

Kinetic coefficients of ion transport in a porous medium based on the Enskog–Landau kinetic equation

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Normal solutions of the Enskog–Vlasov–Landau kinetic equation were obtained within the model of positively and negatively charged solid spheres for the system ion solution – porous medium. The Chapman–Enskog method was applied. Analytical expressions for coefficients of viscosity, thermal conductivity, diffusion of ions in the system ionic solution – porous medium were derived by constructing the equations of hydrodynamics on the basis of normal solutions of the kinetic equation.

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1. Introduction

Studies of ion transport in porous systems are relevant in modern technologies for the creation of new current sources, water purification devices, biological membranes, channels, etc [1–16]. This is important for a deeper understanding of these processes and their management. The importance and justification of such research is noted in many works, including [17–38]. The study of the mechanisms of anomalous dispersion of rheological fluid flows in heterogeneous porous media [27, 32–34] is relevant from the point of view of practical applications. Another aspect of the research is related to the ionic conductivity of ionic solutions in porous and layered structures, channels, in “electrolyte – electrode” systems, which is important in connection with the anomalous behavior of ion diffusion and polarization effects [18, 20, 21, 30, 39–51].

From the point of view of theoretical studies of ion transport in porous systems, approaches based on nonequilibrium thermodynamic equations [36–38, 40, 41, 45] with constant diffusion coefficients are used, in particular equations of Poisson–Nernst–Planck, Smoluchovsky electrodiffusion. In [30, 47], a statistical theory is proposed to describe the processes of electrodiffusion transport of ions in the “electrolyte-electrode” system, taking into account spatial inhomogeneities and memory effects using the statistical operator of the non-equilibrium method (NSO). In [30, 48, 49, 51] an experimental and theoretical study of the subdiffusion impedance for a multi-layer GaSe system with encapsulated β -cyclodextrin, which has a porous fractal structure, was carried out. It should be noted that some methods of calculating ion diffusion coefficients depending on coordinates and time for systems “electrolyte solution – membrane”, “electrolyte solution – glassy materials containing fuel”, “electrolyte solution – soil” is proposed in [52–54]. In [30, 47], a statistical theory is proposed to describe the processes of electrodiffusion transport of ions in the “electrolyte – electrode” system, taking into account spatial inhomogeneities and memory effects using NSO. In the vast majority of works, the equations of diffusion processes with constant values of the diffusion coefficients of the components are used. Their values are taken from experimental studies during numerical modeling in specific cases. On the other hand, diffusion coefficients contain the main mechanisms of how diffusion processes occur through interaction potentials between system particles, the time evolution operator according to Kubo’s formulas. An important feature of these systems is their significant spatial heterogeneity, when the diffusion coef-

ficients are functions of spatial coordinates and time, that is, time correlation functions “flow – flow” $\langle \hat{\mathbf{j}}(\mathbf{r}_l; t) \hat{\mathbf{j}}(\mathbf{r}_s; t') \rangle$ in each of the phases and between phases.

It is interesting to study the processes of self-diffusion of ions in charged nanoporous media (particles that are frozen) using computer modeling methods [55,56]. It is also important to note the recent work of [16], where the self-diffusion of particles along the longitudinal coordinate in a channel of variable cross-section was considered with the application of the two-dimensional Enskog–Boltzmann–Lorentz kinetic equation with appropriate boundary conditions. In work [57], Enskog’s theory was applied to describe the self-diffusion coefficient of the flow of solid spheres in a disordered porous medium.

In this work, a kinetic approach will be applied to the description of ion transport processes in the system ionic solution – porous medium, the basic equations of which were obtained in [58]. The second chapter will detail the generalized kinetic equations of the revised Enskog–Vlasov–Landau theory for non-equilibrium ion distribution functions in the model of charged solid spheres for the system ion solution – porous medium. In the third chapter, normal solutions of these equations, corresponding hydrodynamic equations with analytical determination of mutual diffusion, thermal diffusion, viscosity and thermal conductivity coefficients through particle distribution functions and their nature of interaction for the ionic solution – porous medium system will be obtained using the Chapman–Enskog method.

2. The kinetic equation of the revised Enskog–Landau theory for the electrolyte-porous medium system

As in paper [58], we will consider the system of an ionic solution that interacts with a porous medium, diffusing in it. Positively and negatively charged ions of the solution can penetrate into the structure of the porous medium and move in it, interacting with the particles of the porous medium (matrix). We will take the entire volume of the system equal to $V = V_l + V_s$, where V_l is the volume occupied by the ionic solution, and V_s is the true volume porous matrix. Having entered the volume V_{por} of the porous space of the matrix, we can determine its porosity: $\phi = 1 - \frac{V_{\text{por}}}{V}$. We will consider the ionic solution with certain dielectric properties without explicit consideration of the molecular subsystem, and the porous matrix as formed by structureless moving particles of s varieties. An example of a porous medium can be biological systems (macromolecular structures), polymer, composite materials, electrode materials, which can structurally change in the process of their interaction with ionic solutions. With this consideration of the system, we have $f_s = 1 - \phi$ – the volume fraction of the porous matrix, $f_l = \chi\phi$ is the volume fraction of filling the pores with an ionic solution, where χ is degree of filling of pores with an ionic solution (at $\chi = 1$ is complete saturation of the porous medium with ionic solutions) and $f_n = (1 - \chi)\phi$ is volume capacitive fraction of incomplete pore filling with an ionic solution. We will assume that the kinetic energy of the ions of the solution is much greater than the kinetic energy of the particles of the porous medium. In paper [58], for the description of ion transport processes in the system “ionic solution – porous medium” a kinetic approach based on a modified chain of equations is applied BBGKI for non-equilibrium particle distribution functions. The generalized kinetic equation of the revised Enskog–Vlasov–Landau theory for the non-equilibrium distribution function of ions in the model of charged hard spheres with consideration of short-lived of attractive interactions for the system “ionic solution – porous medium”. We will use these results under the condition that the kinetic energy of the ions is significantly greater than the kinetic energy of the particles of the matrix of the porous medium. So, consider the model of charged hard spheres for the ionic subsystem, when the interaction potential can be represented as a sum [58–61]:

$$\Phi_{\alpha\gamma}(\mathbf{r}, \mathbf{r}') = \Phi_{\alpha\gamma}^{\text{sh}}(\mathbf{r}, \mathbf{r}') + \Phi_{\alpha\gamma}^l(\mathbf{r}, \mathbf{r}'),$$

where $\Phi_{\alpha\gamma}^{\text{sh}}(\mathbf{r}, \mathbf{r}')$ is the potential of hard spheres, $\Phi_{\alpha\gamma}^l(\mathbf{r}, \mathbf{r}')$ is the long-range interaction potential, in particular the Coulomb potential. In addition, we will describe the interaction of ions and particles of the porous medium short-term potential of solid spheres $\Phi_{\alpha s}^{\text{sh}}(\mathbf{r}, \mathbf{r}_s)$. Based on the works of [58–60] in the case of the solid sphere model for the fluid subsystem, we get:

$$\begin{aligned} \left(\frac{\partial}{\partial t} + iL_\alpha(1)\right) f_\alpha(x_1; t) = & - \sum_\gamma \int_0^{\sigma_\gamma} d\mathbf{r}_2 \int d\mathbf{p}_2 i L_{\alpha\gamma}^{\text{sh}}(12) \\ & \times \int_{-\infty}^0 d\tau e^{(\varepsilon + iL_{\alpha\gamma}^0(12) + iL_{\alpha\gamma}^{\text{sh}}(12))\tau} g_{\alpha\gamma}(\mathbf{r}_1, \mathbf{r}_2 | n; t + \tau) f_\alpha(x_1; t + \tau) f_\gamma(x_2; t + \tau) \\ & - \int_0^{\sigma_s} dx_s i L_{\alpha s}^{\text{sh}}(12) \int_{-\infty}^0 d\tau e^{(\varepsilon + iL_\alpha(1) + iL_{\alpha s}^{\text{sh}}(12))\tau} g_{\alpha s}(\mathbf{r}_1, \mathbf{r}_s | n; t + \tau) f_\alpha(x_1; t + \tau) f_1(x_s; t) \\ & - \sum_\gamma \int_{\sigma_\gamma}^\infty d\mathbf{r}_2 \int d\mathbf{p}_2 i L_{\alpha\gamma}^l(12) \int_{-\infty}^0 d\tau e^{(\varepsilon + iL_{\alpha\gamma}^0(12) + iL_{\alpha\gamma}^l(12))\tau} g_{\alpha\gamma}(\mathbf{r}_1, \mathbf{r}_2 | n; t + \tau) f_\alpha(x_1; t + \tau) f_\gamma(x_2; t + \tau) \end{aligned}$$

