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## MATHEMATICAL MODEL OF CONDUCTING NANOPORE FOR MOLECULAR DYNAMICS SIMULATIONS

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*An electrostatic model of conducting nanopore is presented in the paper. The model does not require solution of the Poisson equation for the potential. This model is intended for use in simulation of transport phenomena of charged particles in conducting nanopores by the method of molecular dynamics. This method is based on Newton's equations of motion and it allows one to determine the variation of position, velocity and acceleration of particles with time. The electric field from the charge distributed over the nanopore surface is approximated by the field from fictitious point charges on the same surface. To verify the proposed model of fictitious charges system capacitance is calculated. The obtained values of capacitance are compared with classical results for conducting tubule and with the results obtained by the other similar method. The comparison shows that relative discrepancy between results is less than 10 %. There is a need to further develop the proposed model both in case of a large number of fictitious charges and in case when charged particles are in close proximity to the nanopore surface. The proposed method can be easily applied to an arbitrary shape nanopore. The model can be used in the development of various nanodevices, among them the devices used in life support systems of manned space vehicles.*

*Keywords: conducting nanopore, ion transport, molecular dynamics.*

## МАТЕМАТИЧЕСКАЯ МОДЕЛЬ ПРОВОДЯЩЕЙ НАНОПОРЫ ДЛЯ РАСЧЕТОВ МЕТОДОМ МОЛЕКУЛЯРНОЙ ДИНАМИКИ

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*Представлена электростатическая математическая модель проводящей нанопоры. Расчет потенциала проводящей нанопоры не требует решения уравнения Пуассона. Модель предназначена для компьютерного моделирования транспорта заряженных частиц в проводящих нанопорах методом молекулярной динамики. Этот вычислительный метод основан на втором законе Ньютона и позволяет получить траекторию, которая описывает положения, скорости и ускорения частиц со временем. Электрическое поле распределенного по поверхности нанопоры заряда аппроксимировано полем фиктивных точечных зарядов, расположенных на той же поверхности. Выполнено сравнение электроемкости системы фиктивных зарядов, рассчитанной предложенным методом, с классическими решениями для проводящего тубулена и с решениями, полученными другим подобным методом. Предложенный метод показал достаточную точность (около 10 %) и предсказуемость поведения. Необходимо его дальнейшее исследование и развитие как для случая достаточно большого числа фиктивных зарядов, так и для случая достаточно сильного приближения ионов к поверхности нанопоры. Рассмотренный метод введения фиктивных зарядов может быть легко применен к нанопорам произвольной*

*формы. Результаты выполненного моделирования могут быть использованы при разработке различных нанотехнологических устройств, в том числе используемых в качестве компонентов систем жизнеобеспечения пилотируемых космических аппаратов.*

*Ключевые слова: проводящая нанопора, транспорт ионов, молекулярная динамика.*

**Introduction.** Nanopores represent a type o pores with a diameter of about several nanometers. Channels of such size can be both natural and artificially made objects. Currently researchers take great interest in the issues of studying and modeling of nanopore properties due to their broad application in science and technology [1; 2]. Artificial nanopores can be used, for example, for imitation of biological nanopore functions. They also have attractive potential applications in nanofluid fields [3]. Among these applications are desalination, ionic sieves [4], sensors for biological agents and sequencing of DNA or RNA [5].

Various forms of artificial nanopores using different production technologies and materials, including polymers, inorganic substances, biotic and composite materials have been developed [6; 7].

Conducting nanopores attract considerable attention due to their important potential applications. In a number of works production methods of similar structures are given. For example, such nanopores can be made via integration of carbon structures into the corresponding nanoporous material. A multilayered carbon nanotube was made inside a pore and on the surface of an anode aluminum oxidic membrane, applying the method of chemical sedimentation from a steam phase [8]. Strengthened single-layer metal carbon nanotubes were grown on a silicon plate via chemical sedimentation from a steam phase [9]. Synthesis of conducting carbon tubules inside the pores of the anode aluminum and oxidic membrane was investigated [10]. Similar structures can be of interest in terms of production of selective membranes switched by electric field.

In recent years mathematical and electrostatic models of ion transport in various types of nanopores and nanochannels have been vigorously developed, computer modeling of processes have been carried out as well [11–13].

