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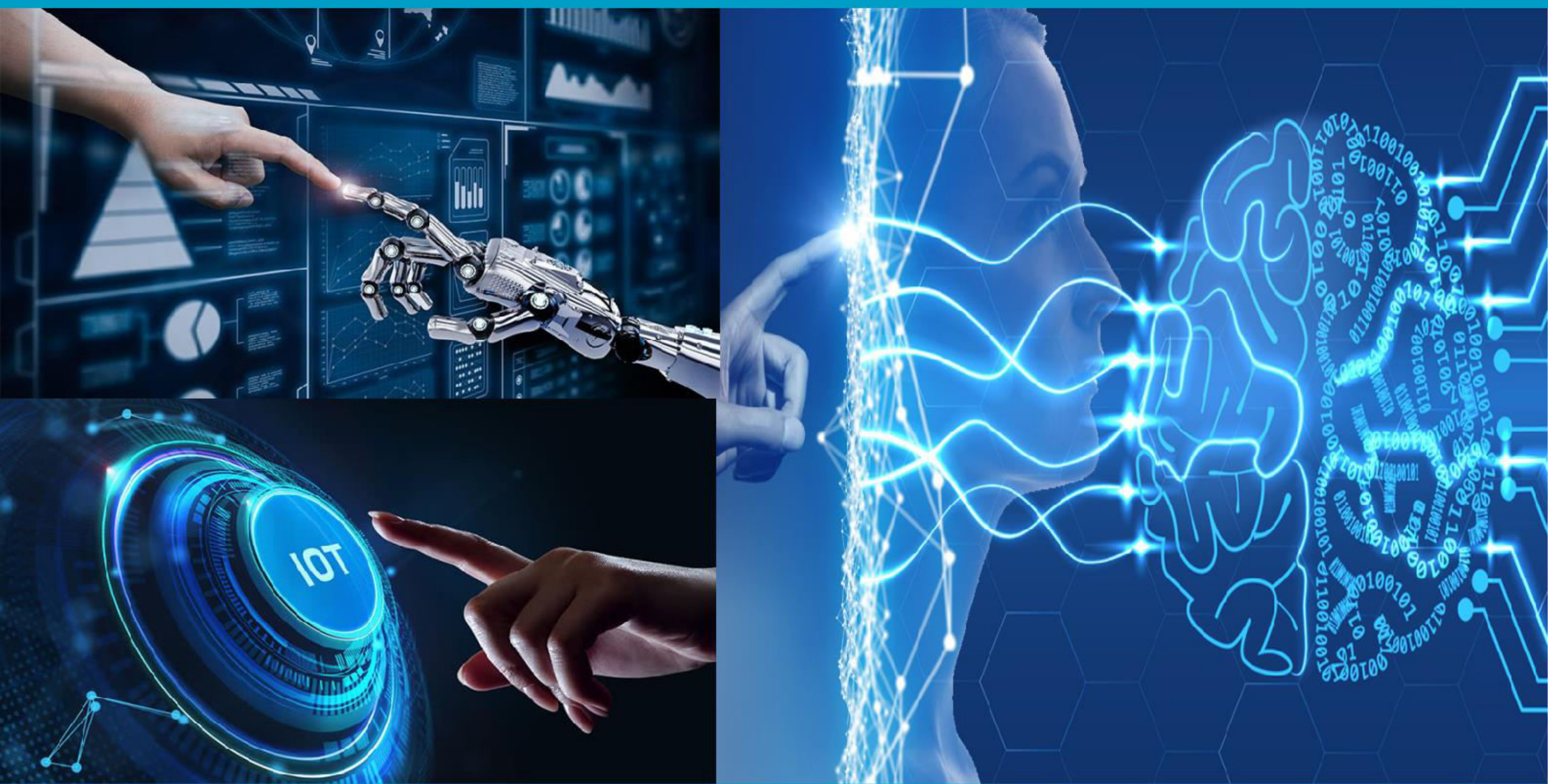

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Reseiving of Distribution Functions Parameters by Sizes from the Experiments of Water Sorbtion by Polymers.

