Condensed Matter Physics 2010, Vol. 13, No 2, 23607: 1–7

http://www.icmp.lviv.ua/journal

CONDENSED MATTER PHYSICS

Analytical theory of one- and two-dimensional hard sphere fluids in random porous media

M.F. Holovko[1], V.I. Shmotolokha[2], W. Dong[3]

[1] Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine

[2] Physico-Mechanical Institute of the National Academy of Sciences of Ukraine, 5 Naukova Str., 79601 Lviv, Ukraine

[3] Ecole Normale Superiere de Lyon, 46 Allee d' Italie, 69364 Lyon, Cedex 07, France

Received April 23, 2010, in final form April 28, 2010

The recently proposed scaled particle theory SPT2 approach to the description of three-dimensional hard sphere fluids in random porous media is extended for one- and two-dimensional cases. Analytical expressions for the chemical potential and pressure of one- and two-dimensional hard sphere fluids in hard sphere and overlapping hard sphere matrices are obtained and discussed. Some improvements and modifications of the obtained results are proposed.

Key words: *confined fluids, porous materials, scaled particle theory*

PACS: *61.20.Gy, 61.43.Gy*

1. Introduction

Much theoretical effort has been devoted to the study of fluids in porous materials for the last two decades starting with a pioneering work of Madden and Gland [1]. In that work, a very simple model for fluid adsorption in random porous media was proposed. Within the framework of this model, a porous medium forms a matrix of randomly distributed particles. With the replica Ornstein-Zernike integral equation [2] for the description of this model, the statistical-mechanics approach of liquid state physics was extended to a description of different fluids confined in a random porous matrix including the chemical reacting fluids adsorbed in porous media [3]. However, in sharp contrast with the bulk fluid, no analytical results have been obtained in the integral equation approach even for a simple model like a hard sphere fluid in a hard sphere matrix. The main difficulty in describing such a model is related to the absence of direct interaction between hard spheres from different replicated copies of fluids. Due to this, the description of such a model is equivalent to the study of a hard-sphere mixture with strongly nonadditive diameters for which it is very difficult to find correct analytical results.

The first very accurate analytical results for a hard-sphere (HS) fluid in HS and overlapping HS matrices were obtained quite recently [4–6] by extending the scaled particle theory (SPT) to a HS fluid confined in random porous media. This approach is based on the combination of the exact treatment of point scaled particle in HS fluid with the thermodynamical consideration of finite size scaled particle [7, 8]. It should be noted that for the bulk thermodynamical properties of HS fluid from SPT there was obtained the same result as for analytical solution of integral equation in Percus-Yevick approximation [9]. The exact result for point scaled particle in HS fluid in random porous media was obtained in [4]. However, the proposed approach, called SPT1, has got some inconsistency. After some improvements to the SPT1 there was developed a SPT2 approach [6] free from this inconsistency. The expressions obtained in SPT2 include two types of porosities. One of them is defined by the geometry of porous media and the second one is defined by the chemical potential of the fluid in infinite dilution. After an additional approximation there was developed a SPT2b approach that reproduces the computer simulation data with a very high accuracy.

All the above discussed results were obtained for three-dimensional systems. In this paper we extend the SPT method to the treatment of one- and two-dimensional HS fluid in random porous media. We should mention that SPT for the pure HS fluid in one-dimensional case [10] reproduces the exact result of Tonks [11] and in two-dimensional case leads to an analytical result which very well reproduces the computer simulation data. In contrast to three-dimensional case for pure HS fluids, in the two-dimensional case, the integral equation theory does not provide analytical results.

2. SPT for one- and two-dimensional hard sphere fluid

The basic idea of SPT is to insert an additional scaled HS particle of a variable size into a HS fluid. This is equivalent to creating a spherical cavity devoid of any other fluid particles. In the original formulation of SPT [7–10], the contact value of the pair distribution function of fluid particle around the scaled particle is the central function of the theory. However, as it was pointed in [4] such formulation cannot be readily extended to fluids in random porous media because no direct relation between pressure and the contact distribution function has been found. Due to this in [4] there was presented a reformulation of SPT which is slightly different from the original one. In this section we consider a generalization of this approach for the one- and two-dimensional HS fluids.

