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Address: 195251 Politekhnicheskaya St. 29, St. Petersburg, Russia.

Phone: (812) 294-22-85.

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CONDENSED MATTER PHYSICS

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CONTRIBUTION OF INTERNAL IONIZATION PROCESSES IN SEMICONDUCTORS TO RADIATIVE LOSSES OF RELATIVISTIC ELECTRONS

A.E. Vasiliev¹, V.V. Kozlovski¹, S.N. Kolgatin²

¹ Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation;

² Bonch-Bruevich St. Petersburg State University of Telecommunications,

St. Petersburg, Russian Federation

The study presents analysis of mass radiative energy losses (RL) incurred by relativistic electrons in different materials commonly used in semiconductor electronics. We have specifically focused on accounting for the processes of 'internal' ionization, resulting in the production of electron-hole pairs in semiconductors and dielectrics. We have established that accounting for these processes is the only method offering consistent explanations on the values of mass RLs observed experimentally. The analysis performed should allow to make more detailed predictions for the performance of semiconductor devices in real conditions, particularly, in space.

Keywords: relativistic electron, ionization potential, radiative energy losses, silicon, germanium, graphene

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ВКЛАД ПРОЦЕССОВ ВНУТРЕННЕЙ ИОНИЗАЦИИ ПОЛУПРОВОДНИКОВ В ТОРМОЗНЫЕ ПОТЕРИ ЭНЕРГИИ РЕЛЯТИВИСТСКИХ ЭЛЕКТРОНОВ

А.Э. Васильев¹, В.В. Козловский¹, С.Н. Колгатин²

¹ Санкт-Петербургский политехнический университет Петра Великого, Санкт-Петербург, Российская Федерация;

² Санкт-Петербургский государственный университет телекоммуникаций им. проф. М.А. Бонч-Бруевича, Санкт-Петербург, Российская Федерация

Выполнен анализ массовых тормозных потерь энергии (ТПЭ) релятивистских электронов в различных материалах, используемых в полупроводниковой электронике. Особое внимание уделено учету процессов «внутренней» ионизации, приводящей к образованию электронно-дырочных пар в полупроводниках и диэлектриках. Показано, что только при таком учете удается непротиворечиво объяснить экспериментально наблюдаемые значения массовых ТПЭ. Проведенный в работе анализ позволит выполнять более детальное прогнозирование работоспособности полупроводниковых приборов в реальных, в частности космических, условиях.

Ключевые слова: релятивистский электрон, потенциал ионизации, тормозные потери энергии, кремний, германий, графен

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Introduction

While the effects of electron irradiation on the properties of semiconductor structures and devices have been considered in numerous papers and books [1 - 4], many aspects of this problem are yet to be fully understood. Most studies tend to focus on the role of elastic processes and the effect of emerging radiation defects on the properties of materials and devices [4 - 8]. The contribution from inelastic energy losses of bombarding particles is discussed to a far lesser extent. However, it is the inelastic processes that determine the resistance to electron radiation for a number of semiconductor devices, e.g., metal-oxide-semiconductor (MOS) structures and field-effect transistors [9].

The goal of our study is to investigate the ionization losses and the absorbed energy of relativistic electrons in different materials semiconductor electronics. used in In particular, we concentrated on the processes of 'internal' ionization leading to production of electron-hole pairs in semiconductors and dielectrics. Relativistic electrons of 0.9 MeV (V = 0.94c) were used as irradiating particles. The particles and the energy were chosen so that the computational data could be verified experimentally with the RTE-1V electron accelerator available at Peter the Great St. Petersburg Polytechnic University.

Estimation of radiative energy losses of relativistic electrons within the Born approximation of scattering theory

In general, calculating the absorbed energy is a complex problem that can be best solved by numerical methods. We confine ourselves to considering the situation when the thickness of the irradiated sample is much lower than the particle range, which is the case in most applied problems.

The absorbed dose D_e depends on linear radiative losses (RL) of the bombarding electrons (dE/dx) in the medium:

$$D_e = (1/\rho) \cdot (dE/dx) F_e.$$
(1)

Here ρ is the density of the medium, F_e is the exposure dose, often referred to as fluence.

The quantity $(1/\rho) \cdot (dE/dx)$ which is called the reduced (or mass) RL, is more common in practice. For convenience, Eq. (1) can be transformed by introducing the units widely used for the quantities included in this formula:

$$D_{\rho} = 1.6 \cdot 10^{-10} (1/\rho) \cdot (dE/dx) F_{\rho}; \qquad (2)$$

 D_e is given here in grays (Gy), mass RL $(1/\rho) \cdot (dE/dx)$ in MeV·(cm²/g), F_e in cm⁻². Eq. (2) allows calculating the absorbed

Eq. (2) allows calculating the absorbed dose at a known particle fluence. The inverse formula for estimation of the fluence required to obtain a known absorbed dose takes the following form:

$$F_e = \frac{1}{1.6 \cdot 10^{-10} (1/\rho) \cdot (dE/dx)}.$$
 (3)