At computer modeling of ion transport, applying methods of molecular dynamics, the problem of electric field defining, created in the system, has to be solved at each step in time. In presence of electro-conductive elements in the system, solving such a task with classical methods becomes rather resource-intensive. Therefore, problem solving methods of such electrostatic tasks should be fairly simple, although they are not as accurate as classical ways. In this regard there is a problem of such methods accuracy assessment in comparison with classical ones. A rather typical assessment might be a comparison of integrated electric parameters of the system, obtained by the offered methods, with classical decisions. In this work electric capacitance parameter will be compared with the data from the reference book [14].

The purpose of this work is to simulate the conducting nanopore electric field in presence of external charges (ions). This model is intended for use in fundamental research of charged particles transfer phenomenon (ions and charged proteinaceous residue) in conducting nanopores.

In the work [15] a method of the conducting nanopore electric field in the presence of external charges (ions) modeling in relation to problems of molecular dynamics was offered. In the present work an alternative for further development of this method is being investigated.

The results of simulation can be used when developing various devices, including, for instance, a component of life support systems in piloted spacecrafts.

**Problem definition.** The membrane containing a nanopore is simulated in the form of L wide uniform dielectric plate. The nanopore is a cylindrical hole with radius $a$ and length $L$ (fig. 1).

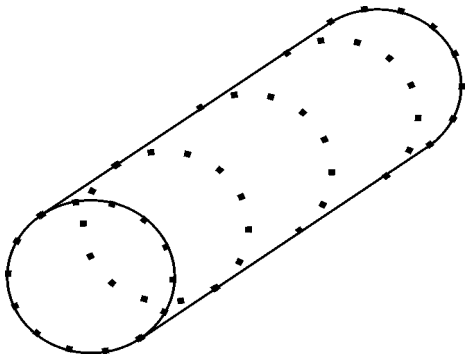

Fig. 1. Model of nanopore. Dots denote fictitious electric charges

Рис. 1. Модель нанопоры. Точками обозначены фиктивные электрические заряды

We shall consider the problem of ion transport in the context of continual electrostatic model. We shall assume that the ion is located in random position $\mathbf{r}^*$. Electrostatic potential of $\varphi(\mathbf{r})$ in and outside the nanopore satisfies the Poisson's equation

$$\Delta\varphi = -\frac{1}{4\pi\varepsilon_0}\sum_{n=1}^{N} q_n \delta\left(\mathbf{r}-\mathbf{r}_n^*\right), \qquad (1)$$

where $\Delta$ – Laplasian operator; $q_n$ – ion charge; $N$ – ion number; $\delta\left(\mathbf{r}-\mathbf{r}_n^*\right)$ – delta-Dirac function. The equation (1) has to be solved across all the space, except the area of membrane material with the potential set of boundary conditions on the tubulen surface. It is also necessary to demand the continuity of the membrane, normal to the surface, components of electric induction vector and, whenever possible, decrease of potential while being removed from the system.

Under consideration of charged particles transport phenomenon, we are interested in the force affecting the ion from the conducting nanopore which is expressed as $\mathbf{f} = -q \cdot \mathrm{grad}\left(\varphi\left(\mathbf{r}^*\right)\right)$.

The solution of the equation (1) with the set boundary conditions is a difficult task. The problem becomes even

more complicated if to consider not only cylindrical, but also other forms of nanopores. Further we will try to present simple and rather universal model of conducting nanopores which does not require solving the Poisson equation for the potential.

**Electrostatic model of conducting nanopore.** We shall approximate electric field distributed on the body (tubulen) of the charge by the field of the dot charges located on the same surface. We shall place these fictitious charges in the chosen in advance surface dots. We will determine their size from the condition of maximum approach to mechanical balance. Assuming that fictitious charges could move on a tubulen surface, then equality to zero projection on the turbulen surface of total force affecting each charge from other charges would be condition of balance. This case is equivalent to the requirement of equality to zero projections on the tubulen surface of total electric field strengths created by all other charges in the point of each fictitious charge. In our case as positions of charges are fixed, the above-stated requirement is generally impracticable. Therefore, we shall demand the minimal sum of these projections squares.