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Annotation:

It has been theoretically considered three kinds of distribution functions of pores by sizes in polymers. On the base of experimental data of water sorption by polymers the following parameters of these distributions functions as the total number of pores per sorbent unit mass and their size distribution have been received. It has been revealed that the sizes of pores in such polymers as PVP, khitozan and cellulose were in nanoscaled area.

Keywords: chitosan, sorbtion, polymer, sizes, distributions functions

During sorption, in principle, two cases are possible: the sorbate occupies the entire pore volume or the pore volume is partially occupied by the sorbate [1]. In the first case, knowing from the experiment [1,2] the total volume occupied by the sorbate, this volume can be identified with the total actual volume of the pores, and the specific surface area is the sum of the surface area of all pores per unit mass of the sorbent. As for the group of pores, in principle, two options for their organization are possible - firstly, assuming that the pores have a spherical shape, they can all be the same size (radius), secondly, they can have a certain spread in size (radius). An interesting problem arises - how to obtain information about the size of pores and the pore size distribution function from experimental data. In the spherical pore approximation, this can be done from fairly general considerations. Let's look at specific cases.

1. Approximation of spherical pores of the same size.

In this case, the pore distribution function can be selected in delta form: $f(R) = \delta(R - R_0)$, where R_0 is the unified pore radius, $\delta(R)$ is the Dirac delta function. Then for the total volume of all pores and their specific surface area we obtain the expressions.

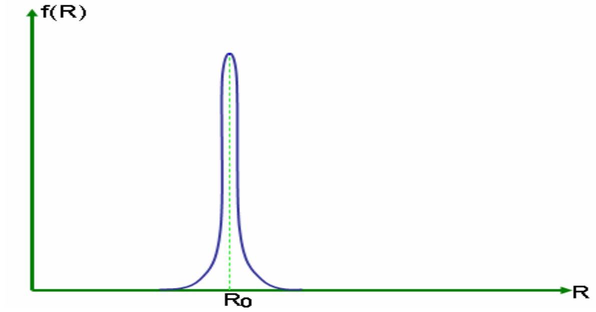

Fig. 1. Delta-shaped distribution function.

$$V_t = N\frac{4\pi}{3}\int_0^\infty R^3 f(R)dR = N\frac{4\pi}{3}\int_0^\infty R^3\delta(R - R_0)dR = N\frac{4\pi}{3}R_0^3$$

$$S_t = N4\pi\int_0^\infty R^2 f(R)dR = N4\pi\int_0^\infty R^2\delta(R - R_0)dR = N4\pi R_0^2$$

In these expressions, N is the total number of pores per unit mass of the sorbent, V_t is the total volume and S_t is the total surface of the pores per unit mass of the sorbent. If V_t and S_t are known from experiment, then we obtain a system of two equations with two unknowns – N and R_0. Solving the system of equations, we obtain expressions for N and R_0.

$$R_0 = 3\frac{V_t}{S_t}$$

$$N = \frac{3}{4\pi}\frac{V_t}{R_0^3}$$

Let us apply the obtained formulas to cases of water sorption by polymers [1]:

a) Polyvinylpyrrolidone (PVP).

$$[V_t = 0.331\cdot 10^{-6}\ м^3/г \quad S_t = 77.6815\ м^2/г]$$

$$R_0 = 3\frac{0.331\times 10^{-6}}{77.6815} = 12.78\times 10^{-9}\ м \approx 13нм$$

$$N = \frac{3}{4\pi}\frac{0.331\times 10^{-6}}{(12.78\times 10^{-9})^3} = 3.78\times 10^{16}\quad 1/г$$

