Investigation of pore size and energy distributions by statistical physics formalism applied to agriculture products

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HIGHLIGHTS

- Investigation allowing to determine the distribution of PSD.
- The radius of olive leaves is macrospores.
- The distribution of energetically different sites deduces from PSD.
- All desorption energy distributions have a Gaussian shape.

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ABSTRACT

In this paper, we present a new investigation that allows determining the pore size distribution (PSD) in a porous medium. This PSD is achieved by using the desorption isotherms of four varieties of olive leaves. This is by the means of statistical physics formalism and Kelvin's law. The results are compared with those obtained with scanning electron microscopy. The effect of temperature on the distribution function of pores has been studied. The influence of each parameter on the PSD is interpreted. A similar function of adsorption energy distribution, AED, is deduced from the PSD.

1. Introduction

Gas adsorption measurements are widely used for determining the surface area and pore size distribution of a variety of different solid materials, e.g. industrial adsorbents, catalysts, pigments, ceramics and building materials [1]. The study of the distribution of pore sizes is an area of investigation that attracted the attention of many researchers. The technological applications of the porous environments are very numerous and will be it still more in the future with the increase of the costs of energy and the awakening of the environmental problems [1–3]. They play a paramount role in the biological processes (vegetable, wood, human skin, cartilage, bone...) [4], natural (grounds, porous rocks...) and in multiple industrial applications (concretes, powders, metal foam, porous ceramics, cement, fabric...) [5,6]. In the literature, there are many techniques, which make it possible to characterize the pores size distribution [1–6]. Moreover, they are more difficult to implement and expensive (thermoporometry, diffusion with the small angles, NMR...) and sometimes destructive, in

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Nomenclature

PSD:	Pore Size Distribution
AED:	Adsorption Energy Distribution
a_w:	The water activity
Q:	The equilibrium moisture content (kg water vapor/kg dry matter)
n:	The number of molecules per site
N_M:	The receptor sites per surface unit
a_1 and a_2:	Dimensionless parameters which are related to the adsorption energy
N_2:	The number of layers formed with energy $(-\varepsilon_2)$
R^2:	The coefficient of determination
P:	The partial pressure of the water vapor
P_0:	The saturated vapor pressure
T:	The absolute temperature
V_L:	The molar volume of liquid ($22.4\ 10^{-3}\ \mathrm{m^3\ mol^{-1}}$)
γ:	The surface tension of the liquid ($75.64 \times 10^{-3}\ \mathrm{N\ m^{-1}}$)
θ_k:	The contact angle between the liquid and the walls (adsorbent)
R:	The ideal gas constant ($8.3144621\ \mathrm{J\ mol^{-1}\ K^{-1}}$)
V_a:	The adsorbed volume
V_M:	The monolayer adsorbed volume
K_k:	Constant of Kelvin
r:	The pore radius

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particular the technique of the stereology, or the direct study of the geometry of the plane sections of a porous environment [7]. The measurement of adsorption at the gas/solid interface also forms an essential part of most fundamental and applied investigations of the nature and behavior of solid surfaces.

Indeed, knowing the distribution of pore sizes from desorption isotherms is a well known method, which has the advantage of being nondestructive unlike methods based on microscopic techniques [7,8]. The measurement of desorption isotherms, in particular a gas over a porous solid, allows access to the pore size distribution.

In general, the surfaces of porous adsorbents have complex geometrical structures of varying affinity for the guest molecule and the adsorption phenomenon is related to the characteristic interactions between the adsorbent and adsorbed molecules [8].

Many adsorbents of high surface area are porous and with such materials, it is often useful to distinguish between the external and internal surfaces [9]. The external surface is usually regarded as the geometrical envelope of discrete particles or agglomerates, but a difficulty arises in defining it because solid surfaces are rarely smooth on an atomic scale. A suggested convention proposes that the external surface is taken to include all the prominences and also the surface of those cracks, which are wider than they are deep. Whereas the internal surface then comprises the walls of all cracks, pores and cavities which are deeper than they are wide and which are accessible to the adsorptive [9–11]. In practice, the demarcation is likely to depend on the methods of assessment and the nature of the pore size distribution because the accessibility of pores may depend on the size and shape of the gas molecules, the area, and the volume enclosed by the internal surface. This latter determined by gas adsorption may be controlled by the dimensions of the adsorbed molecules (molecular sieve effect) [10]. On molecular scale, the roughness of a solid surface may be characterized by a roughness factors i.e. the ratio of the external surface to the chosen geometric surface [9–11]. It is expedient to classify pores according to their sizes [9,11,12]:

- Pores with widths exceeding about 50 nm (0.05 μm) are called macropores.
- Pores with widths not exceeding about 2 nm are called micropores.
- Pores of intermediate size are called mesopores.

The different distributions obtained for each adsorbate do not reflect the size distribution of the actual total pore material used, but they are very useful for representing the interval pores detected by these molecules, which may be called the interval accessibility or penetration range. Thus, despite the fact that these distributions do not show the entire structure of food products, they can inform us about the relationship between the sizes of the pores detected and geometrical characteristics of the adsorbate molecule.

In our previous study [13], we investigated the desorption phenomenon by the use of new model describing the sorption isotherms of water vapor. This model is applied to agriculture product and particularly to Tunisia olive leaves. In this work, we focus interest in the determination of the adsorbent characteristics such as the PSD and AED using the same model proposed in our previous work [13]. The theoretical model was investigated by the use of statistical physics formalism and the Kelvin equation and applied to desorption isotherms of olive leaves. A theoretical study was presented to understand the effect of different parameters on the distribution of pore size. In addition, we described energetically the surface heterogeneities by the calculation of AED.