is the kinetic equation for the non-equilibrium one-particle distribution function of ions, taking into account areas of action of short-acting (hard-sphere) and long-acting potentials. Given that in the field of action of the potential of solid spheres, the interaction time $\tau \rightarrow +0$, as well as the results of works [59–61], the equation can be presented in the form:

$$\begin{aligned} \left(\frac{\partial}{\partial t} + iL_\alpha(1)\right) f_\alpha(x_1; t) = & - \sum_\gamma \int dx_2 \hat{T}_{\alpha\gamma}(12) g_{\alpha\gamma}(\mathbf{r}_1, \mathbf{r}_2 | n; t) f_\alpha(x_1; t) f_\gamma(x_2; t) \\ & - \int dx_s \hat{T}_{\alpha s}(1s) g_{\alpha s}(\mathbf{r}_1, \mathbf{r}_s | n; t) f_\alpha(x_1; t) f_1(x_s; t) \\ & - \sum_\gamma \int_{\sigma_\gamma}^\infty d\mathbf{r}_2 \int d\mathbf{p}_2 i L_{\alpha\gamma}^l(12) \int_{-\infty}^0 d\tau e^{(\varepsilon + iL_{\alpha\gamma}^0(12) + iL_{\alpha\gamma}^l(12))\tau} g_{\alpha\gamma}(\mathbf{r}_1, \mathbf{r}_2 | n; t + \tau) f_\alpha(x_1; t + \tau) f_\gamma(x_2; t + \tau), \end{aligned}$$

where $\hat{T}_{\alpha\gamma}(12)$ is the Enskog collision operator for charged hard spheres (ions) [59], $\hat{T}_{\alpha s}(1s)$ is the operator Enskog collisions for charged hard spheres and hard spheres, describing a porous medium. Next, if in the long-range part of the collision integral, perform the expansion $e^{[\varepsilon + iL_{\alpha\gamma}^0(12) + iL_{\alpha\gamma}^l(12)]\tau}$ by the contribution $iL_{\alpha\gamma}^l(12)$ of the long-range interaction potential and limit ourselves to the first order of the expansion, we get the following kinetic equation:

$$\begin{aligned} \left(\frac{\partial}{\partial t} + iL_\alpha(1)\right) f_\alpha(x_1; t) = & - \sum_\gamma \int dx_2 \hat{T}_{\alpha\gamma}(12) g_{\alpha\gamma}(\mathbf{r}_1, \mathbf{r}_2 | n; t) f_\alpha(x_1; t) f_\gamma(x_2; t) \\ & - \int dx_s \hat{T}_{\alpha s}(1s) g_{\alpha s}(\mathbf{r}_1, \mathbf{r}_s | n; t) f_\alpha(x_1; t) f_1(x_s; t) \\ & - \sum_\gamma \int_{\sigma_\gamma}^\infty d\mathbf{r}_2 \int d\mathbf{p}_2 i L_{\alpha\gamma}^l(12) \int_{-\infty}^0 d\tau e^{(\varepsilon + iL_{\alpha\gamma}^0(12))\tau} (1 + iL_{\alpha\gamma}^l(12)\tau) g_{\alpha\gamma}(\mathbf{r}_1, \mathbf{r}_2 | n; t + \tau) f_\alpha(x_1; t + \tau) f_\gamma(x_2; t + \tau), \end{aligned}$$

where the first term of the expansion is the generalized Vlasov collision operator – the generalized mean field, and the second term is a generalized collision operator of the Landau type, taking into account memory effects.

Having revealed the action of the Enskog operator on the right-hand side, in the spatially inhomogeneous case (with accuracy up to linear values along the gradients and without taking into account memory effects) we get:

$$\left(\frac{\partial}{\partial t} + iL_\alpha(1)\right) f_\alpha(x_1; t) = I_{\alpha E}^{(0)}(x_1; t) + I_{\alpha E}^{(1)}(x_1; t) + I_{\alpha MF}^{(1)}(x_1; t) + I_{\alpha L}^{(1)}(x_1; t), \tag{1}$$

where the terms on the right are collision integrals, due to the contribution from a certain type of interparticle interaction. The first and second of them are Enskog-type collision integrals of the RET theory [58, 59]:

$$\begin{aligned} I_{\alpha E}^{(0)}(x_1; t) = & \sum_\gamma \int d\mathbf{v}_2 \int d\varepsilon \int b db g(12) g_{\alpha\gamma}(\sigma_{\alpha\gamma} | n; t) (f_\alpha(\mathbf{r}_1, \mathbf{v}'_1; t) f_\gamma(\mathbf{r}_2, \mathbf{v}'_2; t) - f_\alpha(\mathbf{r}_1, \mathbf{v}_1; t) f_\gamma(\mathbf{r}_2, \mathbf{v}_2; t)) \\ & + \int d\mathbf{v}_s \int d\varepsilon \int b db g(1s) g_{\alpha s}(\sigma_{\alpha s} | n; t) (f_\alpha(\mathbf{r}_1, \mathbf{v}'_1; t) f_1(\mathbf{r}_s, \mathbf{v}'_s; t) - f_\alpha(\mathbf{r}_1, \mathbf{v}_1; t) f_1(\mathbf{r}_s, \mathbf{v}_s; t)), \tag{2} \end{aligned}$$

$$\begin{aligned}
 I_{\alpha E}^{(1)}(x_1; t) = & \sum_{\gamma} \sigma_{\alpha\gamma}^3 \int d\hat{\mathbf{r}}_{12} \int d\mathbf{v}_2 \Theta(\hat{\mathbf{r}}_{12} \cdot \mathbf{g}(12)) (\hat{\mathbf{r}}_{12} \cdot \mathbf{g}(12)) \\
 & \cdot \left(g_{\alpha\gamma}(\mathbf{r}_{12}|n; t) \mathbf{r}_{12} \cdot [f_{\alpha}(\mathbf{r}_1, \mathbf{v}'_1; t) \nabla_2 f_{\gamma}(\mathbf{r}_2, \mathbf{v}'_2; t) - f_{\alpha}(\mathbf{r}_1, \mathbf{v}_1; t) \nabla_2 f_{\gamma}(\mathbf{r}_2, \mathbf{v}_2; t)] \right. \\
 & + \frac{1}{2} (\hat{\mathbf{r}}_{12} \cdot \nabla_2 g_{\alpha\gamma}(\mathbf{r}_{12}|n; t)) [f_{\alpha}(\mathbf{r}_1, \mathbf{v}'_1; t) f_{\gamma}(\mathbf{r}_2, \mathbf{v}'_2; t) - f_{\alpha}(\mathbf{r}_1, \mathbf{v}_1; t) f_{\gamma}(\mathbf{r}_2, \mathbf{v}_2; t)] \Big) \\
 & + \sigma_{\alpha s}^3 \int d\hat{\mathbf{r}}_{1s} \int d\mathbf{v}_s \Theta(\hat{\mathbf{r}}_{1s} \cdot \mathbf{g}(1s)) (\hat{\mathbf{r}}_{1s} \cdot \mathbf{g}(1s)) \\
 & \cdot \left(g_{\alpha s}(\mathbf{r}_{1s}|n; t) \mathbf{r}_{1s} \cdot [f_{\alpha}(\mathbf{r}_1, \mathbf{v}'_1; t) \nabla_s f_1(\mathbf{r}_s, \mathbf{v}'_s; t) - f_{\alpha}(\mathbf{r}_1, \mathbf{v}_1; t) \nabla_s f_1(\mathbf{r}_s, \mathbf{v}_s; t)] \right. \\
 & \left. + \frac{1}{2} (\hat{\mathbf{r}}_{1s} \cdot \nabla_s g_{\alpha s}(\mathbf{r}_{1s}|n; t)) \cdot [f_{\alpha}(\mathbf{r}_1, \mathbf{v}'_1; t) f_1(\mathbf{r}_s, \mathbf{v}'_s; t) - f_{\alpha}(\mathbf{r}_1, \mathbf{v}_1; t) f_1(\mathbf{r}_s, \mathbf{v}_s; t)] \right), \quad (3)
 \end{aligned}$$

