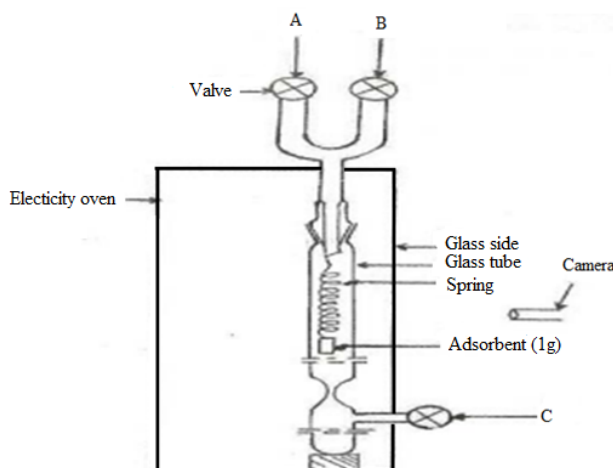
Chemical name	$\text{Na}_{86} \{(\text{AlO}_2)_{86}(\text{SiO}_2)_{106}\} 276 \text{ H}_2\text{O}$
Pore diameter	$\sim 8 \text{ \AA}$
Mecropore volume	$0165 \text{ cm}^3/\text{g}$
Micropore volume	$0.17 \text{ cm}^3/\text{g}$
Langmuir surface	$571 \text{ m}^2/\text{g}$
Mass of the pellet sample	2.37g
Mass of the crushed sample	2.49g
Volumic mass	$1.43 \text{ g/cm}^3$
Molar mass	18391 g
Cp	$0.7 \text{ KJ / kg K}$

All adsorption kinetics measurements were carried out on a fixed bed at the National Engineering School of Monastir at the Thermal and Energy Systems Studies Laboratory.

### 2.1 Experimental Condition

During the experiment, the pressure variation remains small (about 5 mb) and the temperature is maintained constant for each isotherm. The 1g of zeolite13X is placed in the support and introduced into the glass tube, the valves A, B, and C are connected and the pump is set to vacuum. When a satisfactory vacuum is reached, heating is started using an electric oven and pumping continues until the desired temperature stabilizes. In front of the oven, the camera is placed and the first negative for the initial length of the spring is taken, the support is marked by a red line which will serve as a

reference for the measurements of the lengths of the spring. The valve of the inlet of adsorbate C is opened and the negatives at regular time intervals are taken. At the end of the measurements, for each isotherm, the negatives are developed and the quantity adsorbed at each moment is determined, knowing the lengthening (the lengthening measurement accuracy is 0.002 mm) (Mhiri, 2021) (Figure 1).



**Figure 1.** Representative diagram of the installation utilized for the experimental tracing of isotherms: A: measure of the pressure; B: vacuum pump; C: injection of fluids (Mhiri, 2021)

## 2.2 Representation of the kinetic isotherms

**Figure 2** shows the variation of the relative amount of water adsorbed by zeolite 13X as a function of time. These adsorption isotherms are Type I (Duquesne, 2013), exhibited by a rapid increase in the adsorbed amount followed by an approximately horizontal plateau. This type of isotherm is generally in two zones, each zone corresponding to a particular method of fixing the adsorbate to the adsorbent:

- Zone 1: This zone concerns the filling of micropores. It is characteristic of the action of forces interaction of the type of electrostatic between hydrophilic groups and polar molecules (water). Water is in a rigid state due to the strong bonding forces between water molecules and the surface. The adsorption of water molecules takes place gradually until a monolayer forms covering the surface of the adsorbent as described by Jajko *et al.*, 2022; Agboola O.D. and Benson N.U. 2021.

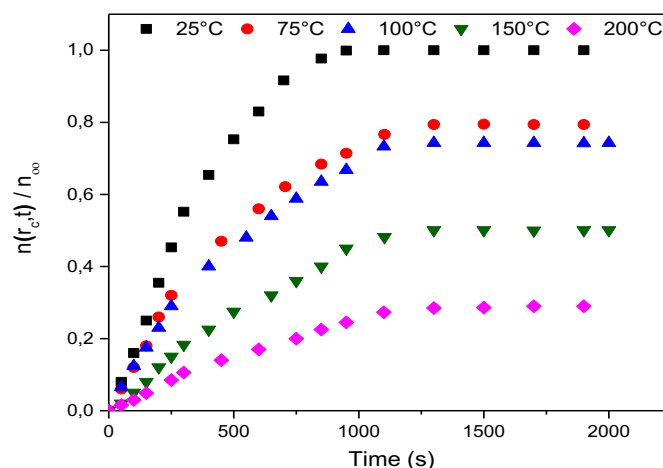
- Zone 2: The isotherm is linear which implies the saturation of the zeolite with adsorbed molecules, i.e. the adsorption of molecules on the initial monolayer (Aouaini *et al.* 2021).