The central point of reformulation of SPT presented in [4] is a direct calculation of chemical potential of the scaled particle. After generalizing this approach to the excess of chemical potential of small scaled particle in n-dimensional HS fluid we have

$$\beta\mu_{\mathrm{s}}^{\mathrm{ex}} = -\ln\left(1-\eta_1\left(1+\frac{R_{\mathrm{S}}}{R_1}\right)^n\right) \quad \text{for} \quad 0 \leqslant R_{\mathrm{S}}+R_1 \leqslant R_1\,, \tag{1}$$

where $\beta = 1/kT$, k is Boltzmann constant, T – is temperature, R_{S} is the radius of scaled particle, R_1 is the radius of HS fluid particle, $\eta_1 = \rho_1 v_1$ is the fluid packing fraction, ρ_1 is fluid density, v_1 is the volume of one fluid particle. For one-dimensional case $v_1 = 2R_1$, for two-dimensional case $v_1 = 4\pi R_1^2$, for three-dimensional case $v_1 = \frac{4}{3}\pi R_1^3$.

For a larger scaled particle ($R_{\mathrm{S}} \geqslant 0$), the excess of chemical potential in SPT is given by a thermodynamic expression for the work needed to create a macroscopic cavity inside a fluid and it can be presented in the following form:

$$\mu_{\mathrm{s}}^{\mathrm{ex}} = w_{\mathrm{S}}(R_{\mathrm{S}}) + Pv_{\mathrm{S}}\,, \tag{2}$$

where P is pressure, v_{S} is the volume of scaled particle.

$w_{\mathrm{S}}(R_{\mathrm{S}})$ is the surface contribution which can be presented in the form of Taylor expansion which we cut off on $(n-1)$th term

$$w_{\mathrm{S}}(R_{\mathrm{S}}) = w_0 + \cdots + \frac{1}{(n-1)!}w_{n-1}R_{\mathrm{S}}^{n-1}. \tag{3}$$

The coefficients of this expansion can be found from the continuity of $\mu_{\mathrm{s}}^{\mathrm{ex}}$ at $R_{\mathrm{S}} = 0$. As a result, for $n = 1$ we will have only the first term

$$\beta w_0 = -\ln(1-\eta_1). \tag{4}$$

For $n = 2$ we will also have the second term

$$\beta w_1 = \frac{n\eta_1}{1-\eta_1}\frac{1}{R_1}\,. \tag{5}$$

For $n = 3$ we will also have the next term

$$\beta w_2 = \left[\frac{n(n-1)\eta_1}{1-\eta_1} + \frac{\eta_1^2 n^2}{(1-\eta_1)^2}\right]\frac{1}{R_1^2}\,. \tag{6}$$

Now it we put $R_{\mathrm{S}}=R_1$, the expression (2) gives us the relation between the pressure and the chemical potential of HS fluid. Using Gibbs-Duhem equation

$$\left(\frac{\partial P}{\partial \rho_1}\right)_T=\rho_1\left(\frac{\partial \mu_1}{\partial \rho_1}\right)_T \tag{7}$$

we will find that for one-dimensional HS fluid

$$\beta\mu_1^{\mathrm{ex}}=-\ln(1-\eta_1)+\frac{\eta_1}{1-\eta_1}\,, \qquad \frac{\beta P}{\rho_1}=\frac{1}{1-\eta_1}\,, \tag{8}$$

for two-dimensional HS fluid

$$\beta\mu_1^{\mathrm{ex}}=-\ln(1-\eta_1)+\frac{2\eta_1}{1-\eta_1}+\frac{\eta_1}{(1-\eta_1)^2}\,, \qquad \frac{\beta P}{\rho_1}=\frac{1}{(1-\eta_1)^2}\,, \tag{9}$$

for three-dimensional HS fluid

$$\begin{aligned}\beta\mu_1^{\mathrm{ex}} &= -\ln(1-\eta_1)+\frac{7\eta_1}{1-\eta_1}+\frac{15\eta_1^2}{2(1-\eta_1)^2}+\frac{6\eta_1^3}{(1-\eta_1)^3}\,,\\ \frac{\beta P}{\rho_1} &= \frac{1}{1-\eta_1}+\frac{3\eta_1}{(1-\eta_1)^2}+\frac{3\eta_1^2}{(1-\eta_1)^3}\,.\end{aligned} \tag{10}$$

All these results were obtained earlier by the standard SPT techniques [7–10].