where b is the aiming parameter, $\nabla_s = \frac{\partial}{\partial \mathbf{r}_s}$, $\nabla_2 = \frac{\partial}{\partial \mathbf{r}_2}$, $g_{\alpha\gamma}(\sigma_{\alpha\gamma}|n; t)$, $g_{\alpha s}(\sigma_{\alpha s}|n; t)$ are the contact values of the paired quasi-equilibrium ion – ion, ion – particle matrix distribution function, $\hat{\mathbf{r}}_{12} = \frac{\mathbf{r}_{12}}{|\mathbf{r}_{12}|}$, $\hat{\mathbf{r}}_{1s} = \frac{\mathbf{r}_{1s}}{|\mathbf{r}_{1s}|}$ are a unit vectors, $\mathbf{v}'_1 = \mathbf{v}_1 + \hat{\mathbf{r}}_{12}(\hat{\mathbf{r}}_{12} \cdot \mathbf{g}(12))$, $\mathbf{v}'_2 = \mathbf{v}_2 - \hat{\mathbf{r}}_{12}(\hat{\mathbf{r}}_{12} \cdot \mathbf{g}(12))$, $\mathbf{v}'_s = \mathbf{v}_s - \hat{\mathbf{r}}_{1s}(\hat{\mathbf{r}}_{1s} \cdot \mathbf{g}(1s))$ are the values of particle velocities 1, 2, s after the collision, while \mathbf{v}_1 , \mathbf{v}_2 , \mathbf{v}_s are the value of their velocities before the collision, where $\mathbf{g}(12) = \mathbf{v}_2 - \mathbf{v}_1$, $\mathbf{g}(1s) = \mathbf{v}_s - \mathbf{v}_1$ are the relative speed. The work assumes that the gradients $\frac{\partial}{\partial \mathbf{r}_s} f_1(\mathbf{r}_s, \mathbf{v}_s; t)$ and $\frac{\partial}{\partial \mathbf{r}_s} g_{\alpha s}(\mathbf{r}_{1s}|n, \beta; t)$ are much smaller than $\frac{\partial}{\partial \mathbf{r}_2} f_{\gamma}(\mathbf{r}_2, \mathbf{v}_2; t)$ and $\frac{\partial}{\partial \mathbf{r}_2} g_{\alpha\gamma}(\mathbf{r}_{12}|n, \beta; t)$, which is characteristic of the matrix structure of the porous medium. Although in real systems, membranes, electrodes, structural changes can be significant, and then it is necessary to take into account these contributions in the collision integrals.

The following term in (1) is the contribution calculated in the KMFT [59, 62] mean field theory approximation:

$$I_{\alpha MF}^{(1)}(x_1; t) = \frac{1}{m_{\alpha}} \sum_{\gamma} \int d\mathbf{r}_2 \frac{\partial}{\partial \mathbf{r}_1} \Phi_{\alpha\gamma}^l(|\mathbf{r}|_{12}) \cdot \frac{\partial}{\partial \mathbf{v}_1} g_{\alpha\gamma}(\mathbf{r}_{12}|n; t) \cdot f_{\gamma}(\mathbf{r}_2, \mathbf{v}_2; t) n_{\alpha}(\mathbf{r}_1; t).$$

The last term in the (1) is the integral of Landau-type collisions [58–60]

$$I_{\alpha L}^{(1)}(x_1; t) = \sum_{\gamma} \int \int d\mathbf{v}_2 d\varepsilon b db \mathbf{g}(12) (f_{\alpha}(\mathbf{r}_1, \mathbf{v}_1^*; t) f_{\gamma}(\mathbf{r}_2, \mathbf{v}_2^*; t) - f_{\alpha}(\mathbf{r}_1, \mathbf{v}_1; t) f_{\gamma}(\mathbf{r}_2, \mathbf{v}_2; t)), \quad (4)$$

which is presented in a simplified Boltzmann form. This formula can be obtained by switching to the cylindrical coordinate system, by entering the aiming parameter b , the azimuthal scattering angle ε , distance along the cylinder axis ξ , and integrating along ξ taking into account $g_{\alpha\gamma}(\mathbf{r}_{12}|n; t) \rightarrow 1$. When solving the equation by the Chapman–Enskog method, this form is convenient. In these expressions, \mathbf{v}_1^* \mathbf{v}_2^* are particle velocities after Coulomb scattering:

$$\begin{aligned}
 \mathbf{v}_1^* &= \mathbf{v}_1 + \Delta \mathbf{v}_{12}, & \mathbf{v}_2^* &= \mathbf{v}_2 - \Delta \mathbf{v}_{12}, \\
 \Delta \mathbf{v}_{12} &= -\frac{1}{m_{\alpha\gamma}} \int_{\sigma_{\alpha\gamma}} d\xi \frac{\partial}{\partial r_{12}} \Phi_{\alpha\gamma}^l(|\mathbf{r}|_{12}) \frac{1}{g_{12}} \Big|_{r_{12}=\sqrt{b^2+\xi^2}},
 \end{aligned}$$

$m_{\alpha\gamma}$ is the reduced mass of particles of the α and γ varieties.

3. Non-equilibrium one-particle distribution function in the first approximation. The Chapman–Enskog method

To construct normal solutions of the kinetic equation of the Enskog–Landau type, we will use the Chapman–Enskog method [63, 64]. Since we will be interested in the solution in the linear approximation by the gradients of the corresponding particle number density $n_{\alpha}(\mathbf{r}; t)$, hydrodynamic velocity $\mathbf{v}(\mathbf{r}; t)$ and temperatures $T(\mathbf{r}; t)$, we will use the corresponding equations of hydrodynamics for the average values of the densities of the number of particles, momentum and energy [61, 65, 66]:

$$\frac{\partial}{\partial t} n_{\alpha}(\mathbf{r}; t) = -\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{j}_{\alpha}(\mathbf{r}; t), \quad (5)$$

$$\rho(\mathbf{r}; t) \frac{\partial}{\partial t} \mathbf{v}(\mathbf{r}; t) = - \frac{\partial}{\partial \mathbf{r}} : \overleftrightarrow{P}(\mathbf{r}; t), \quad (6)$$

$$\begin{aligned} \rho(\mathbf{r}; t) \frac{\partial}{\partial t} e_{\text{kin}}(\mathbf{r}; t) &= - \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{q}(\mathbf{r}; t) - \overleftrightarrow{P}(\mathbf{r}; t) : \frac{\partial}{\partial \mathbf{r}} \mathbf{v}(\mathbf{r}; t) \\ &+ \sum_{\alpha, \gamma} \mathbf{v}_\alpha(\mathbf{r}; t) \int d\mathbf{r}_{12} \frac{\partial}{\partial \mathbf{r}_{12}} \Phi_{\alpha, \gamma}^l(\mathbf{r}_{12}) n_\alpha(\mathbf{r}_1; t) n_\gamma(\mathbf{r}_1 + n_\alpha(\mathbf{r}_1; t); t). \end{aligned} \quad (7)$$

In these equations, the notations are introduced:

$$n_\alpha(\mathbf{r}; t) = \int d\mathbf{v} f_\alpha(\mathbf{r}, \mathbf{v}; t)$$

is the density of particles of grade α ,

$$\rho(\mathbf{r}; t) = \sum_\alpha m_\alpha \int d\mathbf{v} f_\alpha(\mathbf{r}, \mathbf{v}; t)$$

is the total particle mass density,

$$\rho(\mathbf{r}; t) \mathbf{v}(\mathbf{r}; t) = \sum_\alpha \int d\mathbf{v} m_\alpha \mathbf{v} f_\alpha(\mathbf{r}, \mathbf{v}; t),$$