In addition, this result shows that the quantity of adsorbed water decreases as a function of the temperature. Physical adsorption is exothermic. The rise in temperature prevents adsorbed molecules from easily attaching to the adsorbent surface.

## 2.3 Study of the variation of the flux

The variation of the flow of water adsorbed, measured at different temperatures, goes through three regimes (Figure 3). It can be seen that the adsorption is stronger in the first regime than that corresponding to the adsorption in the micropores due to an adsorbate molecule being subjected to the force fields of both walls of the pore. The electrostatic interaction is therefore stronger.

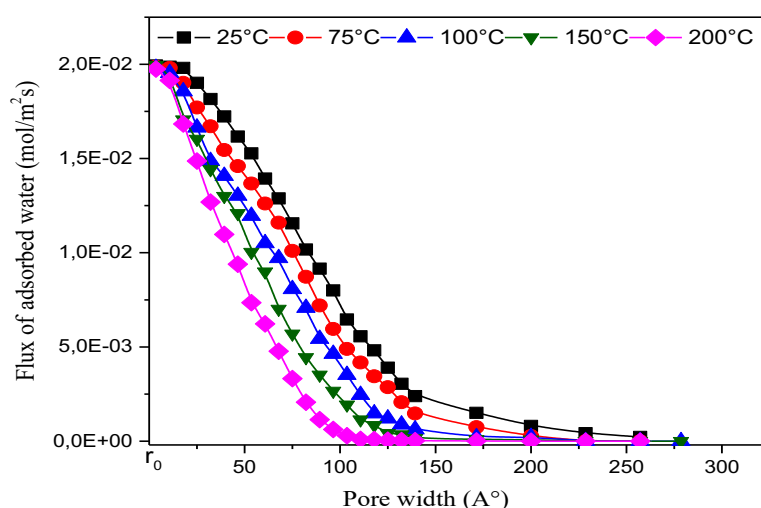
As the pore size increases, the variation in flow decreases linearly. This decrease is due to decreases in the adsorbate-adsorbent interactions and therefore the adsorption is less strong. This region concerns the adsorption in the mesopores.



**Figure 2.** Relative evolution of the quantity of water adsorbed by zeolite 13X measured at different temperatures

Finally, the last regime concerns adsorption in the macropores and on the lateral surface. The flux of adsorbed material is the lowest, which implies that the interactions between the water molecules and macropore and the side surfaces of the adsorbent are weak. The adsorption capacity of macropores is not important, but their importance lies in the fact that they act as transport pores to mesopores and micropores.

Thus the results show that the increase in the temperature of gas implies a reduction in the flow rate of the quantity of material adsorbed, for the two regions of the mesopores, the macropores, and the lateral surface, following the thermal agitation of the molecules of adsorbed gas. Increasing the temperature prevents the adsorbed molecules from easily attaching to the adsorbent surface. For micropores, the flow rate remained constant and higher, regardless of the temperature used. This experimental result is new proof of the strong intensity of the potential for adsorption as a consequence of the interaction forces with respect to the other forces.



**Figure 3.** Variation of the flow of the amount of water adsorbed material as a function of pore width, measured at different temperatures

### 3. Results and Discussion

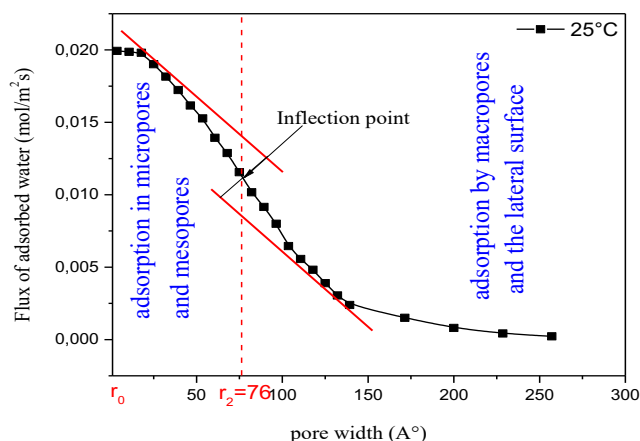
#### 3.1 A mathematical study of the flow

As part of the mathematical study, the evolution of the flux of the adsorbed material as a function of the width of the pores, having an inflection point, is described by two equations. One corresponds to adsorption in micropores and mesopores [ $r_0 < r \leq r_2$ ] and the other corresponds to adsorption by macropores and the lateral surface of the grain of the microporous solid [ $r_2 \leq r$ ] (**Figure 4**).