3. SPT for n-dimensional hard sphere fluid in random porous media

In the presence of porous media the expression for the excess of chemical potential of small scaled particle in n-dimensional HS fluids can be written in the form

$$\beta\mu_{\mathrm{s}}^{\mathrm{ex}} = -\ln\left(p_0(R_{\mathrm{S}})-\eta_1(1+R_{\mathrm{S}}/R_1)^n\right) \tag{11}$$

$$= -\ln p_0(R_{\mathrm{S}})-\ln\left(1-\frac{\eta_1(1+R_{\mathrm{S}}/R_1)^n}{p_0(R_{\mathrm{S}})}\right), \tag{12}$$

where $p_0(R_{\mathrm{S}})=\mathrm{e}^{-\beta\mu_{\mathrm{S}}^0}$ is defined by the excess of the chemical potential μ_{S}^0 of the scaled particle in pure porous media and has the sense of probability of finding a cavity created by the particle of radius R_{S} in the porous media in the absence of fluid particles. $p_{1/0}(R_{\mathrm{S}})=1-\frac{\eta_1(1+R_{\mathrm{S}}/R_1)^n}{p_0(R_{\mathrm{S}})}$ is the conditional probability of finding a cavity created by the particle of radius R_{S} in the fluid-matrix system under condition that the cavity is located entirely inside a pore created by the particle with a radius equal to R_{S}.

For a larger scaled particle ($R_{\mathrm{S}}\geqslant 0$) the excess of chemical potential $\mu_{\mathrm{s}}^{\mathrm{ex}}$ is treated in thermodynamical way. To this end, there are two possibilities described by SPT1 [4] and SPT2 [6] approaches. We will show hereafter that SPT1 can be considered as the special case of SPT2 and due to this we will proceed now to SPT2 approach. According to SPT2 for ($R_{\mathrm{S}}\geqslant 0$)

$$\mu_{\mathrm{s}}^{\mathrm{ex}}-\mu_{\mathrm{S}}^0=w_{\mathrm{S}}(R_{\mathrm{S}})+\frac{1}{p_0(R_{\mathrm{S}})}Pv_{\mathrm{S}}\,, \tag{13}$$

where P is the pressure, which is similar to [6] and is modified here by the presence of porous media, v_{S} is the volume of the scaled particle. $p_0(R_{\mathrm{S}})$ is the probability of finding a cavity created by the particle of radius $R_{\mathrm{S}}\geqslant 0$ in the matrix in the absence of fluid particles.

For $R_{\mathrm{S}}=R_1$

$$p_0(R_{\mathrm{S}}=R_1)=\phi \tag{14}$$

is thermodynamic porosity defined by the excess chemical potential at the infinite dilution.

For $R_{\mathrm{S}}=0$

$$p_0(R_{\mathrm{S}}=0)=\phi_0 \tag{15}$$

is the geometrical porosity of porous media.

Similar to the previous section, $w_{\mathrm{S}}(R_{\mathrm{S}})$ describes the surface contribution and can be presented in the form of expansion (3). The coefficients of this expansion can be found from the continuity of $\mu_{\mathrm{S}}^{\mathrm{ex}}$ at $R_{\mathrm{S}}=0$.

As a result, for $n=1$

$$\beta w_0 = -ln(1-\eta_1/\phi_0). \tag{16}$$

For $n=2$ we have the second term

$$\beta w_1 = \frac{\eta_1/\phi_0}{1-\eta_1/\phi_0}\left[\frac{n}{R_1}-\frac{p_0'}{\phi_0}\right]. \tag{17}$$

For $n=3$ we have the third term

$$\beta w_2 = \frac{\eta_1/\phi_0}{1-\eta_1/\phi_0}\left[\frac{n(n-1)}{R_1^2}-2\frac{n}{R_1}\frac{p_0'}{\phi_0}+2\left(\frac{p_0'}{\phi_0}\right)^2-\frac{p_0''}{\phi_0}\right]+\left(\frac{\eta_1/\phi_0}{1-\eta_1/\phi_0}\right)^2\left[\frac{n}{R_1}-\frac{p_0'}{\phi_0}\right]^2, \tag{18}$$

where $p_0'=\frac{\partial p_0(R_{\mathrm{S}})}{\partial R_{\mathrm{S}}}$, $p_0''=\frac{\partial^2 p_0(R_{\mathrm{S}})}{\partial R_{\mathrm{S}}^2}$ at $R_{\mathrm{S}}=0$.