b) Chitosan $[V_t = 0.045\cdot 10^{-6}\ м^3/г \ S_t = 45.005\ м^2/г]$

$$R_0 = 3\times 10^{-9}\ м \approx 3нм$$

$$N = 3.98\times 10^{17}\quad 1/г$$

v) Cellulose $[V_t = 0.089\cdot 10^{-6}\ м^3/г \quad S_t = 50.044\ м^2/г]$

$$R_0 = 5.3\times 10^{-9}\ м \approx 5{,}3нм$$

$$N = 1.4\times 10^{17}\quad 1/г$$

2. Approximation of spherical pores with a rectangular distribution function.

Let us choose the distribution function in the form

$$f(R) = \frac{1}{R_2 - R_1}.$$

At that $f(R) = \begin{cases} \frac{1}{R_2 - R_1} & R_1 < R < R_2 \\ & \text{at } R < R_1 \\ 0 & R > R_2 \end{cases}$ then

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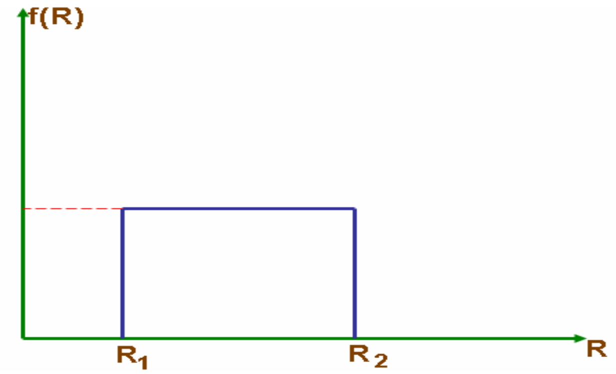

Fig. 2. Rectangular distribution function.

The total specific volume and specific pore surface area will be equal

$$V_t = \frac{4\pi}{3} N \int_{R_1}^{R_2} \frac{R^3 dR}{R_2 - R_1} = \frac{1}{3} \frac{\pi N}{R_2 - R_1} (R_2{}^4 - R_1{}^4)$$

$$S_t = 4\pi N \int_{R_1}^{R_2} \frac{R^2 dR}{R_2 - R_1} = \frac{4}{3} \frac{\pi N}{R_2 - R_1} (R_2{}^3 - R_1{}^3)$$

From a system of two equations with two unknowns at $R_1 = 0$ we obtain N and R_2. Taking relationships and we get

$$\frac{V_t}{S_t} = \frac{1}{4} \frac{R_2{}^4 - R_1{}^4}{R_2{}^3 - R_1{}^3}$$

Let us apply this approximation for, i.e., assuming that the pore size distribution begins with very small values.

Then for PVP we get [1]: $[V_t = 0.331 \cdot 10^{-6}\ м^3/г \quad S_t = 77.6815\ м^2/г]$

$R_2 = 17 \times 10^{-9}\ м \approx 17\ нм$

$N = 6.4 \times 10^{16} \quad 1/г$

For Chitosan $[V_t = 0.045 \cdot 10^{-6}\ м^3/г \quad S_t = 45.005\ м^2/г]$

$R_2 = 4 \times 10^{-9}\ м \approx 4\ нм$

$N = 6.7 \times 10^{17} \quad 1/г$

For Cellulose $[V_t = 0.089 \cdot 10^{-6}\ м^3/г \quad S_t = 50.044\ м^2/г]$

$R_2 = 7.1 \times 10^{-9}\ м \approx 7{,}1\ нм$

$N = 2.4 \times 10^{17} \quad 1/г$

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3. Approximation of spherical pores with a normal distribution function [3].

$$f(R) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(R-R_0)^2}{2\sigma^2}}$$

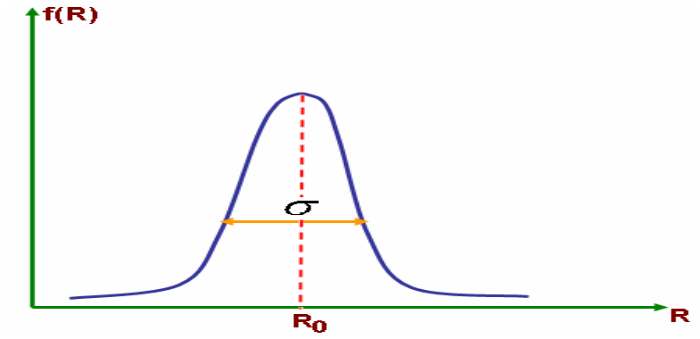

Fig.3. Normal distribution function.