The stopping power of MeV electrons is mainly due to ionization and excitation of bound electrons in target atoms (ionizing losses). Therefore, the notions of radiative and ionizing energy losses are virtually identical in this case. Ionizing energy losses (IEL) of relativistic electrons due to excitation and ionization of target electrons are described by the Bethe formula obtained within the Born approximation of scattering theory [10]:

$$-\left(\frac{dE}{dx}\right)_{ion} = \frac{2pN_{ai}Ze^{4}}{m_{e}V^{2}} \times \left(ln \ \frac{m_{e}V^{2}E}{2\ I^{2}(1-\beta^{2})} - ln2\left(2(1-\beta^{2})^{1/2}-1\ +\beta^{2}\right) + 1-\beta^{2} + \frac{\left[1-(1-\beta^{2})^{1/2}\right]^{2}}{8}\right),$$
(4)

where *E* is the kinetic energy of the relativistic electron, *V* is the velocity of the incident electron, $\beta = V/c$ is the relativistic factor, *I* is the mean ionization potential of the target atoms. IEL linearly depend on the number of electrons per unit of the target volume (electron density), N_e . Electron density, in turn, is known to be proportional to the density of the medium:

$$N_e = Z \cdot N_{at} = Z \cdot \rho \cdot N_0 / A.$$
 (5)

Here N_0 is the Avogadro constant; A is the atomic mass of the medium.

The first (logarithmic) term in curly brackets in the Bethe formula (4) exceeds the remaining terms by an order of magnitude in the given examples. For this reason, Eq. (4) can be simplified by omitting all terms except the first one.

$$-\left(\frac{dE}{dx}\right)_{ion} = \frac{2\pi N_{at} Z e^4}{m_e V^2} \left(ln \frac{m_e V^2 E}{2 I^2 (1-\beta^2)} \right).$$
 (6)

Let us express the squared initial velocity of the incident electron in terms of the relativistic factor

$$-\left(\frac{dE}{dx}\right)_{ion} = \frac{2\pi N_{at} Z e^4}{m_e \beta^2 c^2} \left(ln \ \frac{m_e \beta^2 c^2 E}{2 \ I^2 (1-\beta^2)} \right).$$
(7)

Let us rewrite the factor in front of the logarithm in expression (7), introducing the Rydberg energy $(E_{\rm R})$ and the Bohr radius (r_0) widely used in atomic physics

$$\left(\frac{dE}{dx}\right)_{an} = \frac{8\pi N_{ac} Z E_{k}^{2} r_{0}^{2}}{m_{e} \beta^{2} c^{2}} \times \\
\times \left(b\pi \frac{m_{e} \beta^{2} c^{2} E}{2I^{2} (1-\beta^{2})}\right),$$
(8)

$$E_{R} = -\frac{m_{e}e^{4}}{2(4\pi\varepsilon_{0})^{2}\hbar^{2}} = 13.6 \text{ eV};$$

$$r_{0} = \frac{4\pi\varepsilon_{0}\hbar^{2}}{m_{e}e^{2}} = 0.53 \ 10^{-8} \text{ cm}.$$
(9)

Now Eq. (8) can be used for linear IEL to obtain the formula for mass RL $(1/\rho) \cdot (dE/dx)$, given that the density of the medium $\rho = A \cdot N_{at}/N_0$.

$$-\frac{1}{\rho} \left(\frac{dE}{dx} \right)_{ion} = \frac{8\pi N_{\hat{A}\hat{A}\hat{I}\hat{A}} E_R^2 r_0^2}{m_e c^2} \times \\ \times \frac{Z}{A \cdot \beta^2} \left(ln \frac{m_e \beta^2 c^2 E}{2I^2 (1 - \beta^2)} \right).$$
(10)

Or, substituting the universal constants, we arrive to:

$$-\frac{1}{\rho} \left(\frac{dE}{dx} \right)_{ion} \left(\text{MeV} \cdot \text{cm}^2/\text{g} \right) =$$
$$= 0.154 \cdot \frac{Z}{A \cdot \beta^2} \left(ln \frac{0.511 \cdot 10^6 \cdot \beta^2 E}{2I^2 (1 - \beta^2)} \right), \quad (11)$$

It is often assumed that normalized linear IEL reduced to electron density in the target (or normalized mass RL reduced to mass-tocharge ratio of the target nucleus),

$$\frac{1}{\rho} \left(\frac{dE}{dx} \right)_{ion} \left(\frac{A}{Z} \right) =$$

$$= \frac{1}{\beta^2} \left(ln \frac{m_e \beta^2 c^2 E}{2I^2 (1 - \beta^2)} \right) = K(Z),$$
(12)

is a quantity independent of the material of the stopping target, equal to $18/\beta^2$ [11].