$\mathbf{v}(\mathbf{r}; t)$ is the full hydrodynamic velocity of the particles,

$$\rho(\mathbf{r}; t) e_{\text{kin}}(\mathbf{r}; t) = \sum_\alpha \int d\mathbf{v} \frac{m_\alpha c_\alpha^2(\mathbf{r}; t)}{2} f_\alpha(\mathbf{r}, \mathbf{v}; t),$$

where $c_\alpha(\mathbf{r}; t) = \mathbf{v} - \mathbf{v}(\mathbf{r}; t)$ is the thermal velocity, $\mathbf{v}_\alpha(\mathbf{r}; t) = \int d\mathbf{v} f_\alpha(\mathbf{r}, \mathbf{v}; t) \mathbf{v}$ is the average speed particles of sort α . In the linear approximation by gradients, the partial flow $\mathbf{j}_\alpha(\mathbf{r}; t)$ of particles of sort α , the full tensor of viscous stresses $\overleftrightarrow{P}(\mathbf{r}; t)$ and heat flow $\mathbf{q}(\mathbf{r}; t)$ can be represented by gradients and transfer coefficients:

$$\mathbf{j}_\alpha(\mathbf{r}; t) = -n^2 \sum_\xi \frac{m_\alpha m_\xi}{\rho} D^{\alpha\xi} \mathbf{d}_\alpha(\mathbf{r}; t) - D_T^\alpha \frac{\partial}{\partial \mathbf{r}} \ln T(\mathbf{r}; t), \quad (8)$$

$$\overleftrightarrow{P}(\mathbf{r}; t) = P(\mathbf{r}; t) \overleftrightarrow{I} - \kappa \left(\frac{\partial}{\partial \mathbf{r}} : \mathbf{v}(\mathbf{r}; t) \right) - 2\eta \overleftrightarrow{S}(\mathbf{r}; t), \quad (9)$$

$$\mathbf{q}(\mathbf{r}; t) = -\lambda \frac{\partial}{\partial \mathbf{r}} T(\mathbf{r}; t) + \sum_\alpha w_\alpha \mathbf{d}_\alpha(\mathbf{r}; t), \quad (10)$$

where $\xi = \gamma, s$, $D^{\alpha\gamma}$ is the mutual diffusion coefficient, D_T^α is the thermal diffusion coefficient, κ is the bulk viscosity coefficient, η is the coefficient of shear viscosity and λ is the coefficient of thermal conductivity of solution particles in the solution-porous medium system. $\mathbf{d}_\alpha(\mathbf{r}; t)$ is the diffusion thermodynamic force of α grade particles, for which the condition $\sum_\alpha \mathbf{d}_\alpha(\mathbf{r}; t) = 0$ is fulfilled.

The presented equations of hydrodynamics can be constructed on the basis of solutions of the kinetic equation (1). To find the appropriate expressions for the transfer coefficients according to the method. We will look for the Chapman–Enskog [61, 63, 64] solution of the equation (1) in the form:

$$f_\alpha(\mathbf{r}_1, \mathbf{v}_1; t) = f_\alpha^0(\mathbf{r}_1, \mathbf{v}_1; t) (1 + \varphi_\alpha(\mathbf{r}_1, \mathbf{v}_1; t)),$$

where $f_\alpha^0(\mathbf{r}_1, \mathbf{v}_1; t)$ is the locally-equilibrium Maxwell function as a zero approximation corresponding to ideal hydrodynamics,

$$f_1 \equiv f_\alpha^0(x_1; t) = n_\alpha(\mathbf{r}_1; t) \left(\frac{m_\alpha}{2\pi k_B T(\mathbf{r}_1; t)} \right)^{3/2} \exp \left(- \frac{m_\alpha c_\alpha^2(\mathbf{r}_1; t)}{2k_B T(\mathbf{r}_1; t)} \right).$$

The correction $\varphi_\alpha(\mathbf{r}_1, \mathbf{v}_1; t)$ is written in terms of Sonin–Lager polynomials [61, 63, 64]:

$$\begin{aligned} \varphi_\alpha(\mathbf{r}_1, \mathbf{v}_1; t) &= - \sqrt{\frac{m_\alpha}{2k_B T}} E^\alpha \left(\frac{m_\alpha (c_\alpha)^2}{2} \right) n c_\alpha \cdot \mathbf{d}_\alpha - \sqrt{\frac{m_\alpha}{2k_B T}} A^\alpha \left(\frac{m_\alpha (c_\alpha)^2}{2} \right) c_\alpha \cdot \frac{\partial}{\partial \mathbf{r}} \ln T(\mathbf{r}_1; t) \\ &- \frac{m_\alpha}{2k_B T} B^\alpha \left(\frac{m_\alpha (c_\alpha)^2}{2} \right) \left(c_\alpha c_\alpha - \frac{1}{3} (c_\alpha)^2 \overleftrightarrow{I} \right), \end{aligned}$$

where

$$E^\alpha(x) = \sum_{j=0}^\infty E_j^\alpha L_j^{3/2}(x), \quad A^\alpha(x) = \sum_{j=0}^\infty A_j^\alpha L_j^{3/2}(x), \quad B^\alpha(x) = \sum_{j=0}^\infty B_j^\alpha L_j^{5/2}(x),$$

$$L_j^r(x) = \sum_{s=0}^j (-1)^s x^s \frac{j! \Gamma(j+r+1)}{s! \Gamma(s+r+1) \Gamma(j-s+1)}.$$

Based on the works [61], we define the functions $E^\alpha(x)$, $A^\alpha(x)$, $B^\alpha(x)$, after which the zero polynomial approximation we obtain the following expressions for the transfer coefficients taking into account the porosity ϕ of the matrix and the fraction χ of filling the porous space with an ionic solution:

$$D^{\alpha\gamma} = -\frac{n_\alpha \rho}{m_\gamma n} \sqrt{\frac{k_B T}{2m_\alpha}} E_0^\alpha$$

is the mutual diffusion coefficient of ions,

$$D_T^\alpha = m_\alpha n_\alpha \sqrt{\frac{k_B T}{2m_\alpha}} A_0^\alpha$$

is the thermal diffusion coefficient of ions of the sort α ,

$$\begin{aligned} \kappa = \frac{8}{9} \sum_{\alpha\gamma} \sigma_{\alpha\gamma}^4 \chi \phi g_{\alpha\gamma}(\sigma_{\alpha\gamma}|n, \beta) n_\alpha n_\gamma \frac{m_{\alpha\gamma}}{m_\gamma} \sqrt{2\pi m_{\alpha\gamma} k_B T} \\ + \frac{8}{9} \sum_{\alpha} \sigma_{\alpha s}^4 (1 - \phi) g_{\alpha s}(\sigma_{\alpha s}|n, \beta) n_\alpha n_s \frac{m_{\alpha s}}{m_s} \sqrt{2\pi m_{\alpha s} k_B T} = \sum_{\alpha\xi} \kappa_{\alpha\xi} \end{aligned}$$

is the volume viscosity coefficient,

$$\eta = \frac{3}{5} \kappa + \sum_{\alpha} n_\alpha k_B T \left[1 + \frac{2\pi}{15} \sum_{\xi} n_\xi \sigma_{\alpha\xi}^3 f_\xi g_{\alpha\xi}(\sigma_{\alpha\xi}|n, \beta) \left(1 + \frac{m_\alpha B_0^\xi}{m_\xi B_0^\alpha} \right) \right] B_0^\alpha \tag{11}$$

is the coefficient of shear viscosity, $f_\xi = f_\gamma, f_s, f_\gamma = \chi\phi, f_s = 1 - \phi$ and

$$\begin{aligned} \lambda = \frac{3}{2} \sum_{\alpha\xi} k_B m_\alpha m_\xi \left(\frac{1}{2} (m_\alpha + m_\xi) - \frac{1}{8} \frac{(m_\alpha - m_\xi)^2}{m_\alpha + m_\xi} \right)^{-3} \kappa_{\alpha\xi} \\ + \frac{5}{4} \sum_{\alpha} n_\alpha k_B \sqrt{\frac{2k_B T}{m_\alpha}} \left[1 - \frac{A_0^\alpha}{A_1^\alpha} + \frac{\pi}{5} \sum_{\xi} n_\xi \sigma_{\alpha\xi}^3 f_\xi g_{\alpha\xi}(\sigma_{\alpha\xi}|n, \beta) \left(1 + \frac{m_\alpha^{3/2} A_1^\xi}{m_\xi^{3/2} A_1^\alpha} \right) \right] A_1^\alpha \end{aligned}$$

is the thermal conductivity coefficient of the system, where

$$w_\alpha = \frac{5}{4} n n_\alpha \sqrt{\frac{2(k_B T)^3}{m_\alpha}} E_0^\alpha. \tag{12}$$

