PHYSICAL CHEMISTRY OF FRACTAL STRUCTURE MATERIALS

OLDŘICH ZMEŠKAL[a], MARTIN VALA[a], PAVEL BEDNÁŘ[a]

[a]*Institute of Physical and Applied Chemistry, Faculty of Chemistry, Brno University of Technology, Purkyňova 118, 61200 Brno, Czech Republic, e-mail: zmeskal@fch.vutbr.cz*

Introduction

Fractal geometry is widely used nowadays in many scientific areas. Fractals seem to be very powerful in describing natural objects on all scales. Fractal dimension and fractal measure, are crucial parameters for such description [1].

Fundamental laws describing the heat diffusion in fractal environment are discussed. It is shown that for the three-dimensional space the heat radiation process occur in structures with fractal dimension $0 < D < 1$, whereas in structures with $1 < D < 3$ heat conduction and convection have the upper hand (generally in the real gases).

It is shown that the results are comparable to the kinetics theory of real (ideal) gas (compressibility factor, Boyle's temperature) [2]. For the critical temperature the compressibility factor gains $Z = 1$ (except for the ideal gas case $D = 3$) also for the fractal dimension $D = 1/\phi = 1.618033989$, where ϕ is the golden mean value of the El Nashie's golden mean field theory [2].

Theoretical background

In papers [4], [5], [6] the density of fractal physical quantity $C(r)$ in E - dimensional Euclidean space E_n ($E = n$) (the density of heat capacity) was defined as

$$C(r) = k\,n(r) = k\,K\,r^{D-E}\,, \tag{1}$$

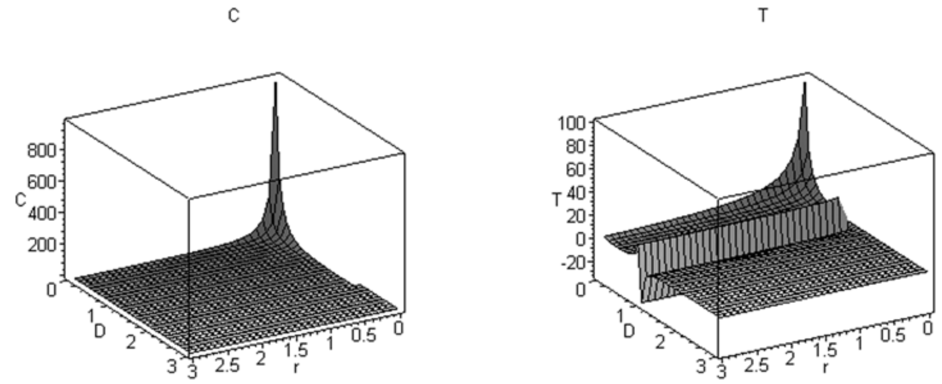
where $n(r)$ is the coverage of space – distribution of particles concentration [4], $k = 1.380658\cdot 10^{-23}\ \mathrm{J.K^{-1}}$ is the quantum of heat capacity (Boltzmann constant), r is the radius of elementary quantity, K the fractal measure and D is the fractal dimension.

For radial temperature field we can write the dependence of temperature on radius using (1), see [5] as:

$$T_{\mathrm{r}}(r) = -\frac{\hbar c}{k} \cdot \frac{K\, r^{D-E+2}}{D(D-E+2)} \,. \tag{1}$$

From this equation it is obvious that in the space with constant density of the heat capacity $C(r)$ (i.e. for $D = E$) the temperature increases with second power. In the case of point-like source of the heat radiation (i.e. for $D = E - 3, E = 3$) the temperature decreases with the distance by $1/r$. Assuming that there is linear source of heat (hot wire, $D = E - 2, E = 3$), the temperature is constant over the whole space.