Thus, we shall place the fictitious charges $Q_k$, $k = 1, \ldots, K$, at the point with coordinates $\mathbf{r}_k$. Then we obtain electric-field vector Projection $\mathbf{E}_{i\tau}$ at point $\mathbf{r}_i$:

$$\mathbf{E}_{i\tau}(\mathbf{r}_i) = \frac{1}{4\pi\varepsilon_0}\sum_{k\neq i} Q_k \frac{(\mathbf{r}_i - \mathbf{r}_k) - \mathbf{n}_i(\mathbf{n}_i * (\mathbf{r}_i - \mathbf{r}_k))}{|\mathbf{r}_i - \mathbf{r}_k|^3}, \quad (2)$$

where $\mathbf{n}_i$ – normal vector to the surface at the point $\mathbf{r}_i$; * is dot product of vectors.

By summing squares (2) where all $i = 1, \ldots, K$, we obtain

$$\sum_{i=1}^{K} \mathbf{E}_{i\tau}^2(\mathbf{r}_i) = \frac{1}{16\pi^2\varepsilon_0^2} \times$$

$$\times \sum_{i=1}^{K}\sum_{k\neq i}\sum_{l\neq i} Q_k Q_l \frac{(\mathbf{r}_i - \mathbf{r}_k) * (\mathbf{r}_i - \mathbf{r}_l) - (\mathbf{n}_i * (\mathbf{r}_i - \mathbf{r}_k))(\mathbf{n}_i * (\mathbf{r}_i - \mathbf{r}_l))}{|\mathbf{r}_i - \mathbf{r}_k|^3 |\mathbf{r}_i - \mathbf{r}_l|^3}. \quad (3)$$

We shall look for the minimum (3) on condition of specified total charge $q$ of conducting tubulen:

$$q = \sum_{i=1}^{K} Q_i . \quad (4)$$

Considering that a set of unknown charges is vector $\mathbf{Q} = (Q_k)$, than we have a standard problem of square form minimization of (3):

$$\sum_{i=1}^{K} \mathbf{E}_{i\tau}^2(\mathbf{r}_i) = \frac{1}{16\pi^2\varepsilon_0^2} \mathbf{Q}' \times \hat{\mathbf{A}} \times \mathbf{Q}, \quad (5)$$

$$\hat{\mathbf{A}}_{kl} = \sum_{i\neq k,l} \frac{(\mathbf{r}_i - \mathbf{r}_k) * (\mathbf{r}_i - \mathbf{r}_l) - (\mathbf{n}_i * (\mathbf{r}_i - \mathbf{r}_k))(\mathbf{n}_i * (\mathbf{r}_i - \mathbf{r}_l))}{|\mathbf{r}_i - \mathbf{r}_k|^3 |\mathbf{r}_i - \mathbf{r}_l|^3}.$$

Under condition (4):

$$q = \mathbf{1}' \times \mathbf{Q}. \quad (6)$$

Here $\times$ denotes dot product of vectors of $K$ dimension and vectors and dimensional matrix $K \times K$; stroke denotes transposing operation of a vector column in a vector line; $\mathbf{1} = (1,1,1,\ldots 1)$ – made of units dimension vector $K$.

Solution to variational problem (5), (6), on condition that nondegenerate matrix $\hat{\mathbf{A}}$, will be vector

$$\mathbf{Q} = q \frac{\hat{\mathbf{A}}^{-1} \times \mathbf{1}}{\mathbf{1}' \times \hat{\mathbf{A}}^{-1} \times \mathbf{1}}. \quad (7)$$

In case of nondegenerate matrics $\hat{\mathbf{A}}$, under condition that $\mathbf{a}_0$ – evector $\hat{\mathbf{A}}$, corresponding to zero evalue, non-orthogonal $\mathbf{1}$, we obtain

$$\mathbf{Q} = q \frac{\mathbf{a}_0}{\mathbf{1}' \times \mathbf{a}_0}. \quad (8)$$

The result (8) can be easily summarized and in case of greater 1 dimension of the evector subspace, corresponding to zero evalue $\hat{\mathbf{A}}$: in this case $\mathbf{a}_0$ – any non orthogonal to $\mathbf{1}$ vector from that subspace. However, in case $\mathbf{a}_0$ is orthogonal to $\mathbf{1}$, the task should be reduced, while decreasing $\hat{\mathbf{A}}$ size and leaving behind only zero evalues. It should be noted that from the method $\hat{\mathbf{A}}$ it is clear that $\hat{\mathbf{A}}$ is symmetrical non-negative matrix.