The most interesting among the transfer coefficients are the diffusion coefficients of the ions of the solution in the porous space of the medium. This is related to the important question of how much and how quickly the ionic solution can fill the porous space of the medium. Therefore, let's consider the structure of the ion diffusion coefficient in more detail. To do this, we will calculate the function E_0^α [61] for our model

$$\begin{aligned} E_0^\alpha = - \sum_{\gamma} \frac{3\pi m_\gamma}{8\rho n_\alpha} \sqrt{\frac{\pi m_\alpha}{m_{\alpha\gamma}}} \left(\chi\phi \left(g_{\alpha\gamma}(\sigma_{\alpha\gamma}|n, \beta)^{\alpha\gamma} \Omega_{hs}^{(1,1)} + {}^{\alpha\gamma} \Omega_l^{(1,1)} \right) \right)^{-1} \\ - \frac{3\pi m_s}{8\rho n_\alpha} \sqrt{\frac{\pi m_\alpha}{m_{\alpha s}}} \left((1 - \phi) g_{\alpha\gamma}(\sigma_{\alpha s}|n, \beta)^{\alpha s} \Omega_{hs}^{(1,1)} \right)^{-1}, \end{aligned}$$

for the mutual diffusion coefficient, we obtain the following expression:

$$D^{\alpha\gamma} = \frac{3\pi}{8n} \sqrt{\frac{\pi k_B T}{m_{\alpha\gamma}}} \left(\chi\phi \left(g_{\alpha\gamma}(\sigma_{\alpha\gamma}, n)^{\alpha\gamma} \Omega_{hs}^{(1,1)} + {}^{\alpha\gamma} \Omega_l^{(1,1)} \right) \right)^{-1}. \tag{13}$$

The quantities ${}^{\alpha\gamma}\Omega_{hs}^{(1,1)}$ and ${}^{\alpha\gamma}\Omega_l^{(1,1)}$ are called Ω -integrals [59, 61, 64]. For this system, they have the following form:

$$\begin{aligned} {}^{\alpha\gamma}\Omega_{hs}^{(1,1)} &= \sqrt{\frac{k_B T}{2\pi m_{\alpha\gamma}}} \pi \sigma_{\alpha\gamma}^2, \\ {}^{\alpha s}\Omega_{hs}^{(1,1)} &= \sqrt{\frac{k_B T}{2\pi m_{\alpha s}}} \pi \sigma_{\alpha s}^2, \\ {}^{\alpha\gamma}\Omega_l^{(1,1)} &= \sqrt{\frac{k_B T}{2\pi m_{\alpha\gamma}}} \frac{\pi}{2} \left(\frac{Z_\alpha Z_\gamma e^2}{\varepsilon k_B T} \right)^2 \ln \frac{D}{\sigma_{\alpha\gamma}}, \end{aligned}$$

where ε is the dielectric constant, Z_α is the valence of ions of the α sort, D is the Coulomb shielding radius. For the diffusion coefficient of α particles in the system, the ionic solution is porous environment we get:

$$\begin{aligned} D^\alpha &= \frac{3\pi}{8n} \sqrt{\frac{\pi k_B T}{m_{\alpha\alpha}}} \left(\chi \phi \left(g_{\alpha\alpha}(\sigma_{\alpha\alpha}, n) {}^{\alpha\alpha}\Omega_{hs}^{(1,1)} + {}^{\alpha\alpha}\Omega_l^{(1,1)} \right) \right)^{-1} \\ &+ \frac{3\pi}{8n} \sqrt{\frac{\pi k_B T}{m_{\alpha\gamma}}} \left(\chi \phi \left(g_{\alpha\gamma}(\sigma_{\alpha\gamma}, n) {}^{\alpha\gamma}\Omega_{hs}^{(1,1)} + {}^{\alpha\gamma}\Omega_l^{(1,1)} \right) \right)^{-1} \\ &+ \frac{3\pi}{8n} \sqrt{\frac{\pi k_B T}{m_{\alpha s}}} \left((1 - \phi) g_{\alpha s}(\sigma_{\alpha s}, n) {}^{\alpha s}\Omega_{hs}^{(1,1)} \right)^{-1}. \end{aligned} \quad (14)$$

It is important to note that we can account for the charge of the porous medium Z_s by introducing the function $(1 - \phi) {}^{\alpha s}\Omega_l^{(1,1)}$ in the last term in (14). As we can see, for further numerical calculation of the diffusion coefficient, it is necessary to calculate the contact values of the paired distribution functions of the particles of the solution and the porous medium, as well as the corresponding shielding radius D . In the case of the model without taking into account long-range interactions, we obtain the diffusion coefficient for the fluid system – a porous medium based on the solid sphere model:

$$\begin{aligned} D_{sh}^\alpha &= \frac{3\pi}{8n} \sqrt{\frac{\pi k_B T}{m_{\alpha\alpha}}} \left(\chi \phi g_{\alpha\alpha}(\sigma_{\alpha\alpha}, n) {}^{\alpha\alpha}\Omega_{hs}^{(1,1)} \right)^{-1} \\ &+ \frac{3\pi}{8n} \sqrt{\frac{\pi k_B T}{m_{\alpha\gamma}}} \left(\chi \phi g_{\alpha\gamma}(\sigma_{\alpha\gamma}, n) {}^{\alpha\gamma}\Omega_{hs}^{(1,1)} \right)^{-1} \\ &+ \frac{3\pi}{8n} \sqrt{\frac{\pi k_B T}{m_{\alpha s}}} \left((1 - \phi) g_{\alpha s}(\sigma_{\alpha s}, n) {}^{\alpha s}\Omega_{hs}^{(1,1)} \right)^{-1}. \end{aligned}$$

It is important to note that in (14) the shielding radius D can be calculated according to the work of [67] as $D = \frac{1}{2}\Gamma$, and Γ is the solution of the equations:

$$\begin{aligned} 4\Gamma^2 &= \frac{e^2}{\varepsilon} \sum_{\alpha=1}^M n_\alpha X_\alpha^2, \\ X_\alpha &= \left(Z_\alpha - \frac{\pi}{2} \frac{\sigma_\alpha^2}{1 - \Delta} P_m \right) (1 + \Gamma \sigma_\alpha)^{-1}, \\ P_m &= \sum_{\alpha=1}^M \frac{n_\alpha \sigma_\alpha Z_\alpha}{1 + \Gamma \sigma_\alpha} \left(1 + \frac{\pi}{2(1 - \Delta)} \sum_{\alpha=1}^M \frac{n_\alpha \sigma_\alpha^3}{1 + \Gamma \sigma_\alpha} \right)^{-1}, \end{aligned}$$

where $\Delta = \sum_{\alpha=1}^M \Delta_\alpha \sigma_\alpha^3$, $\Delta_\alpha = \frac{\pi n_\alpha}{6}$.