This implies that the contribution from variation of the mean ionization potential under the logarithm in Eq. (11) is small. Making this assumption, we can use Eq. (11) to easily calculate mass RL in any medium based on the experimentally found RL, for example, in aluminum [12]:

$$\left(\frac{1}{\rho} \cdot \frac{dE}{dx}\right)_{x} = \left(\frac{1}{\rho} \cdot \frac{dE}{dx}\right)_{Al} \times \left(\frac{Z}{A}\right)_{x} / \left(\frac{Z}{A}\right)_{Al}.$$
(13)

We believe that neglecting the contribution from the ionization potential of the target atoms and using Eq. (13) is ill-suited for our problems. For this reason, Eq. (11) was used to calculate RL in some materials common for semiconductor electronics. Semiconductors with different band gaps, and metals with different ohmic and rectifying contacts were selected. The mean ionization potential I and mass RL of electrons were approximated for these materials. The value of I was taken equal to [13]:

$$I = 11.5Z$$
 (for $Z < 15$),
 $I = 9.0Z$ (for large Z). (14)

The data obtained are given in Table 1. The table also lists the coefficients for calculating the absorbed dose at a known fluence (by Eq. (2)) and calculating the fluence at a known absorbed dose (by Eq. (3)).

Table 1

Target	Ι	$(1/\rho) \cdot (dE/dx)$	F/D
material	eV	$MeV \cdot (cm^2/g)$	$1/Gy \cdot cm^2$
Graphene	69	1.72	3.6·10 ⁹
Aluminum	150	1.53	$4.1 \cdot 10^9$
Silicon	161	1.56	$4.0 \cdot 10^9$
Germanium	288	1.29	$4.8 \cdot 10^9$
Gold	711	1.04	$6.0.10^{9}$

As evident from Table 1, mass RL and conversion factors between the exposure and absorbed doses can differ by 1.7 times for most materials (with the atomic number Z ranging from 6 to 79).

The Bragg rule was used for the case when the stopping medium was a chemical compound consisting of several elements [13]. According to this rule, the stopping power of a complex substance is equal to the weighted sum of stopping powers of the constituent elements:

$$\frac{1}{\rho} \cdot \frac{dE}{dx} = \frac{\omega_1}{\rho_1} \cdot \left(\frac{dE}{dx}\right)_1 + \frac{\omega_2}{\rho_2} \cdot \left(\frac{dE}{dx}\right)_2. \quad (15)$$

where ω_1 and ω_2 are the relative proportions of elements in the compound (wt. %).

Eq. (15) was used to calculate the stopping powers of silicon oxide (dielectric) and silicon carbide (wide-bandgap semiconductor). Both values of $1/\rho \cdot (dE/dx)$ coincided and were equal to 1.61 MeV·(cm²/g).

Fig. 1 shows the curve for mass RL normalized to mass-to-charge ratio of the target nucleus K(Z), as a function of the nuclear charge; the dependence was obtained by Eq. (12). This curve can be extrapolated by the dependence

$$K(Z) \sim \frac{1}{\beta^2} \ln\left(\frac{const}{Z^2}\right).$$
 (16)

As follows from Fig. 1, substituting the curve with a straight line $K(Z) = 18/\beta^2$ is not entirely acceptable for light and heavy targets.

According to the Bethe formula, targets with close values of Z should also have close values of mass RL. For example, it can be

seen from Table 1 that the elements with Z = 13 (aluminum) and Z = 14 (silicon) have virtually the same calculated values of mass RL (1.53 and 1.56 MeV·(cm²/g), respectively). However, it was experimentally confirmed in Ref. [14] that RL in silicon are higher than in aluminum by almost 1.5 times (1.5 and 2.1 MeV·(cm²/g), respectively). Possible explanations for this difference may lie in the mechanism of internal ionization in semiconductors.

Contribution from internal ionization of semiconductors to radiative energy losses of relativistic electrons

The concept of internal ionization is introduced for condensed matter. Internal ionization in semiconductors and dielectrics corresponds to the transition of valence electrons to the conduction band (band-to-band transition). Klein [15] suggested an equation relating the energy for production of an electronhole pair E_i and the band gap E_{σ} (in eV):

$$E_i = 2.67 E_a + 0.87, \tag{17}$$

establishing that the internal ionization energy is approximately three times more than the band gap.

 E_i is higher than E_g because the energy of relativistic electrons is spent not only for ionization but also for generation of excited states in a solid, i.e., plasmons and phonons. Table 2 gives the energies E_i and E_g for the main materials used in modern semiconductor electronics (silicon, germanium) and graphene.