With

$r_0$  is the minimum width of the micropores for adsorption to take place.

$r_2$  is the effective pore width, determined experimentally from the point of inflection.



**Figure 4.** Variation of the flow of the amount of water adsorbed material as a function of pore width at  $T = 25^\circ\text{C}$

By analogy, each of the flux variation curves of the water adsorbed by the zeolite in the interval [ $r_0 < r \leq r_2$ ] is similar to the curve of gain as a function of pulsation for a low pass circuit in electricity. Then the first flow equation is defined by (**Benkahla and Mhiri, 2019**):

$$r_0 < r \leq r_2 \quad \Phi_1 = \frac{B}{1+(r/r_2)^2} \quad \text{Eqn. 1}$$

Then, in the interval [ $r_2 \leq r$ ] and from the curves, it is about a Coulomb potential of form  $1/r^2$ . The second proposed equation is then, described by (**Benkahla and Mhiri, 2019**):

$$r_2 \leq r \quad \Phi_2 = \frac{A}{(r/r_2)^2} \quad \text{Eqn. 2}$$

The continuity of the flow in  $r_2$  implies  $\Phi_1(r_2) = \Phi_2(r_2)$  and according to Equations **Eqn. 1** and **Eqn. 2**, B defined as follows:  $B=2A$ .

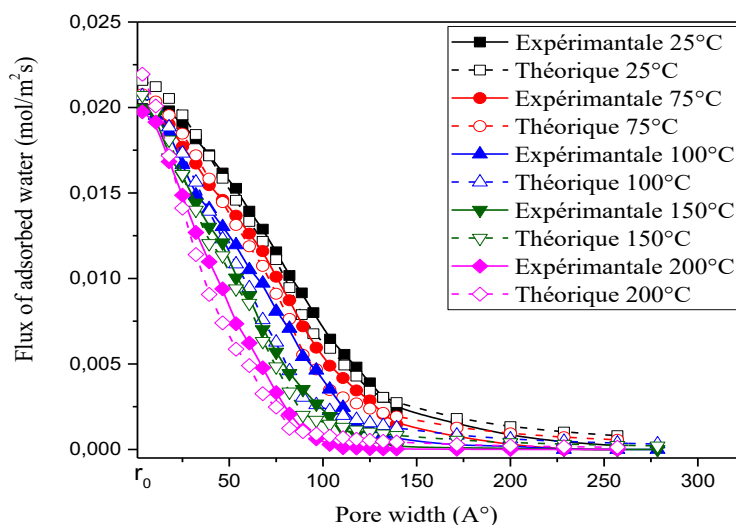
#### 3.2 Validation of the mathematical model

The comparison of the theoretical flow with the experimental flow allows checking the validity of the mathematical model. Note the good agreement between the two results on the curves of the variation of the flux as a function of the width of the pores ( $\Phi = f(r)$ ), illustrated in **Figure 5**, using the two theoretical proposed Equations **Eqn. 1** and **Eqn. 2**.

Mathematically, the three regions found experimentally on the curve of the flux as a function of the width of the pores were reduced to two: adsorption in the micropores and the mesopores (a filling



in volume), multilayer adsorption in the macropores, and on the lateral surface. These results justify the existence of the two most commonly used models, Dubinin-Astakov (in the case of microporous filling) (Dubinin and Astakhov, 1971; Benkahla and Mhiri, 2019), and BET (in the case of multilayer adsorption) (Brunauer *et al.*, 1938; Benkahla and Mhiri, 2019).