Now if we put $R_{\mathrm{S}}=R_1$ the expression (13) gives us the following relation between pressure P and the excess chemical potential of the fluid in porous media

$$\beta(\mu_1^{\mathrm{ex}}-\mu_1^0) = -\ln(1-\eta_1/\phi_0)+A\frac{\eta_1/\phi_0}{1-\eta_1/\phi_0}+B\frac{(\eta_1/\phi_0)^2}{(1-\eta_1/\phi_0)^2}+\frac{\beta P}{\rho_1}\frac{\eta_1}{\phi}\,, \tag{19}$$

where for one-dimensional case $A=B=0$, for two-dimensional case

$$A = n-\frac{p_0'}{\phi_0}R_1, \qquad B=0, \tag{20}$$

for three-dimensional case

$$\begin{aligned} A &= n-\frac{p_0'}{\phi_0}R_1+\frac{1}{2}\left[n(n-1)-2n\frac{p_0'}{\phi_0}R_1+2\left(\frac{p_0'}{\phi_0}\right)^2R_1^2-\frac{p_0''}{\phi_0}R_1^2\right], \\ B &= \frac{1}{2}\left(n-\frac{p_0'}{\phi_0}R_1\right)^2. \end{aligned} \tag{21}$$

Using Gibbs-Duhem equation (7) from (19) we have

$$\begin{aligned} \beta\left(\frac{\partial P}{\partial \rho_1}\right) &= 1+\frac{\eta_1/\phi}{1-\eta_1/\phi}+(A+1)\frac{\eta_1/\phi_0}{(1-\eta_1/\phi)(1-\eta_1/\phi_0)} \\ &\quad +(A+2B)\frac{(\eta_1/\phi_0)^2}{(1-\eta_1/\phi)(1-\eta_1/\phi_0)^2}+2B\frac{(\eta_1/\phi_0)^3}{(1-\eta_1/\phi)(1-\eta_1/\phi_0)^3} \end{aligned} \tag{22}$$

which is of the same form as in [6]. The general result for the chemical potential and pressure for three-dimensional case is presented in [6]. Here we present the results for one- and two-dimensional cases. For one-dimensional case

$$\beta(\mu_1^{\mathrm{ex}}-\mu_1^0) = -ln(1-\eta_1/\phi)+\frac{\phi}{\phi-\phi_0}ln\frac{1-\eta_1/\phi}{1-\eta_1/\phi_0}\,, \tag{23}$$

$$\frac{\beta P}{\rho_1} = \frac{\phi_0}{\eta_1}\frac{\phi}{\phi-\phi_0}ln\frac{1-\eta_1/\phi}{1-\eta_1/\phi_0} \tag{24}$$

and for two-dimensional case

$$\begin{aligned} \beta(\mu_1^{\mathrm{ex}}-\mu_1^0) &= -ln(1-\eta_1/\phi)+(A+1)\frac{\phi}{\phi-\phi_0}ln\frac{1-\eta_1/\phi}{1-\eta_1/\phi_0} \\ &\quad +A\frac{\phi}{\phi-\phi_0}\left[\frac{\eta_1/\phi_0}{1-\eta_1/\phi_0}-\frac{\phi}{\phi-\phi_0}ln\frac{1-\eta_1/\phi}{1-\eta_1/\phi_0}\right], \end{aligned} \tag{25}$$

$$\begin{aligned}\frac{\beta P}{\rho_1} &= -\frac{\phi}{\eta_1}ln\frac{1-\eta_1/\phi}{1-\eta_1/\phi_0}+(A+1)\frac{\phi}{\eta_1}\frac{\phi}{\phi-\phi_0}ln\frac{1-\eta_1/\phi}{1-\eta_1/\phi_0}\\ &\quad + A\frac{\phi}{\phi-\phi_0}\left[\frac{1}{1-\eta_1/\phi_0}-\frac{\phi}{\eta_1}\frac{\phi}{\phi-\phi_0}ln\frac{1-\eta_1/\phi}{1-\eta_1/\phi_0}\right]\end{aligned} \tag{26}$$

where A is given by (20).