It is evident that the density of the quantity (the density of heat capacity $C(r)$) depends on the fractal dimension *D*, on the fractal measure *K*, and on its distribution in the *E*-dimensional space. This distribution is expressed by *Figure 1a* (in appropriate units). It turns out that, for the fully covered space ($D = E$) the distribution of the physical quantity is homogenous in the space. For the space where just one elementary cell is placed the charge density in the cell of size *r* is given by $\rho(r) = 1/r^E$ (with the growing size of the cell, the coverage of space decreases). The dependence of the potential of physical field's radial part for different values of fractal dimension is presented on *Figure 1b*. The potential of physical field (the temperature $T_r(r)$) is positive for $D < E - 2$ and negative for $D > E - 2$. For $D = E - 2$ is potential (temperature) constant (in special case equal to zero: intensity of field is constant – homogenous field).



a) b)

Figure 1 The dependences of physical quantities on the distance *r* and fractal dimension *D* for topological dimension $E = 3$: a) the density of the heat capacity $C(r, D)$, b) the temperature $T_{\mathrm{r}}(r, D)$.

From the density of the heat capacity (1) and from the temperature (2) the density of energy

$$w(r) = C(r)T_{\mathrm{r}}(r) = -\hbar c\frac{K^2 r^{2(D-E+1)}}{D(D-E+2)} \tag{2}$$

respectively

$$w(T_{\mathrm{r}}) = KkT_r\left[\frac{kT_{\mathrm{r}}D(E-D-2)}{K\hbar c}\right]^{\frac{E-D}{E-D-2}} \tag{3}$$

can be determined.

The heat radiation

Let's first consider the properties of heat transfer in the three-dimensional space ($E = 3$) just for the fractal dimensions $D \in \langle 0,1)$ of the heat source. In this case, the heat density (4) can be written using generalised Planck radiation law

$$w(T_{\mathrm{r}}) = KkT_{\mathrm{r}}\left[\frac{kT_r D(1-D)}{K\hbar c}\right]^{\frac{3-D}{1-D}}. \tag{4}$$

The power of the temperature T_{r} can gain values from interval $\langle 4,\infty)$.

The wavelength and the fractal dimension are connected by the following equation [7]

$$\overline{\alpha}_w = \frac{\lambda}{\lambda_0} = \frac{1-D}{D}, \tag{5}$$

where $\overline{\alpha}_w = \overline{\alpha} + 1$ is the inverse coupling constant of the mass energy ($\overline{\alpha}$ is the inverse coupling constant of energy [6]) and λ_0 is the wavelength for fractal dimension D = 1/2 (maximum of function $D(1 - D)$).

The *Figure 2* shows the dependency of the energy density on fractal dimension for a specific number of oscillators ($K \approx 2.2\times10^6\,\mathrm{m}^{-3}$). The parameter of the dependences is temperature. Its values were chosen to allow comparison with experimentally gained values for the Sun.

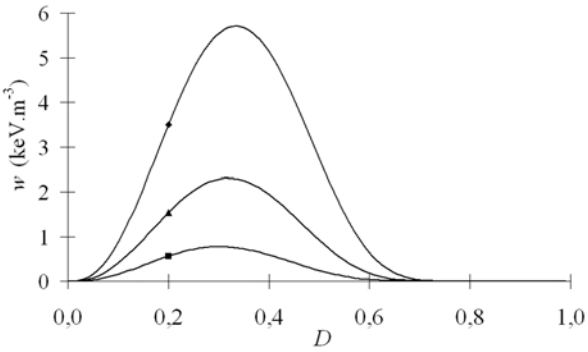


Figure 2 The dependency of energy density of heat oscillators on their fractal dimension plotted for three different temperatures ($\blacksquare\, T = 4000\,\mathrm{K}$, $\blacktriangle\, T = 5000\,\mathrm{K}$, $\blacklozenge\, T = 6000\,\mathrm{K}$) and constant number of oscillators ($K = 2.2\times10^{6}\,\mathrm{m}^{-3}$).

Analysing the dependencies expressing the Planck's radiation law, similar results are obtained

$$w_\nu = \frac{\mathrm{d}w_s}{\mathrm{d}\nu} = \frac{\lambda^2}{c}\frac{\mathrm{d}w_s}{\mathrm{d}\lambda} = \frac{2\pi h\nu^3}{c^3\left[\exp\left(h\nu/kT\right)-1\right]} = \frac{2\pi h}{\lambda^3\left[\exp\left(hc/\lambda kT\right)-1\right]}, \tag{6}$$

where $\nu = c/\lambda$ is the frequency of the electromagnetic wave.