**Figure 5.** Comparison between experimental and theoretical flows, measured at different temperatures

### 3.3 A mathematical study of the adsorbate–adsorbent interaction potential

This study has made a simple and obvious assumption: The flow of the quantity of adsorbed material is proportional to the variation of the adsorbate-adsorbent interaction potential ([appendix 1](#)):

$$\Phi = \beta \frac{dU}{dr} \quad \text{Eqn.3}$$

With  $\beta$  being the proportionality constant for a given adsorbate-adsorbent pair (mol s/m<sup>3</sup> kg), this is the adsorbate-adsorbent affinity coefficient. If there is no affinity,  $\beta$  is zero, the flux is zero and the interaction potential is zero and not infinite because in this case A and B (equations [Eqn. 5](#) and [Eqn. 6](#)) are zero.

From expression ([Eqn.3](#)), the expression of the variation of the adsorption potential is defined by:

$$U = \frac{1}{\beta} \int \Phi(r) dr \quad \text{Eqn. 4}$$

Then the mathematical equations of the adsorbate-adsorbent interaction potential, as a function of the pore widths are described by (Benkahla and Mhiri, 2019):

➤ Adsorption in micropores and mésopores:

$$\Phi_1(r) = \beta \frac{dU_1}{dr} = \frac{B}{1+(r/r_2)^2} \rightarrow U_1 = \frac{B r_2}{\beta} \text{Arctan}\left(\frac{r}{r_2}\right) + c_1 \quad \text{for } r_0 < r \leq r_2 \quad \text{Eqn. 5}$$

➤ Adsorption by macropores and the lateral surface:

$$\Phi_2(r) = \beta \frac{dU_2}{dr} = \frac{A}{(\frac{r}{r_2})^2} \rightarrow U_2 = -\frac{A r_2}{\beta (\frac{r}{r_2})} + c_2 \quad \text{for } r_2 \leq r \quad \text{Eqn. 6}$$

With A and B are constants, proportional to the intensities of the forces of interaction (for each couple). The continuity of the potential U(r) in the interval  $[r_0, \infty[$  implies  $U_1(r_2) = U_2(r_2)$  ([appendix 2](#)):

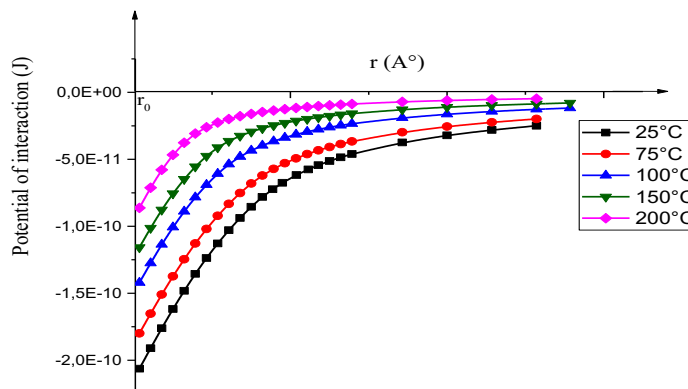
$$U_1(r) = \frac{B r_2}{\beta} \left\{ \text{Arctan} \left( \frac{r}{r_2} \right) - \text{Arctan} (1) - \frac{1}{2} \right\} + c_2 \quad \text{Eqn. 7}$$

$$U_2(r) = -\frac{B r_2^2}{2\beta r} + c_2 \quad \text{Eqn. 8}$$

With  $c_2$  being a negative constant which is nothing other than the interaction potential for a flat surface (when  $r$  approaches infinity).

### 3.4 Study of the variation of the adsorbate–adsorbent interaction potential

The **Figure 6** shows the variation of the adsorbate-adsorbent interaction potential as a function of the pore width, determined at different temperatures.



**Figure 6.** Variation of the adsorbate–adsorbent interaction potential as a function of the pore width, measured at different temperatures

Mathematically, this implies that the curve of **Figure 6** described by two functions (Arctangent and  $1/r$ ), one relating to the part corresponds to the adsorption in the micropores and the mesopores ( $r_0 < r \leq r_2$ ) and the other relating to the monolayer and multilayer adsorption in the macropores and on the side surface of the zeolite13X ( $r_2 \leq r < \infty$ ). The variation of the adsorption potential increases as a function of the width of the pores. These findings are in good agreement with those obtained by [Fernández-Reyes \*et al.\*, 2021](#). The relatively high values of the potential implications a relatively strong electrostatic interaction between the adsorbed polar molecules and the adsorbent surface. Each adsorbed molecule undergoes a force field generated by the walls of the pores. When  $r$  tends to infinity, the limit of the potential is the constant  $c_2$  which represents the adsorption potential on a plane surface.