As is known, this distribution corresponds to a symmetrical curve with one maximum corresponding to the pore radius equal to R_0 and dispersion σ. [3].

Let us calculate the total specific volume of all pores and their specific surface area with such a distribution function in a similar way to what was done above.

$$V_t = N\frac{4\pi}{3}\int_0^\infty R^3 f(R)dR = N\frac{4\pi}{3}\frac{1}{\sqrt{2\pi\sigma}}\int_0^\infty R^3 e^{-\frac{(R-R_0)^2}{2\sigma^2}} dR =$$

$$N\frac{4\pi}{3}\frac{1}{\sqrt{2\pi\sigma}}[2\sigma^4 + 3\sqrt{\frac{\pi}{2}}R_0\sigma^3 + 3R_0{}^2\sigma^2 + \sqrt{\frac{\pi}{2}}R_0{}^3\sigma]$$

$$S_t = N4\pi\int_0^\infty R^2 f(R)dR = N4\pi\frac{1}{\sqrt{2\pi\sigma}}\int_0^\infty R^2 e^{-\frac{(R-R_0)^2}{2\sigma^2}} dR =$$

$$N4\pi\frac{1}{\sqrt{2\pi\sigma}}[\sqrt{\frac{\pi}{2}}\sigma^3 + 2R_0\sigma^2 + \sqrt{\frac{\pi}{2}}R_0{}^2\sigma]$$

R_0 is selected from the delta function approximation (Section 1). Then we solve a system of two equations with two unknowns N and σ. Taking the ratio of V_t to S_t

$$\frac{V_t}{S_t} = \frac{1}{3}\frac{[2\sigma^4 + 3\sqrt{\frac{\pi}{2}}R_0\sigma^3 + 3R_0{}^2\sigma^2 + \sqrt{\frac{\pi}{2}}R_0{}^3\sigma]}{[\sqrt{\frac{\pi}{2}}\sigma^3 + 2R_0\sigma^2 + \sqrt{\frac{\pi}{2}}R_0{}^2\sigma]}$$

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$$N = \frac{3V_t}{2\sqrt{2\pi}[2\sigma^4 + 3\sqrt{\frac{\pi}{2}}R_0\sigma^3 + 3R_0^2\sigma^2 + \sqrt{\frac{\pi}{2}}R_0^3\sigma]}$$

Let us calculate the unknown parameters N and σ for the case of water sorption [1]:

a) For PVP.

$$N = 7.57 \times 10^{16} \ \ 1/г$$

$$\sigma = 3.72 \times 10^{-12} \ м = 3.72 \cdot 10^{-3} \, нм$$

b) For Chitosan

$$N = 2.42 \times 10^{18} \ \ 1/г$$

$$\sigma = 1.88 \times 10^{-9} \ м = 1.88 \, нм$$

v) For Cellulose

$$N = 2.8 \times 10^{17} \ \ 1/г$$

$$\sigma = 4.39 \times 10^{-11} \ м = 4.39 \cdot 10^{-2} \, нм$$

Conclusion

Thus, the developed mathematical formalism makes it possible from the analysis of experiment [1] to approximately obtain important parameters of sorption by polymers: the total specific number of pores, pore size [2]. As the results show, the pore sizes in three different polymer sorbents turn out to be different and have a characteristic size of the order of nanometers. Moreover, for chitosan the pore sizes are the smallest, and for PVP they are the largest. These results are especially important given their potential application in nanotechnology: during sorption or doping, a sorbate (dopant) is placed in the pores, so that nanoclusters are formed, the sizes of which depend on the pore size [4, 5].

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