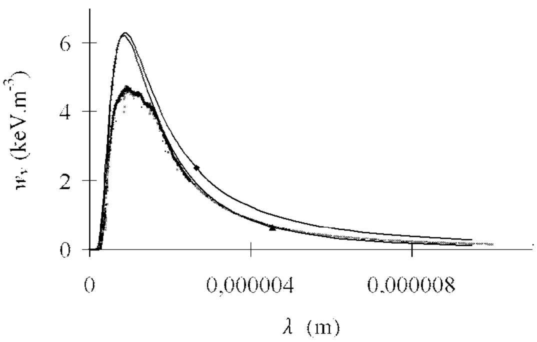


Figure 3 The spectral energy density of heat oscillators computed for temperature T = 5800 K and $K = 2.53\times10^{6}\,\mathrm{m}^{-3}$ using the Plank's radiation law (♦) and dependency defining the energy density of fractal structure (▲). The results are compared with measured values of the Sun.

The *Figure 3* shows the heat density dependency on wavelength (5) computed from Eq. (4) at temperature T = 5800 K and assuming that $K\hbar c/kT \approx K\lambda_0 \approx 1$. Experimental results of Sun give (see *Figure 3*) better agreement with the fractal model than with the quantum theory calculations for higher wavelengths. The significant divergences around the maximum, which is at the visible part of the spectrum, are caused by the absorption in the atmosphere.

Heat conduction and flow

This kind of heat transport occurs when the fractal dimension lies in the interval $D \in \langle 1, 3 \rangle$. In this case the $D(1-D)$ term in Eq. (4) is negative and relation for energy density, which in this case represents the gas pressure (i.e. $w(T_\mathrm{r}) = p(T_\mathrm{r})$), has to be rewritten into

$$p(T_\mathrm{r}) = K k T_\mathrm{r} \left(-1\right)^{\frac{3-D}{1-D}} \left[\frac{k T_r \, D(D-1)}{K\hbar c}\right]^{\frac{3-D}{1-D}}, \tag{7}$$

where using the Moivre's theorem

$$\left(-1\right)^{\frac{D-3}{D-1}} = \exp\left(\mathrm{j}\pi \frac{D-3}{D-1}\right) = \cos\left(\frac{D-3}{D-1}\pi\right) + \mathrm{j} \cdot \sin\left(\frac{D-3}{D-1}\pi\right). \tag{8}$$

To describe the behaviour of real gases it is more practical to use the so-called compressibility factor. With the help of $p_\mathrm{id} = RT_\mathrm{r}/V_\mathrm{M} = KkT_\mathrm{r}$, where $V_\mathrm{M} = N_\mathrm{A}/K$ is the molar gas volume, $R = k\,N_\mathrm{A}$ is the molar gas constant, N_A is the Avogadro constant, which represents the ideal gas equation, it can be defined by the equation

$$Z = \frac{p}{p_\mathrm{id}} = \frac{pV_\mathrm{M}}{RT_\mathrm{r}} = \left(-1\right)^{\frac{D}{1-D}} \left[\frac{k T_r \, D(D-1)}{K\hbar c}\right]^{\frac{3-D}{1-D}}. \tag{9}$$

It is possible to establish from the dependency shown in [2] the condition

$$\left(\frac{\mathrm{d}Z}{\mathrm{d}p}\right)_{T_B} = \left(\frac{\mathrm{d}Z}{\mathrm{d}D}\right)_{T_B} \left(\frac{\mathrm{d}D}{\mathrm{d}p}\right)_{T_B} = 0, \tag{10}$$

so-called Boyle temperature (temperature at which real gasses behave as the ideal one - when the pressure is low or the volume is small). The minimum of the dependence (9) function arise when the fractal dimension $D = 3$. According to Eq. (9) we can thus write: $Z_B = 1$, $T_B = K\hbar c/6k$, $p_B = K(K\hbar c)/6$.