Since the average ionization potential, which is equal to $\sim 9Z$ for most elements,



Fig. 1. Mass RL normalized to mass-to-charge ratio of target nucleus K(Z) as a function of nuclear charge; obtained by Eq. (12). The inset shows mass RL as a function of the nuclear charge calculated by Eq. (11)

within the Born approximation of scattering theory. The black dots indicate mass RL values obtained taking into account the internal ionization for graphene, silicon, and germanium

is significantly (by orders of magnitude) higher than the energy for the production of electron-hole pairs in semiconductors, the main result of electron stopping is a sharp increase in the concentration of charge carriers. Mass RL are estimated by substituting into Eq. (10) the energies for production of electron-hole pairs for the materials listed in Table 2. The results obtained are given in column 3 of Table 2. Comparing the data in Table 1 and Table 2, we can conclude that taking into account internal ionization changes (that is, increases) the capacities for RL: for example, by almost 50 % for silicon and germanium (up to 2.23 MeV·(cm²/g)). With this factor taken into account, the calculated values of mass RL (2.23 MeV·(cm²/g)) are much closer to the experimental ones (2.21 MeV·(cm²/g)) [14]. The black dots in the inset at Fig. 1 correspond to the values of mass RL normalized to mass-to-charge ratio of the target nucleus, accounting for internal ionization for graphene, silicon, and germanium. Let us estimate the concentration of electron-hole pairs produced by a single relativistic electron (N_{e-p}/F) , dividing linear RL by pair production energy. This data is given in column 4. For example, this value for silicon is $1.4 \cdot 10^6$ cm⁻¹. Let us estimate the production rate of electron-hole pairs for the real electron accelerator running at Peter the

Table 2

Band gap, energy for production of electron-hole pairs, mass RL and pair production rate by single relativistic electron for three semiconductor materials

T (E	E_i	$(1/\rho) \cdot (dE/dx)$	N_{e-p}/F
material	e	V	$MeV \cdot (cm^2/g)$	cm^{-1}
Graphene	5.2	18.7	1.94	1.6.105
Silicon	1.12	3.6	2.23	$1.4 \cdot 10^{6}$
Germanium	0.67	2.9	1.99	$3.7 \cdot 10^{6}$

Great St. Petersburg Polytechnic University. Irradiation with electrons is performed using an RTE-1V pulse accelerator. Pulse frequency is 450 Hz, pulse duration 370 µs, duty cycle 1/6. A beam with a current of 1 mA and a cross-sectional diameter of 0.9 cm scans over an area of 2×40 cm. The mean current density of the beam during irradiation with electrons is taken to be 12.5 μ A·cm⁻²; however, the current density in the pulse is much higher, reaching 6 mA·cm⁻². The electron flux density in the pulse at such currents is $3.6 \cdot 10^{16}$ cm⁻²s⁻¹, and the total production rate for electron-hole pairs upon electron irradiation reaches a huge value $(1.4 \cdot 10^{6} \cdot 3.6 \cdot 10^{16}) = 5 \cdot 10^{22} \text{ cm}^{-3} \text{s}^{-1}$. An additional charge is generated upon irradiation of MOS structures and field-effect transistors at the insulator-semiconductor interface and in the bulk of the insulator due to production of electron-hole pairs, resulting in a change in the main characteristic, which is the threshold voltage of the device [9].

Summary

The results obtained in the course of our investigation led us to the following conclusions:

1. Accounting for internal ionization of semiconductors due to production of electronhole pairs changes (increases) the stopping powers of relativistic electrons, for example, by almost 50% for silicon and germanium.

2. This in turn offers a consistent explanation for the values of mass RL observed experimentally.

3. The analysis carried out in the study should allow making more effective and more detailed predictions for the performance of semiconductor devices in real conditions, particularly, in space.

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THE AUTHORS

VASILIEV Alexander E.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation vasiliev_ae@spbstu.ru

KOZLOVSKI Vitaly V.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation vkozlovski@phmf.spbstu.ru

KOLGATIN Sergey N.

Bonch-Bruevich St. Petersburg State University of Telecommunications 61 Moika Emb., St. Petersburg, 191186, Russian Federation kolgatins@gmail.com

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СВЕДЕНИЯ ОБ АВТОРАХ

ВАСИЛЬЕВ Александр Электронович — кандидат физико-математических наук, доцент кафедры экспериментальной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 vasiliev_ae@spbstu.ru

КОЗЛОВСКИЙ Виталий Васильевич — доктор физико-математических наук, профессор кафедры экспериментальной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 vkozlovski@phmf.spbstu.ru

КОЛГАТИН Сергей Николаевич — доктор технических наук, заведующий кафедрой физики Санкт-Петербургского государственного университета телекоммуникаций им. проф. М.А. Бонч-Бруевича, Санкт-Петербург, Российская Федерация.