Thus the results show that the temperature also influences the variation of the adsorption potential. The increase in the temperature of gas automatically implies an increase in the speed and the mean free path of the molecules. This prevents the adsorbed molecules from being easily picked up by the available sites of the adsorbent due to the thermal agitation of the molecules adsorbed in the gaseous state. This implies a rapid decrease in the potential for adsorbate-adsorbent interaction, a transition to adsorption on the flat surface is observed.

### Conclusion

The law presented in this paper presents an excellent agreement with the experimental measurements, which is logical; it is deduced from these experimental data. The interpretation of the different terms of this law makes the difference with other existing potentials.



Mathematically, the three regions found experimentally on the curve of flux versus pore size are reduced to two: adsorption in micropores and mesopores (one filling in volume), multilayer adsorption in macropores, and on the lateral surface of grains of the microporous solid, this implies the existence of two types of interaction forces between the molecules of adsorbate and the adsorbent, each type of forces corresponds to one of the regions. Thus the variation of the adsorption potential depends on the effect of temperature.

The increase in temperature implies a decrease in the quantity of material adsorbed because the increase in temperature prevents the adsorbed molecules from being easily picked up by the available sites of the adsorbent due to the thermal agitation of the molecules adsorbed to the surface gaseous state.

Determining the adsorption potential as a function of pore size opens the door to the development of technologies. In the event that there is an affinity between the adsorbent and the adsorbate. The study of the variation in interaction potential allows the manufacture of specific microporous solids for each adsorbent-adsorbate pair according to their utility. For example, if you want the recovery of Volatile Organic Compounds in a microporous solid. The radius of the pores of the solid must be in the zone where the potential is the highest to ensure a strong adsorbate-adsorbent interaction.

## Annexes1

The flow of the adsorbed quantity is given by:  $\Phi = \iint_{\text{surface}} \rho \vec{u} \cdot d\vec{S}$

Where  $\rho$  is the density of the fluid,  $\vec{u}$  is its velocity, and  $d\vec{S}$  is the oriented surface ( $d\vec{S} = ds\vec{n}$  where  $\vec{n}$  is the unit vector normal to the surface).

The equation of quantity conservation of motion is defined by:  $m \frac{d\vec{u}}{dt} = -\vec{\sigma} \cdot \vec{U} - \lambda \vec{u}$

Where  $U$  is the interaction potential and  $\lambda$  is a constant. If the flow is at a constant speed ( $\frac{d\vec{u}}{dt} = 0$ ) we will then have  $\vec{u} = -\frac{1}{\lambda} \vec{\sigma} \cdot \vec{U}$ , this implies that the adsorption rate depends on the potential and consequently on the flow as well. In fact, this observation and this demonstration have given us the idea of drawing the following hypothesis: the flux is proportional to the variation of the interaction potential as a function of the pore width:

$$\Phi = \beta \frac{dU}{dr}$$

## Annexes 2

The function  $\Phi(r)$  is continuous over the interval  $[r_0, \infty[$ , the derivative of the potential  $\frac{dU}{dr}$  exists and is continuous over the same interval, which implies that the potential  $U(r)$  is continuous over this interval:

$$\text{Then } U_1(r_2) = U_1(r_2) \quad \text{Eqn.1}$$

$$\frac{B r_2}{\beta} \text{Arctan}(1) + c_1 = -\frac{A r_2}{\beta} + c_2 \quad \text{Eqn. 2}$$

Where  $B = 2A$

$$c_1 = -\frac{B r_2}{\beta} \left\{ \text{Arctan}(1) + \frac{1}{2} \right\} + c_2 \quad \text{Eqn. 3}$$

$$\text{So } U_1(r) = \frac{B r_2}{\beta} \left\{ \text{Arctan}\left(\frac{r}{r_2}\right) - \text{Arctan}(1) - \frac{1}{2} \right\} + c_2 \quad \text{Eqn. 4}$$

$$U_2(r) = -\frac{B r_2^2}{2\beta r} + c_2 \quad \text{Eqn. 5}$$

With  $c_2$  being a negative constant which is nothing other than the interaction potential for a flat surface (when  $r$  approaches infinity).

**Disclosure statement:** *Conflict of Interest:* The authors declare that there are no conflicts of interest.

*Compliance with Ethical Standards:* This article does not contain any studies involving human or animal subjects.

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