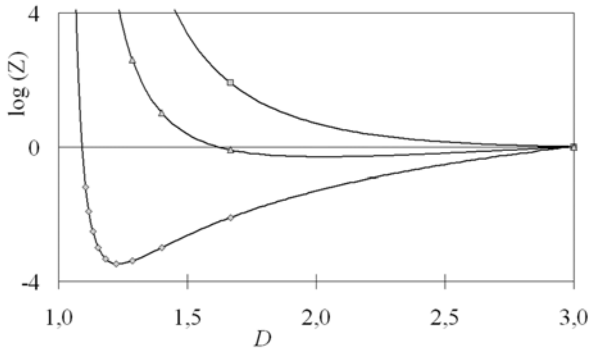


Figure 4 The dependency of compressibility factor size on fractal dimension plotted for three different temperatures ■ $T = 50000\,\mathrm{K}$, ▲ $T = 5000\,\mathrm{K}$ (i.e. for $K\hbar c \approx kT_{\mathrm{r}}$), ♦ $T = 500\,\mathrm{K}$, and constant number of oscillators ($K = 2.2\times10^{6}\,\mathrm{m}^{-3}$).

The dependency of the compressibility factor size on the fractal dimension at three different temperatures is plotted in *Figure 4*. Assuming that the temperature is low the compressibility factor has a growing tendency straight away from the beginning (when the fractal dimension decreases). In the other cases the compressibility factor begins to grow only after previous decreasing period. At critical temperature the system ($K\hbar c = kT_{\mathrm{r}}$) gains $Z = 1$ (except for the case of the ideal gas $D = 3$) also for the fractal dimension $D = 1/\phi = 1.618033989$, where ϕ is the golden mean value of El Nashie's golden mean field theory.

Conclusion

The properties of heat radiation conduction and convection in fractal structures were discussed.

It is shown that the dependency of energy density on fractal dimension $w = \mathrm{f}(D)$ (4) is connected with the Planck radiation law (i.e. the spectral radiant excitance on wavelength $H_\lambda = \mathrm{f}(\lambda)$) for structures with fractal dimensions from the interval $D \in \langle 0,1)$.

On the other hand, structures with fractal dimensions $D \in (1,3\rangle$ behave as real gases.

The energy density $w = \mathrm{f}(D)$ gains generally complex values within this interval (7) and describes the behaviour of a real (cohesive) gas. Only at specific values of fractal dimension the gas behave as the ideal one (the energy density is real-valued). Again, it was shown that in three-dimensional space ($E = 3$) at temperatures above the critical temperature ($kT > K\hbar c$) the maximum of the dependency $p = \mathrm{f}(D)$ (7) gives results reconcilable with the kinetic theory of real (ideal) gasses (van der Waals equation of state, compressibility factor, Boyle's temperature). At the critical temperature ($K\hbar c = kT_{\mathrm{r}}$) the compressibility factor gains value $Z = 1$ (except for the case of $D = 3$) also for the fractal dimension $D = 1/\phi = 1.618033989$, which is the golden mean value of the El Nashie's golden mean field theory [3].

REFERENCES

[1] Mandelbrot B.B.: Fractal geometry of nature. New York: W.H. Freeman and Co.; 1983

[2] Atkins P.W.: Physical Chemistry. Oxford University Press, 1998

[3] El Naschie M.S.: Chaos, Solitons & Fractals 16, 353 (2004)

[4] Zmeskal O., Nezadal M., Buchnicek M.: Chaos, Solitons & Fractals *17*, 113 (2003)

[5] Zmeskal O., Nezadal M., Buchnicek M.: Chaos, Solitons & Fractals *19*, 1013 (2004)

[6] Zmeskal O., Buchnicek M., Bednar P.: Chaos, Solitons & Fractals *22*, 985 (2004)

[7] Zmeskal O., Buchnicek M., Vala M.: Chaos, Solitons & Fractals *25*, 941 (2005)