4. Discussion and conclusions

The expressions (23)–(26) are the main results of this paper. At the beginning of this discussion we will consider the application of the obtained results to HS and overlapping HS matrices.

For the HS matrix for $R_\mathrm{S} \leqslant 0$

$$p_0(R_\mathrm{S}) = 1-\eta_0(1+R_\mathrm{S}/R_0)^n, \tag{27}$$

where $\eta_0=\rho_0 v_0$, $\rho_0=\frac{N_0}{V}$, N_0 is the number of matrix particles, V is the volume of the system, R_0 is the radius of matrix particle, v_0 is the volume of matrix particle. For the considered case

$$\phi_0 = p_0(R_\mathrm{S}=0)=1-\eta_0\,, \qquad -\frac{p_0'}{\phi_0}R_1=\frac{n\eta_0}{1-\eta_0}\tau, \tag{28}$$

where $\tau=\frac{R_1}{R_0}$.

The excess chemical potential in infinite dilution $\mu_1^0=\mu_\mathrm{S}^0(R_\mathrm{S}=R_1)$ related to the thermodynamical porosity

$$\phi=\exp(-\beta\mu_1^0) \tag{29}$$

can be found from the usual SPT theory discussed in the second section.

For one-dimensional case

$$\beta\mu_1^0=-ln(1-\eta_0)+\beta\frac{\eta_0}{\rho_0}P_0\tau, \qquad \frac{\beta P_0}{\rho_0}=\frac{1}{1-\eta_0}\,. \tag{30}$$

For two-dimensional case

$$\beta\mu_1^0=-ln(1-\eta_0)+\frac{2\eta_0}{1-\eta_0}\tau+\frac{\beta\eta_0 P_0}{\rho_0}\tau^2, \qquad \frac{\beta P_0}{\rho_0}=\frac{1}{(1-\eta_0)^2}\,. \tag{31}$$

For the overlapping HS matrix for $R_\mathrm{S} \leqslant 0$

$$p_0(R_\mathrm{S})=\exp\left(-\eta_0(1+R_\mathrm{S}/R_0)^n\right) \tag{32}$$

and

$$\phi_0=p_0(R_\mathrm{S}=0)=\mathrm{e}^{-\eta_0}, \qquad -\frac{p_0'}{\phi_0}R_1=n\eta_0\tau, \qquad \beta\mu_1^0=\eta_0(1+\tau)^n. \tag{33}$$

For two-dimensional case in accordance with (20) and (28) for HS matrix

$$A=2\left(1+\frac{\eta_0}{1-\eta_0}\tau\right) \tag{34}$$

and for overlapping HS according to (33)

$$A=2(1+\tau\eta_0). \tag{35}$$

Now all expressions are defined for one- and two-dimensional HS fluids in HS and overlapping HS matrices. Corresponding expressions for three-dimensional case are presented in [6].

From (22) it is easy to obtain virial expansions for pressure and for chemical potential. The second virial coefficient was obtained in [6]

$$B_2=v_1\left(\frac{1}{\phi}+\frac{A+1}{\phi_0}\right) \tag{36}$$

and it was shown that in three-dimensional case it is very accurate. As was shown in [6] for the three-dimensional case, SPT2 overestimates the role of porosity ϕ for the third and higher virial coefficients. A better description can be provided by SPT2b approximation which can be obtained by a slight modification of the expression (22)

$$\beta\left(\frac{\partial P}{\partial\rho_1}\right) = \frac{1}{1-\eta_1/\phi} + (A+1)\frac{\eta_1/\phi_0}{(1-\eta_1/\phi_0)^2} + (2B+A)\frac{(\eta_1/\phi_0)^2}{(1-\eta_1/\phi_0)^3} + 2B\frac{(\eta_1/\phi_0)^3}{(1-\eta_1/\phi_0)^4}\,. \quad (37)$$