Expressions for the coordinate distribution functions $g_{\alpha\gamma}(r)$ can be obtained based on the results of the works [68–71]. It is important to note that in [68] the Percus–Yevick equation for the radial function of the distribution of particles in a liquid is generalized to the case of an n -component mixture, in [69] $g_{\alpha\gamma}(r)$ was calculated for ionic mixtures in the case of Coulomb and shielded Coulomb interactions. A more accurate formula for calculations of $g_{\alpha\gamma}(r)$ based on the Percus–Yevick approximation is given

in [70], and [71] applies a new closure for the Ornstein–Zernike equation for a system of charged particles with a specific interaction potential. Based on this, $g_{\alpha\gamma}(r)$ at the contact of solid spheres can be used in calculations of transfer coefficients in the form:

$$\begin{aligned} g_{\alpha\alpha}(\sigma_\alpha) &= \left(\left(1 + \frac{\Delta}{2}\right) + \frac{3}{2}\Delta_\gamma\sigma_\gamma^2(\sigma_\alpha - \sigma_\gamma) \right) (1 - \Delta)^{-2}, \\ g_{\gamma\gamma}(\sigma_\gamma) &= \left(\left(1 + \frac{\Delta}{2}\right) + \frac{3}{2}\Delta_\alpha\sigma_\alpha^2(\sigma_\gamma - \sigma_\alpha) \right) (1 - \Delta)^{-2}, \\ g_{\alpha\gamma}(\sigma_{\alpha\gamma}) &= (\sigma_\gamma g_{\alpha\alpha}(\sigma_\alpha) + \sigma_\alpha g_{\gamma\gamma}(\sigma_\gamma)) / 2\sigma_{\alpha\gamma}. \end{aligned}$$

In the case of considering a simple model of the system ionic solution – porous medium, we have a three-component system: positively and negatively charged ions of the solution σ_α , $\alpha = +, -$ and particles of the porous medium σ_s , which are considered stationary and can have a charge Z_s . For such a model, the shielding radius D is determined from the corresponding equations:

$$\begin{aligned} 4\Gamma^2 &= \frac{e^2}{\varepsilon l} (n_+ X_+^2 + n_- X_-^2 + n_s X_s^2), \\ X_+ &= \left(Z_+ - \frac{\pi}{2} \frac{\sigma_+^2}{1 - \Delta} P_m \right) (1 + \Gamma\sigma_+)^{-1}, \\ X_- &= \left(Z_- - \frac{\pi}{2} \frac{\sigma_-^2}{1 - \Delta} P_m \right) (1 + \Gamma\sigma_-)^{-1}, \\ X_s &= \left(Z_s - \frac{\pi}{2} \frac{\sigma_s^2}{1 - \Delta} P_m \right) (1 + \Gamma\sigma_s)^{-1}, \\ P_m &= \left(\frac{n_+\sigma_+Z_+}{1 + \Gamma\sigma_+} + \frac{n_-\sigma_-Z_-}{1 + \Gamma\sigma_-} + \frac{n_s\sigma_sZ_s}{1 + \Gamma\sigma_s} \right) \left(1 + \frac{\pi}{2(1 - \Delta)} \left(\frac{n_+\sigma_+^3}{1 + \Gamma\sigma_+} + \frac{n_-\sigma_-^3}{1 + \Gamma\sigma_-} + \frac{n_s\sigma_s^3}{1 + \Gamma\sigma_s} \right) \right)^{-1}, \\ \Delta &= \frac{\pi}{6} (n_+\sigma_+^3 + n_-\sigma_-^3 + n_s\sigma_s^3), \end{aligned}$$

and the contact values of even distribution functions have the following form:

$$\begin{aligned} g_{++}(\sigma_+) &= \left(\left(1 + \frac{\Delta}{2}\right) + \frac{3}{2} (\Delta_- \sigma_-^2 (\sigma_+ - \sigma_-) + \Delta_s \sigma_s^2 (\sigma_+ - \sigma_s)) \right) (1 - \Delta)^{-2}, \\ g_{--}(\sigma_-) &= \left(\left(1 + \frac{\Delta}{2}\right) + \frac{3}{2} (\Delta_+ \sigma_+^2 (\sigma_- - \sigma_+) + \Delta_s \sigma_s^2 (\sigma_- - \sigma_s)) \right) (1 - \Delta)^{-2}, \\ g_{ss}(\sigma_s) &= \left(\left(1 + \frac{\Delta}{2}\right) + \frac{3}{2} (\Delta_+ \sigma_+^2 (\sigma_s - \sigma_+) + \Delta_- \sigma_-^2 (\sigma_s - \sigma_-)) \right) (1 - \Delta)^{-2}, \\ g_{+-}(\sigma_{+-}) &= \frac{(\sigma_- g_{++}(\sigma_+) + \sigma_+ g_{--}(\sigma_-))}{2\sigma_{+-}}, \\ g_{s-}(\sigma_{s-}) &= \frac{(\sigma_- g_{ss}(\sigma_s) + \sigma_s g_{--}(\sigma_-))}{2\sigma_{s-}}, \\ g_{s+}(\sigma_{s+}) &= \frac{(\sigma_+ g_{ss}(\sigma_s) + \sigma_s g_{++}(\sigma_+))}{2\sigma_{s+}}, \end{aligned}$$

where $\Delta_+ = \frac{\pi}{6}n_+$, $\Delta_- = \frac{\pi}{6}n_-$, $\Delta_s = \frac{\pi}{6}n_s$.

4. Conclusions

The kinetic approach is applied to the description of ion transport processes in the ionic solution-porous medium system. By solving the Enskog–Landau kinetic equations for charged solid spheres, constructing hydrodynamic equations, analytical expressions for mutual diffusion, thermal diffusion, viscosity, and thermal conductivity coefficients due to particle distribution functions and their nature of interaction were obtained. Their structure fully reflects the character of the model of interaction of system particles, namely, at small distances – the model of hard spheres, at large – Coulomb shielded interaction.

The transfer coefficients in such a model depend on the contact values of the paired distribution functions of the charged solid spheres, the shielding radius D , the porosity ϕ of the medium, its density, and the parameter χ of the proportion of filling the porous space with an ionic solution. We discussed

one of the ways of calculating D above. However, these problems are related to the approximation of $g_{\alpha\gamma}(\mathbf{r}_{12}|n;t) \rightarrow 1$ in the Landau-type collision integral (4). To find $g_{\alpha\gamma}(\mathbf{r}_{12}|n;t)$, it is necessary to use the system of equations of the Ornstein–Zernike type in the non-equilibrium case [72–74], or the method of collective variables [75], which will be applied in the following works in the case of ionic solutions. This is important from the point of view of consideration of non-stationary transport processes in the system ionic solution – porous medium.