191186, Российская Федерация, г. Санкт-Петербург, наб. р. Мойки, 61. kolgatins@gmail.com

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PHASE TRANSITIONS IN COMPOSITES BASED ON DIISOPROPYLAMMONIUM CHLORIDE AND LEAD TITANATE

E.V. Stukova¹, S.V. Baryshnikov²

¹ Amur State University, Blagoveshchensk, Russian Federation;

² Blagoveschensk State Pedagogical University, Blagoveshchensk, Russian Federation

The paper presents the results of studies in the dielectric properties of $(DIPAC)_{1-x}/(PbTiO_3)_{x}$ composites with the x volume fraction of lead titanate in composite from 0.10 to 0.40. It has been shown that the addition of lead titanate to diisopropylammonium chloride leads to an increase in the dielectric constant and the appearance of additional phase transitions during heating and cooling. The appearance of a new phase transition was explained in the framework of the Landau–Ginzburg theory, taking into account the dipole-dipole interaction between the components.

Keywords: ferroelectric composite, phase transition, dielectric constant, lead titanate, diisopropylammonium chloride

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ФАЗОВЫЕ ПЕРЕХОДЫ В КОМПОЗИТАХ НА ОСНОВЕ ХЛОРИДА ДИИЗОПРОПИЛАММОНИЯ И ТИТАНАТА СВИНЦА

Е.В. Стукова¹, С.В. Барышников²

¹ Амурский государственный университет, г. Благовещенск, Российская Федерация;

² Благовещенский государственный педагогический университет,

г. Благовещенск, Российская Федерация

В работе представлены результаты исследований диэлектрических свойств композитов $(DIPAC)_{1-x}/(PbTiO_3)_x$ с объемной долей x титаната свинца в композите от 0,10 до 0,40. Показано, что добавка титаната свинца к хлориду диизопропиламмония приводит к увеличению диэлектрической проницаемости и возникновению дополнительного фазового перехода при нагреве и охлаждении. Появление нового фазового перехода объясняется в рамках теории Ландау–Гинзбурга с учетом диполь-дипольного взаимодействия между компонентами.

Ключевые слова: сегнетоэлектрический композит, фазовый переход, диэлектрическая проницаемость, титанат свинца, хлорид диизопропиламмония

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Introduction

Ferroelectrics are multifunctional materials with vast potential for practical applications in various devices, such as nonlinear capacitors, piezoelectric, pyroelectric, and electro-optical devices. Spontaneous polarization switching by an applied electric field makes it possible to use these materials in data storage devices.

Recently, there has been a great focus on novel organic ferroelectrics. For example, diisopropylammonium chloride $(C_6H_{16}NCl,$ DIPAC), with polarization spontaneous $P_{a} \approx 8.9 \ \mu C/cm^{2}$ and the Curie temperature $\vec{T} = 440$ K [2], was discovered in 2006 [1]. New crystals were obtained several years later by replacing chlorine with bromine and iodine (characterized by larger ionic radii): diisopropylammonium bromide (C₆H₁₆NBr, DIPAB) with the Curie temperature $T_c = 426$ K and spontaneous polarization $P_{a} \approx 23 \ \mu C/cm^{2}$ [3], as well as diisopropylammonium iodide ($C_6H_{16}NI$, DIPAI) with the parameters $T_c = 378^{\circ}$ K, $P_s \approx 5.17 \ \mu C/cm^2 \ [4].$

^s In particular, DIPAB has a spontaneous polarization value close to that in barium titanate, a high Curie temperature, and exhibits good piezoelectric response. These attributes make ferroelectrics of the diisopropylammonium group an alternative to perovskite-type ferroelectrics. This is the reason for the growing interest in studies of these materials [2–6].

Furthermore, the structures incorporating ferroelectric composites based on such materials may have unusual properties uncharacteristic for homogeneous substances.

The dielectric properties of diisopropylammonium chloride (DIPAC) nanoparticles embedded in opal and MCM-41 silica matrices were considered in [7], where it was found that embedding such a compound into the opal pores shifts the phase transition temperature of the composite towards low temperatures and increases its expansion coefficient compared to the bulk sample. In addition, the thermal hysteresis of the phase transition increases in the opal nanopores. No anomalies of the dielectric constant related to the ferroelectric transition were observed for DIPAC embedded into MCM-41 molecular sieves because this compound is amorphous.

Ref. [8] reports on the studies of linear and nonlinear dielectric properties, accompanied by calorimetric measurements, for a ferroelectric composite $(\text{DIPAB})_{1-x}/(\text{PbTiO}_3)_x$ with the volume fraction of lead titanate particles x = 0.1, 0.2and 0.3. It was established that adding lead titanate particles to diisopropylammonium bromide leads to a change in the sequence of structural phase transitions, an increase in the effective dielectric constant and dielectric loss tangent (tg\delta) of the composite. Two phases are observed in C₆H₁₆NBr in the temperature range from 423 to 411 K (the ferroelectric phase *P*2₁ and the non-ferroelectric one *P*2₁2₁2₁); the ratio between the phases depends on the fraction of lead titanate particles in the composite.

The goal of this study consists establishing the effect of lead in properties of titanate particles on the diisopropylammonium chloride in the $(DIPAC)_{1-x}/(PbTiO_3)_x$ composite.