We shall consider the alternative where $\hat{\mathbf{A}}$ is a degenerate matrix. Generally this is true: we shall place nonzero dot charges of one sign on the tubulen surface and allow them to move on a tubulen surface. It is obvious that such system has a stationary position of charges. If to arrange fictitious charges similarly, then the matrix $\hat{\mathbf{A}}$ will degenerate as there are charge values at which vector projection of electric field strength affecting each charge is equal to zero. Moreover, another stationary position, mostly continuously depending on charges, corresponds to a different set of value sizes which are freely moving on the tubulen surface. Therefore, we have a rather big area of coordinates of fictitious charges at which the matrix degenerate. At numerical calculations it will mean that if we chose the "wrong" positions of fictitious charges, and the matrix is not degenerated, then, while increasing in number of fictitious charges, generally, conditionality ratio of this matrix will grow.

The present work is devoted to preliminary assessment of the offered method practical applicability under molecular and dynamic calculations, therefore further cases of small number of fictitious charges at which in the reviewed examples matrix $\hat{\mathbf{A}}$ is not degenerated are investigated.

The offered method is a further development of [15]. In the work [15] comparative analysis of the presented method of electrostatic task solution with other methods of electrostatics is carried out. As a comparative criterion, the results of electric capacitance calculation given in the reference book [14] were used. In this work for the above method applicability assessment we will use the results of electric capacitance of the conducting tubulen calculations and compare them with the results [14] and [15].

We shall continue the above suggested calculations in order to obtain estimates of conducting tubulen electric capacitance. We shall receive these estimates, comparing

the energy of the system considered with the expression for the energy of the conducting body:

$$W = \frac{1}{4\pi\varepsilon_0}\sum_{i\neq j}\frac{Q_iQ_j}{|\mathbf{r}_i-\mathbf{r}_j|} = \frac{q^2}{2C}, \qquad (9)$$

where $C$ – conducting tubulen electric capacitance. Adding (7) to (9), finally obtain the expression for electric capacitance:

$$C = 2\pi\varepsilon_0\frac{\left(\mathbf{1}'\times\hat{\mathbf{A}}^{-1}\times\mathbf{1}\right)^2}{\mathbf{1}'\times\hat{\mathbf{A}}^{-1}\times\hat{\mathbf{B}}\times\hat{\mathbf{A}}^{-1}\times\mathbf{1}},$$
$$\hat{\mathbf{B}}_{ij} = \begin{cases}\dfrac{1}{|\mathbf{r}_i-\mathbf{r}_j|}, & i\neq j;\\ 0 & i=j.\end{cases} \qquad (10)$$

It shall be noted that in [15] nondegenerate matrics $\hat{\mathbf{B}}$ was proved

**Model validation.** In order to validate the accuracy of the model suggested, we shall calculate the self-capacitance of the cylindrical hole of radius $a$ and length $L$ and compare it with the data given in the table [14].

We shall place the fictitious charges in points $(z_n, a, \theta_m)$ of the cylindrical system of coordinates, where

$$z_n = (n-1)\frac{L}{N-1},\ n=1,...,N,$$
$$\theta_m = (m-1)\frac{2\pi}{N-1},\ m=1,...,N. \qquad (11)$$

Then $K = N^2$. Calculations are given in table for $5 \le L/a \le 20$ и $N = 10, 20, 30$. Electrical capacitance value form the reference book [14] are marked $C_0$, discrepancy between calculated and table-based [14] capacitance value $d = (C - C_0)/C_0$.

In fig. 2 the obtained results are presented graphically, the best results from the work [15] obtained under the same algorithm of fictitious charges arrangement and $N = 80$ are given.

Results presented in table and fig. 2 show that when $L/a > 8$, discrepancy amounts to less than 15 % already for $N = 20$, and smoothly decreases under increase both $L/a$ , and $N$, which is also an advantage of the suggested method. For comparison we must note that given in fig. 2 works [15] do not possess this property. From the practical point of view it might be expected that at $L/a > 10$, $N = 30$ parameters of charged particles interaction with the conducting nanopore are defined to a precision of less than 10 %.

**Conclusion.** One electrostatic model of conducting nanopore is presented in the work. The model is intended for use when modeling a nanopore, applying the method of molecular dynamics. This computing method is based on the second law of Newton. In case force intensity operating on each of atoms is known, integration of the movement equations allows to obtain a trajectory which describes positions, velocities and accelerations of particles over the time.