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- [1] Kondori A., Esmailirad M., Harzandi A. M., Amine R., Saray M. T., Yu L., Liu T., Wen J. et al. A room temperature rechargeable Li_2O -based lithium-air battery enabled by a solid electrolyte. *Science*. **379** (6631), 499–505 (2023).
 - [2] Han G., Vasylenko A., Daniels L. M., Collins C. M., Corti L., Chen R., Niu H., Manning T. D. et al. Superionic lithium transport via multiple coordination environments defined by two anion packing. *Science*. **383** (6684), 739–745 (2024).
 - [3] Yu W., Shen Z., Yoshii T., Iwamura S., Ono M., Matsuda S., Aoki M., Kondo T., Mukai S. R. et al. Hierarchically Porous and Minimally Stacked Graphene Cathodes for High-Performance Lithium–Oxygen Batteries. *Advanced Energy Materials*. **14** (2), 2303055 (2024).
 - [4] Ding J., Du T., Thomsen E. H., Andresen D., Fischer M. R., Møller A. K., Petersen A. R. et al. Metal-Organic Framework Glass as a Functional Filler Enables Enhanced Performance of Solid-State Polymer Electrolytes for Lithium Metal Batteries. *Advanced Science*. **11** (10), 2306698 (2024).
 - [5] Biesheuvel P. M., Zhang L., Gasquet P., Blankert B., Elimelech M., van der Meer W. G. J. Ion Selectivity in Brackish Water Desalination by Reverse Osmosis: Theory, Measurements, and Implications. *Environmental Science & Technology Letters*. **7** (1), 42–47 (2019).
 - [6] Joekar-Niasar V., Schreyer L., Sedighi M., Icardi M., Huyghe J. Coupled Processes in Charged Porous Media: From Theory to Applications. *Transport in Porous Media*. **130**, 183–214 (2019).
 - [7] Yang Z., Zhou Y., Feng Z., Rui X., Zhang T., Zhang Z. A Review on Reverse Osmosis and Nanofiltration Membranes for Water Purification. *Polymers*. **11** (8), 1252 (2019).
 - [8] Heiranian M., Fan H., Wang L., Lu X., Elimelech M. Mechanisms and models for water transport in reverse osmosis membranes: history, critical, assessment, and recent developments. *Chemical Society Reviews*. **52** (24), 8455–8480 (2023).
 - [9] Fan H., Huang Y., Yip N. Y. Advancing ion-exchange membranes to ion-selective membranes: principles, status, and opportunities. *Frontiers of Environmental Science & Engineering*. **17** (2), 25 (2023).
 - [10] Miao J., Hu Q., Zhang Z., Hu Y. Bioinspired cell membrane-based nanofiltration membranes with hierarchical pore channels for fast molecular separation. *Journal of Membrane Science*. **697**, 122578 (2024).
 - [11] Ye Z., Galvanetto N., Puppulin L., Pifferi S., Flechsig H., Arndt M., Trivino C. A. S., Di Palma M., Guo S., Vogel H., Menini A., Franz C. M., Torre V., Marchesi A. Structural heterogeneity of the ion and lipid channel TMEM16F. *Nature Communications*. **15**, 110 (2024).
 - [12] Stabilini S., Menini A., Pifferi S. Anion and Cation Permeability of the Mouse TMEM16F Calcium-Activated Channel. *International Journal of Molecular Sciences*. **22** (16), 8578 (2021).
 - [13] Hou J., Zhang H. Advanced Methods for Ion Selectivity Measurement in Nanofluidic Devices. *Advanced Materials Technologies*. **8** (9), 2201433 (2023).
 - [14] Keene S. T., Rao A., Malliaras G. G. The relationship between ionic-electronic coupling and transport in organic mixed conductors. *Science Advances*. **9** (35), eadi3536 (2023).
 - [15] Zech A., de Winter M. A Probabilistic Formulation of the Diffusion Coefficient in Porous Media as Function of Porosity. *Transport in Porous Media*. **146**, 475–492 (2023).
 - [16] Brey J., García de Soria M. I., Maynar P. Kinetic theory of diffusion in a channel of varying cross section. *Molecular Physics*. e2378116 (2024).
 - [17] Sahimi M. Non-linear and non-local transport processes in heterogeneous media: from long-range correlated percolation to fracture and materials breakdown. *Physics Reports*. **306** (4–6), 213–395 (1998).
 - [18] Hatano Y., Hatano N. Dispersive transport of ions in column experiments: An explanation of long-tailed profiles. *Water Resources Research*. **34** (5), 1027–1033 (1998).

- [19] Gelb L. D., Gubbins K. E., Radhakrishnan R., Sliwinska-Bartkowiak M. Phase separation in confined systems. *Reports on Progress in Physics*. **62** (12), 1573–1659 (1999).
- [20] *Advances in Lithium-Ion Batteries*. Eds.: W. A. van Schalkwijk, B. Scrosati. Springer New York, NY (2002).
- [21] Wagemaker M. *Structure and Dynamics of Lithium in Anatase TiO₂*. Delft University Press, Netherland (2002).
- [22] Berkowitz B., Klafter J., Metzler R., Scher H. Physical pictures of transport in heterogeneous media: Advection-dispersion, random-walk, and fractional derivative formulations. *Water Resources Research*. **38** (10), 1191 (2002).
- [23] Berkowitz B., Cortis A., Dentz M., Scher H. Modeling non-Fickian transport in geological formations as a continuous time random walk. *Reviews of Geophysics*. **44** (2), RG2003 (2006).
- [24] Smith J. J., Zharov I. Ion Transport in Sulfonated Nanoporous Colloidal Films. *Langmuir*. **24** (6), 2650–2654 (2008).
- [25] Neuman S. P., Tartakovsky D. M. Perspective on theories of non-Fickian transport in heterogeneous media. *Advances in Water Resources*. **32** (5), 670–680 (2009).
- [26] Rotenberg B., Pagonabarrag I., Frenkel D. Coarse-grained simulations of charge, current and flow in heterogeneous media. *Faraday Discussions*. **144**, 223–243 (2010).
- [27] Yang C., Nakayama A. A synthesis of tortuosity and dispersion in effective thermal conductivity of porous media. *International Journal of Heat and Mass Transfer*. **53** (15–16), 3222–3230 (2010).
- [28] Maffeo C., Bhattacharya S., Yoo J., Wells D., Aksimentiev A. Modeling and Simulation of Ion Channels. *Chemical Reviews*. **112** (12), 6250–6284 (2012).
- [29] Bijeljic B., Raeini A., Mostaghimi P., Blunt M. J. Predictions of non-Fickian solute transport in different classes of porous media using direct simulation on pore-scale images. *Physical Review E*. **87** (1), 013011 (2013).
- [30] Grygorchak I. I., Kostrobij P. P., Stasiuk I. V., Tokarchuk M. V., Velychko O. V., Ivashchyshyn F. O., Markovych B. M. Physical processes and their microscopic models in periodic inorganic/organic clathrates. Lviv, Rastr-7 (2015), (in Ukrainian).
- [31] *Lithium batteries*. Eds.: G.-A. Nazri, G. Pistoia. USA, Springer (2009).
- [32] Tyukhova A., Dentz M., Kinzelbach W., Willmann M. Mechanisms of Anomalous Dispersion in Flow Through Heterogeneous Porous Media. *Physical Review Fluids*. **1** (7), 074002 (2016).
- [33] Comolli A., Dentz M. Anomalous dispersion in correlated porous media: a coupled continuous time random walk approach. *The European Physical Journal B*. **90**, 166 (2017).
- [34] Waisbord N., Stoop N., Walkama D. M., Dunkel J., Guasto J. S. Anomalous percolation flow transition of yield stress fluids in porous media. *Physical Review Fluids*. **4** (6), 063303 (2019).
- [35] Zhao T., Qing L., Long T., Xu X., Zhao S., Lu X. Dynamical coupling of ion adsorption with fluid flow in nanopores. *AIChE Journal*. **67** (7), e17266 (2021).
- [36] Schmuck M., Bazant M. Z. Homogenization of the Poisson–Nernst–Planck equation for ion transport in charged porous media. *SIAM Journal on Applied Mathematics*. **75** (3), 1369–1401 (2015).
- [37] Revil A. Transport of water and ions in partially water-saturated porous media. Part 1. Constitutive equations. *Advances in Water Resources*. **103**, 119–138 (2017).
- [38] Revil A. Transport of water and ions in partially water-saturated porous media. Part 2. Filtration effects. *Advances in Water Resources*. **103**, 139–152 (2017).
- [39] Bisquert J., Compte A. Theory of the electrochemical impedance of anomalous diffusion. *Journal of Electroanalytical Chemistry*. **499** (1), 112–120 (2001).
- [40] Fuliński A., Kosińska I. D., Siwy Z. On the validity of continuous modelling of ion transport through nanochannels. *Europhysics Letters*. **67** (4), 683–689 (2004).
- [41] Fuliński A., Kosińska I. D., Siwy Z. Transport properties of nanopores in electrolyte solutions: the diffusional model and surface currents. *New Journal of Physics*. **7** (1), 132 (2005).
- [42] Sibatov R. T., Uchaikin V. V. Fractional differential approach to dispersive transport in semiconductors. *Physics-USpekhi*. **52** (10), 1019–1043 (2009).