Samples and experimental procedure

Diisopropylammonium chloride was obtained by reacting diisopropylamine with a 30% aqueous solution of HCl followed by recrystallization from methyl alcohol. According to X-ray spectroscopy data, the obtained diisopropylammonium chloride was in the polar phase $P2_1$ at room temperature, which corresponds to ICDD card 00-009-0589. A non-polar crystal structure is observed in DIPAC at temperatures above $T_c \approx 440$ K; it belongs to space group 2/m. The phase transition in DIPAC is classified as a first-order transition because there is a thermal hysteresis of about 4 K.

Lead titanate is a classical perovskite-type ferroelectric with the Curie temperature $T_c = 763$ K. PbTiO 3 is in a tetragonal ferroelectric phase at room temperature, with $P_c \approx 60 \ \mu \text{K/cm}^2$ [9].

Diisopropylammonium chloride powder with an average particle size of about 10 µm and lead titanate powder with an average particle size of about 1 µm were used to prepare the $(DIPAC)_{1-x}/(PbTiO_3)_x$ samples. The PbTiO₂ content was varied from x = 0.10to 0.40 (x is the volume fraction of lead titanate). Samples for measurement were prepared by thorough mixing, followed by molding under a pressure of about 10⁴ kg/cm² into disks 10 mm in diameter and 1.5 mm thick. Silver electrodes were deposited on the surface of the samples to conduct dielectric measurements. An electron micrograph of the surface of a composite sample without electrodes is shown in Fig. 1.



Fig. 1. Electron micrograph for surface of (DIPAC)_{0.90}/(PbTiO₃)_{0.10} composite sample at a magnification of 2,000 times (dark matrix corresponds to diisopropylammonium chloride particles, light inclusions to lead titanate particles)

Analysis of dielectric properties of the $(DIPAC)_{1-x}/(PbTiO_3)_x$ composite samples was carried out using an E7-25 digital LCR meter with a frequency range of 25–10⁶ Hz and an operating voltage of 0.7 V. A TC-6621 thermometer with a chromel-alumel thermocouple was used to measure the temperature. The temperature was determined with an accuracy of 0.1 K. The studies were carried during successive heating-cooling cycles at a rate of 1 K/min in the temperature range from 290 to 450 K in computer-controlled automatic mode.

Experimental results and discussion

The results of studies on the dielectric properties of polycrystalline DIPAC samples and $(DIPAC)_{1-x}/(PbTiO_3)_x$ composites at x = 0.10, 0.20 and 0.25 are shown in Fig. 2. Analysis of the dependences for $\varepsilon'(T)$ indicates that an additional peak appears on the curves in the composite with x = 0.10 both upon heating and upon cooling; the peak is also observed for composites with a volume fraction of PbTiO_3 up to 0.30. If x > 0.30, the temperature peaks of the phase transition are smoothed out with a further increase in the volume fraction of inclusion particles in pure DIPAC upon heating (T_1) and upon cooling (T_2) . At the same time, the amplitudes of additional peaks on the temperature dependences of the dielectric constant upon heating (T_3) and upon cooling (T_4) increase with increasing volume fraction of lead titanate particles.

The temperature value of the main phase transition in composite samples with the volume fraction of inclusions up to 0.30 does not change significantly compared to the pure DIPAC sample (Fig. 3). The temperature of the additional peak in composite samples with x ranging from 0.10 to 0.30 is virtually independent of the fraction of inclusions, and decreases slightly (by about 5 K) for the sample with x = 0.40.

To explain the appearance of new phase transitions in the composite, let us consider a system of interacting particles. According to phenomenological theory, the



Fig. 2. Temperature dependences for dielectric constant of $(DIPAC)_{1-x}/(PbTiO_3)_x$ composite, recorded at a frequency of 10 kHz in a heating-cooling cycle; x = 0 (1), 0.10 (2), 0.20 (3), 0.25 (4)

Landau-Ginzburg expansion in terms of the degree of polarization, serving as the order parameter, is used to describe the phase transition in a homogeneous ferroelectric [10]. The free energy for composites that are a mixture of ferroelectric powders is the sum of the energy of the particles included in the composite and the energy of their interaction. In view of these considerations, the free energy can be written in the following form:

$$F = \sum_{i} \int_{V_{i}} \left(F_{0i} + \frac{1}{2} \alpha_{i} P_{i}^{2} + \frac{1}{4} \beta_{i} P_{i}^{4} + \dots \right) dv_{i} + \sum_{j} \int_{V_{j}} \left(F_{0j} + \frac{1}{2} \alpha_{j} P_{j}^{2} + \frac{1}{4} \beta_{j} P_{j}^{4} + \dots \right) dv_{i} + (1) + \Delta F_{ii}.$$

where P_i , P_j are the polarization values for particles of the first kind (for example, DIPAC) and particles of the second kind (for example, PbTiO₃), respectively; ΔF_{ij} is the interaction energy between particles, which is mainly electrical in nature in case of composites.