The SPT2b approximation does not change the value of the second virial coefficient but for higher densities it is more accurate than SPT2. For one-dimensional case SPT2b gives the following results

$$\begin{aligned} \beta(\mu_1^{\mathrm{ex}} - \mu_1^0) &= -ln(1-\eta_1/\phi) + \frac{\eta_1/\phi_0}{1-\eta_1/\phi_0}\,, \\ \frac{\beta P}{\rho_1} &= -\frac{\phi}{\eta_1}ln(1-\eta_1/\phi) + \frac{\phi_0}{\eta_1}ln(1-\eta_1/\phi_0) + \frac{1}{1-\eta_1/\phi_0} \end{aligned} \quad (38)$$

and for two-dimensional case

$$\begin{aligned} \beta(\mu_1^{\mathrm{ex}} - \mu_1^0) &= -ln(1-\eta_1/\phi) + (1+A)\frac{\eta_1/\phi_0}{1-\eta_1/\phi_0} + \frac{1}{2}A\frac{(\eta_1/\phi_0)^2}{(1-\eta_1/\phi_0)^2}\,, \\ \frac{\beta P}{\rho_1} &= -\frac{\phi}{\eta_1}ln(1-\eta_1/\phi) + \frac{\phi_0}{\eta_1}ln(1-\eta_1/\phi_0) + \frac{1}{1-\eta_1/\phi_0} + \frac{1}{2}A\frac{\eta_1/\phi_0}{(1-\eta_1/\phi_0)^2}\,. \end{aligned} \quad (39)$$

The comparison of the obtained results with computer simulation data will be presented elsewhere [12].

Finally, we discussed the possibility of applying the SPT1 approach. From (13) and (3) it is possible to show that SPT2 reduces to SPT1 if we put in (13) $p(R_{\mathrm{S}}) = 1$ and subtract in (29) of [4] the infinite dilution part μ_1^0 from the excess chemical potential. As a result, from (23)–(26) it is possible to obtain the corresponding expressions for one- and two-dimensional case by a simple substitution $\phi = 1$. Since usually $\phi < \phi_0$, this approximation is not quite correct at least for small densities.

Acknowledgements

We thank T. Patsahan for some interesting discussions. The support from the CNRS-NASU cooperation project is acknowledged.

References

1. Madden W.G., Glandt E.D., J. Stat. Phys., 1988, **51**, 537.
2. Given J.A., Stell G., J. Chem. Phys., 1992, **97**, 4573.
3. Trokhymchuk A., Pizio O., Holovko M., Sokolowski S., J. Chem. Phys., 1997,**106**, 200.
4. Holovko M., Dong W., J. Phys. Chem. B, 2009,**113**, 6360, 16091.
5. Chen W., Dong W., Holovko M., Chen X.S., J. Phys. Chem. B, 2010, **114**, 1225.
6. Patsahan T., Holovko M., Dong W., J. Chem. Phys., 2010. (in press)
7. Reiss H., Frisch H.L., Lebowitz J.L., J. Chem. Phys., 1959, **31**, 369.
8. Reiss H., Frisch H.L., Helfand E., Lebowitz J.L., J. Chem. Phys., 1960, **32**, 119.
9. Yukhnovskij I.R., Holovko M., Statistical Theory of Classical Equilibrium Systems. Naukova Dumka, Kyiv, 1980.
10. Helfand E., Frisch H.L., Lebowitz J.L., J. Chem. Phys., 1961, **34**, 1037.
11. Tonks L., Phys. Rev., 1936, **50**, 955.
12. Patsahan T., Shmotolokha V., Holovko M., Dong W. (in preparation).

Аналітична теорія одно- та двовимірних плинів твердих сфер у випадковому пористому середовищі

М.Ф. Головко[1], В.І. Шмотолоха[2], В. Донг [3]

[1] Інститут фізики конденсованих систем НАН України, 79011 Львів, вул. Свєнціцького, 1

[2] Фізико-механічний інститут ім. Г.В. Карпенка НАН України, 79061 Львів, вул. Наукова, 5

[3] Нормальна вища школа в Ліоні, 69364 Ліон, Алея Італії, 46, Франція

Недавно запропонована теорія масштабної частинки SPT2 для опису тривимірного плину твердих сфер у випадковому пористому середовищі узагальнена на одно- та двовимірні випадки. Аналітичні вирази для хімічного потенціалу та тиску одно- та двовимірних твердих сфер у матрицях твердих сфер та твердих сфер, що перетинаються, отримані та обговорюються. Запропоновано деякі покращення та модифікації отриманих результатів.

Ключові слова: *обмежені плини, пористі матеріали, метод масштабної частинки*