- [43] Sibatov R. T. Drobno-differencialnaja teorija anomalnoj kinetiki nositelej zarjada v neuporjadochennyh poluprovodnikovyh sistemah. Thesis for the Degree of Doctor of Sciences in Physics and Mathematics. Uljanovsk (2012).
- [44] Khamzin A. A., Popov I. I., Nigmatullin R. R. Correction of the power law of ac conductivity in ion-conducting materials due to the electrode polarization effect. *Physical Review E*. **89** (3), 032303 (2014).
- [45] Ferguson T. R., Bazant M. Z. Nonequilibrium Thermodynamics of Porous Electrodes. *Journal of The Electrochemical Society*. **159** (12), A1967–A1985 (2012).
- [46] Xie Y., Li J., Yuan C. Mathematical modeling of the electrochemical impedance spectroscopy in lithium ion battery cycling. *Electrochimica Acta*. **127**, 266–275 (2014).
- [47] Kostrobij P. P., Markovych B. M., Chernomorets Yu. I., Tokarchuk R. M., Tokarchuk M. V. Statistical description of electro-diffusion processes of ions intercalation in “electrolyte–electrode” system. *Mathematical Modeling and Computing*. **1** (2), 178–194 (2014).
- [48] Kostrobij P., Markovych B., Viznovych O., Tokarchuk M. Generalized electrodiffusion equation with fractality of space-time. *Mathematical Modeling and Computing*. **3** (2), 163–172 (2017).
- [49] Grygorchak I. I., Ivashchyshyn F. O., Tokarchuk M. V., Pokladok N. T., Viznovych O. V. Modification of properties of GaSe(β -cyclodextrin(FeSO_4)) Clathrat by synthesis in superposed electric and light-wave fields. *Journal of Applied Physics*. **121** (18), 185501 (2017).
- [50] Kostrobij P. P., Ivashchyshyn F. O., Markovych B. M., Tokarchuk M. V. Microscopic theory of the influence of dipole superparamagnetics (type $\langle\beta\text{-CD}\langle\text{FeSO}_4\rangle\rangle$) on current flow in semiconductor layered structures (type GaSe, InSe). *Mathematical Modeling and Computing*. **8** (1), 89–105 (2021).
- [51] Kostrobij P., Grygorchak I., Ivashchyshyn I., Markovych B., Viznovych O., Tokarchuk M. Generalized electrodiffusion equation with fractality of space time: experiment and theory. *The Journal of Physical Chemistry A*. **122** (16), 4099–4110 (2018).
- [52] Omelyan I. P., Zhelem R. I., Sovyak E. M., Tokarchuk M. V. Calculation of distribution functions and diffusion coefficients for ions in the system “initial electrolyte solution – membrane”. *Condensed Matter Physics*. **2** (1), 53–62 (1999).
- [53] Yukhnovskii I. R., Zhelem R. I., Tokarchuk M. V. Physical processes in the fuel containing masses interacting with aqueous solutions in the “Shelter” object. Inhomogeneous diffusion of ions UO_2^{2+} , Cs^+ in the system “glassy nuclear magma – water”. *Condensed Matter Physics*. **2** (2), 351–360 (1999).
- [54] Yukhnovskii I. R., Omelyan I. P., Zhelem R. I., Tokarchuk M. V. Statistical theory for diffusion of radionuclides in ground and subterranean water. *Radiation Physics and Chemistry*. **59** (4), 361–375 (2000).
- [55] Jardat M., Hribar-Lee B., Vlachy V. Self-diffusion of ions in charged nanoporous media. *Soft Matter*. **8**, 954–964 (2012).
- [56] Jardat M., Hribar-Lee B., Dahirel V., Vlachy V. Self-diffusion and activity coefficients of ions in charged disordered media. *The Journal of Chemical Physics*. **137** (11), 114507 (2012).
- [57] Holovko M. F., Korvatska M. Ya. Diffusion of hard sphere fluids in disordered porous media: Enskog theory description. *Condensed Matter Physics*. **23** (2), 23605 (2020).
- [58] Tokarchuk M. V. Kinetic description of ion transport in the system “ionic solution – porous environment”. *Mathematical Modeling and Computing*. **9** (3), 719–733 (2022).
- [59] Zubarev D. N., Morozov V. G., Omelyan I. P., Tokarchuk M. V. Kinetic equations for dense gases and liquids. *Theoretical and Mathematical Physics*. **87** (1), 412–424 (1991).
- [60] Zubarev D. N., Morozov V. G., Omelyan I. P., Tokarchuk M. V. The Enskog–Landau kinetic equation for charged hard spheres. *Problems of atomic science and technique. Series: Nuclear physics investigations (theory and experiment)*. Kharkov, Kharkov Physico Technical Institute. **3** (24), 60–65 (1992).
- [61] Kobryn A. E., Morozov V. G., Omelyan I. P., Tokarchuk M. V. Enskog–Landau kinetic equation. Calculation of the transport coefficient for charged hard spheres. *Physica A: Statistical Mechanics and its Applications*. **230** (1–2), 189–201 (1996).
- [62] Tokarchuk M. V., Omelyan I. P. Model kinetic equations for dense gases and liquids. *Ukrainian Journal of Physics*. **35** (8), 1255–1261 (1990), (in Ukrainian).
- [63] Chapman S., Cowling T. G. *The Mathematical Theory of Nonuniform Gases*. Cambridge, Cambridge University Press (1952).

- [64] Ferziger J. H., Kaper H. G. Mathematical theory of transport processes in gases. North-Holland, Amsterdam (1972).
- [65] Kobryn O. E., Omelyan I. P., Tokarchuk M. V. Normal solutions and transport coefficient to the Enskog–Landau kinetic equation for a two-component system of charged hard spheres. The Chapman–Enskog method. *Physica A*. **268** (3–4), 607–628 (1999).
- [66] Kobryn O. E., Omelyan I. P., Tokarchuk M. V. Enskog–Landau kinetic equation for multicomponent mixture. Analytical calculation of transport coefficient. *The European Physical Journal B – Condensed Matter and Complex Systems*. **13**, 579–583 (2000).
- [67] Blum L., Hoye J. S. Mean spherical model for asymmetric electrolytes. II. Thermodynamic properties and pair correlation function. *Journal of Physical Chemistry*. **81** (13), 1311–1316 (1977).
- [68] Lebowitz J. L. Exact solution of generalized Percus–Yevick equation for a mixture of hard spheres. *Physical Review*. **133** (4A), 895–889 (1964).
- [69] Copestake A. P., Evans R. Charge ordering and the structure of ionic liquids: screened Coulomb versus Coulomb interionic potentials. *Journal of Physics C: Solid State Physics*. **15**, 4961–4974 (1982).
- [70] Kahl G., Pastore G. Percus–Yevick pair-distribution functions of a binary hard-sphere system covering the whole r -range. *Journal of Physics A: Mathematical and General*. **24** (13), 2995–3011 (1991).
- [71] Babu C. S., Ichiye T. New integral equation theory for primitive model ionic liquids: from electrolytes to molten salts. *Journal of Chemical Physics*. **100** (12), 9147–9155 (1994).
- [72] Ramshaw J. D. Time-dependent direct correlation function. *Physical Review A*. **24** (3), 1567–1570 (1981).
- [73] Eu B. C. Dynamic Ornstein–Zernike Equation. In: *Transport Coefficients of Fluids*. *Chemical physics*. **82**, 221–240 (2006).
- [74] Gan H. H., Eu B. C. Theory of the nonequilibrium structure of dense simple fluids: Effects of shearing. *Physical Review A*. **45** (6), 3670–3686 (1992).
- [75] Tokarchuk M. V. To the kinetic theory of dense gases and liquids. Calculation of quasi-equilibrium particle distribution functions by the method of collective variables. *Mathematical Modeling and Computing*. **9** (2), 440–458 (2022).

Кінетичні коефіцієнти транспорту іонів у пористому середовищі на основі кінетичного рівняння Енскога–Ландау

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Отримано нормальні розв'язки кінетичного рівняння Енскога–Власова–Ландау в межах моделі позитивно і негативно заряджених твердих сфер для системи іонний розчин – пористе середовище. Застосовано метод Чепмена–Енскога. Шляхом побудови рівнянь гідродинаміки на основі нормальних розв'язків кінетичного рівняння отримано аналітичні вирази для коефіцієнтів в'язкості, теплопровідності, дифузії іонів в системі іонний розчин – пористе середовище.

Ключові слова: *кінетичні рівняння; функція розподілу; рівняння гідродинаміки; коефіцієнти переносу; дифузія; радіус екранування; іонний розчин – система пористе середовище.*