The strength of the electric field generated by a single-domain particle 1 μ m in diameter at a distance of 50 μ m from it in the direction of polarization can be estimated as approximately 5·10⁶ V/cm for lead titanate and 7·10⁵ V/cm for DIPAC. The energy of electrical interaction between dipole particles is the sum of the Keesom and Debye energies. The maximum interaction energy of two dipole particles can be written as

$$\Delta F_{ij} \approx \frac{1}{4\pi\varepsilon_o} \left[\frac{2p_1p_2}{R^3} + \frac{\varepsilon_1p_2^2}{\pi R^6} + \frac{\varepsilon_2p_1^2}{\pi R^6} \right], \quad (2)$$

where the first term is the Keesom energy (describing the interaction of particles with complete dipole moments), and the second and the third are the Debye energy (the interaction of dipole and non-dipole particles due to induced polarization); p_1 , p_2 are the dipole moments of particles.

The energy ΔF_{ij} for a system of dipole particles has the form

$$\Delta F_{ij} = \frac{1}{4\pi\varepsilon_o} \sum_{i,j} \left[\iint_{V_i V_j} \left(\frac{2(P_i P_j)}{R_{ij}^3} \right) dv_i dv_j + \\ + \iint_{V_i J} \left(\frac{\varepsilon_i P_j^2}{\pi R_{ij}^6} \right) dv_i dv_j + \\ + \iint_{V_i V_j} \left(\frac{\varepsilon_j P_i^2}{\pi R_{ij}^6} \right) dv_i dv_j \right],$$
(3)

where P_i and P_j refer to some average values of particle polarization; this is due to the scatter in the values of dipole moments of particles both in magnitude and in direction.

The phase transition temperatures of DIPAC particles in the composite are found from the condition of minimum free energy, taking into account the interaction:

$$\frac{dF_i}{dP_i} = \frac{d}{dP_i} \left[\sum_i \int_{V_i} \left(\frac{1}{2} \alpha_i P_i^2 + \frac{1}{4} \beta_i P_i^4 + \dots \right) dV_i + \Delta F_{ij} \right] = 0.$$
(4)

According to expressions (3) and (4), the interaction energy of particles and, consequently, the phase transition temperatures for DIPAC in the composite differ from the phase transition temperatures of homogeneous DIPAC. The temperature shift of the phase transition depends on several quantities:

concentration and size of inclusion particles, the values of spontaneous polarization of these particles,

the degree of their polarization,

+

the dielectric constant of these particles.

Analyzing the dependence of phase transition temperatures of the composite on the volume fraction of lead titanate (see Fig. 3), we can assume that the mixture contains two states of DIPAC particles:

the first is particles with no PbTiO₃ particles in their immediate vicinity; their phase transitions correspond to phase transitions in isotropic DIPAC (T_1 and T_2);

the second is the particles adjacent to dipole

PbTiO₃ particles; their phase transition temperatures are determined taking into account the interaction energy (T_3 and T_4), as follows from relations (3) and (4).

This is confirmed by the fact that the amplitudes of the curves $\varepsilon'(T)$ (Fig. 3) increase with increasing concentration of PbTiO₃ for particles of the second type, and the number of particles of the first kind is negligible with x > 0.30. The phase transition temperatures T_3 and T_4 are virtually independent of the concentration of lead titanate particles in the range of x values from 0.10 to 0.30, which may point to some anomalies in the thermodynamic potential of DIPAC at these temperatures, while a small change in the interaction energy leads to phase transitions.

Conclusion

We have carried out studies on the dielectric properties of polycrystalline DIPAC samples and $(\text{DIPAC})_{1-x}/(\text{PbTiO}_3)_x$ composites at x = 0.10, 0.20 and 0.25. Analysis of the obtained data indicates that an increase in the volume fraction x (PbTiO₃ content) from 0.10 to 0.30 produces additional phase transitions for composites based on diisopropylammonium chloride and lead titanate. The main transition peak was practically indistinguishable at x > 0.30. The appearance of an additional phase transition can be explained by the dipole-dipole interaction of the components of the composite.



Fig. 3. Positions of temperature peaks depending on volume fraction of inclusions in $(DIPAC)_{1-x}/(PbTiO_3)_x$ composite samples:

 T_1 , T_2 are the temperatures of the main peak during heating and cooling, respectively; T_3 , T_4 are the temperatures of the additional peak during heating and cooling, respectively

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THE AUTHORS

STUKOVA Elena V.

Amur State University 21 Ignatievskoe Ave., Blagoveshchensk, 675027, Russian Federation lenast@bk.ru

BARYSHNIKOV Sergey V.

Blagoveschensk State Pedagogical University 104 Lenina St., Blagoveshchensk, 675000, Russian Federation svbar2003@list.ru

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СВЕДЕНИЯ ОБ АВТОРАХ

СТУКОВА Елена Владимировна — доктор физико-математических наук, профессор, заведующая кафедрой физики Амурского государственного университета, г. Благовещенск, Российская Федерация.