If fictitious charges are not entered, then to find the force operating on charged particle from the conducting nanopore, at first it is necessary to solve the equation (1) in each timepoint. In [15] the method allowing a single invert of the matrix of equation system by fictitious charges introduction is offered. The method presented in this work is similar, but demonstrates a better accuracy as it is shown in table and fig. 2. It is obvious that the offered model can be easily applied to nanopores of any form.

Thus, the offered method showed the sufficient accuracy and predictability. Therefore, its further research and development is necessary for both large number of fictitious charges leading to significant growth of matrix conditionality and for the case of rather close approximation of ions to a nanopore surface.

**The results of calculations of the electrical capacitance of a conducting nanopore**

| $L/a$, relative units. | $N = 10$ | | $N = 20$ | | $N = 30$ | | $C_0/2\pi\varepsilon_0 a$, [14], relative units. |
|---|---|---|---|---|---|---|---|
| | $C/2\pi\varepsilon_0 a$, relative units. | $d$, % | $C/2\pi\varepsilon_0 a$, relative units. | $d$, % | $C/2\pi\varepsilon_0 a$, relative units. | $d$, % | |
| 5 | 2.294 | 35.58 | 2.129 | 25.83 | 2.073 | 22.52 | 1.692 |
| 6 | 2.457 | 30.90 | 2.283 | 21.63 | 2.223 | 18.43 | 1.877 |
| 7 | 2.604 | 28.34 | 2.418 | 19.17 | 2.354 | 16.02 | 2.029 |
| 8 | 2.740 | 25.75 | 2.543 | 16.70 | 2.475 | 13.58 | 2.179 |
| 9 | 2.869 | 23.45 | 2.660 | 14.46 | 2.588 | 11.36 | 2.324 |
| 10 | 2.993 | 21.47 | 2.772 | 12.50 | 2.696 | 9.42 | 2.464 |
| 11 | 3.113 | 19.68 | 2.879 | 10.69 | 2.799 | 7.61 | 2.601 |
| 12 | 3.229 | 18.06 | 2.983 | 9.07 | 2.899 | 6.00 | 2.735 |
| 13 | 3.342 | 16.65 | 3.083 | 7.61 | 2.995 | 4.54 | 2.865 |
| 14 | 3.451 | 15.30 | 3.180 | 6.25 | 3.088 | 3.17 | 2.993 |
| 15 | 3.557 | 14.08 | 3.276 | 5.07 | 3.179 | 1.96 | 3.118 |
| 16 | 3.659 | 12.90 | 3.369 | 3.95 | 3.268 | 0.83 | 3.241 |
| 17 | 3.759 | 11.84 | 3.461 | 2.98 | 3.355 | –0.18 | 3.361 |
| 18 | 3.855 | 10.78 | 3.551 | 2.04 | 3.441 | –1.12 | 3.480 |
| 19 | 3.948 | 9.73 | 3.639 | 1.14 | 3.524 | –2.06 | 3.598 |
| 20 | 4.038 | 8.75 | 3.726 | 0.35 | 3.607 | –2.85 | 3.713 |

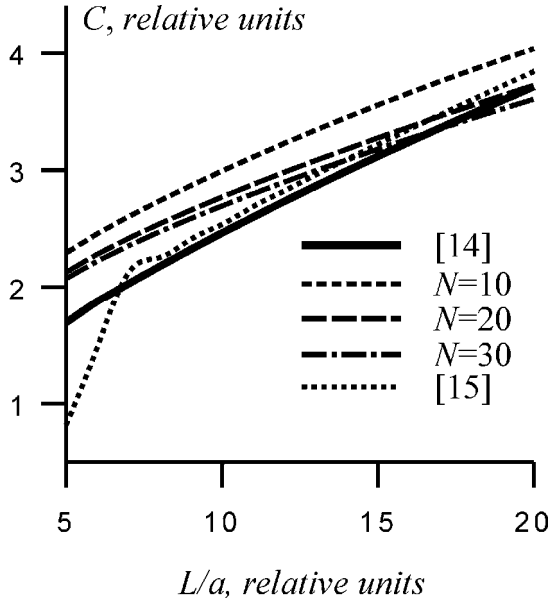


Fig. 2. Relationship between capacitance of a nanopore and the value of *L*/*a* for various numbers of fictitious charges. Solid line – tabulated data on capacitance [14]

Рис. 2. Зависимость емкости нанопоры от величины *L*/*a* при различном количестве фиктивных зарядов. Сплошная жирная линия – табличные значения емкости [14]

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