675027, Российская Федерация, г. Благовещенск, Игнатьевское шоссе, 21 lenast@bk.ru

БАРЫШНИКОВ Сергей Васильевич — доктор физико-математических наук, профессор кафедры физического и математического образования Благовещенского государственного педагогического университета, г. Благовещенск, Российская Федерация.

675000, Российская Федерация, г. Благовещенск, ул. Ленина, 104 svbar2003@list.ru

SIMULATION OF PHYSICAL PROCESSES

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GENERALIZED CORRECTION TO EMBEDDED-ATOM POTENTIALS FOR SIMULATION OF EQUILIBRIUM AND NON-EQUILIBRIUM PROPERTIES OF METALS

A.V. Verkhovtsev¹, A.V. Korol¹, G.B. Sushko¹, S. Schramm², A.V. Solov'yov¹

¹ MBN Research Center at Frankfurt Innovation Center of Biotechnology, Frankfurt am Main, Germany;

² Goethe University Frankfurt, Frankfurt am Main, Germany

A modification of an embedded-atom method (EAM)-type potential is proposed for a quantitative description of equilibrium and non-equilibrium properties of metal systems within the molecular dynamics framework. The modification generalizes the previously developed linear correction to EAM-type potentials and asymptotically approaches zero at large interatomic distances. A general procedure for constructing this modification is outlined and its relation to the linear correction is elaborated. To benchmark this procedure, we examine the melting phase transition and several equilibrium properties of finite-size nanosystems made of silver, gold and titanium. The simulations performed with the modified potential predict higher bulk melting temperatures of the metals and agree better with experimental values as compared to the original EAM-type potential. Our results show that the modification works well for metals with both cubic and hexagonal lattice structures. The Gupta potential is chosen as an example but the modification proposed can also be applied to other potentials of the EAM type.

Keywords: molecular dynamics simulations, many-body potential, phase transitions, equilibrium properties, metal nanoparticles

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ОБОБЩЕННАЯ ПОПРАВКА К ПОТЕНЦИАЛАМ ПОГРУЖЕННОГО АТОМА ДЛЯ МОДЕЛИРОВАНИЯ РАВНОВЕСНЫХ И НЕРАВНОВЕСНЫХ СВОЙСТВ МЕТАЛЛОВ

А.В. Верховцев¹, А.В. Король¹, Г.Б. Сушко¹, Ш. Шрамм², А.В. Соловьёв¹

¹ Научно-исследовательский центр мезобионаносистем, г. Франкфурт-на-Майне, Германия;

² Университет им. Гёте, г. Франкфурт-на-Майне, Германия;

Предложена модификация потенциалов погруженного атома (EAM) для описания равновесных и неравновесных свойств металлических систем в рамках классической молекулярной динамики. Данная модификация обобщает разработанную ранее авторами линейную поправку к потенциалам типа EAM и асимптотически убывает на больших межатомных расстояниях. Описана процедура построения модифицированных

потенциалов и показана связъданной модификации с линейной поправкой. Предложенная модификация использована для моделирования процесса плавления и изучения ряда равновесных свойств наносистем из серебра, золота и титана. Результаты расчетов, проведенных при помощи модифицированного потенциала, предсказывают более высокие температуры плавления металлов, по сравнению с изначальным потенциалом типа EAM, что лучше согласуется с экспериментальными данными. Многочастичный потенциал типа Гупта рассмотрен в качестве примера, но предложенная модификация может также применяться и к другим потенциалам типа EAM.

Ключевые слова: метод молекулярной динамики, многочастичный потенциал, фазовый переход, металлическая наночастица

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Introduction

Computer simulations based on atomistic models have emerged as a powerful tool for the analysis of physicochemical processes occurring in materials and related materials properties [1]. A vast number of atomistic simulations employ molecular dynamics (MD) methods that require the evaluation of total potential energy of manyatom systems and the forces acting on constituent atoms [2, 3]. MD simulations provide insights into many physical processes, such as diffusion [4–6], plastic deformation [7, 8], melting [9– 11], crystallization [10, 12] and other phase transformations [13, 14]. All of these processes happen on temporal and spatial scales exceeding by far those accessible by ab initio methods. In order to reach these scales, semi-empirical interatomic potentials parameterized for specific material compositions and structures are used [3, 15–17]. A potential constructed by fitting to a specific set of properties should perform well for other properties that were not explicitly considered during its construction phase [18].

Different interatomic potentials [19-24] belonging to a general class of embedded-atom method (EAM)-type potentials are commonly used in MD simulations of metal systems [25]. In the past decades, more complex potentials, based on the modified EAM (MEAM) or the second-neighbor (2NN) MEAM, have also been developed for different metals and alloys (see, e.g., a few recent examples [26, 27]). Parameters of these potentials are usually fitted to reproduce experimental data on the properties of bulk materials (e.g., cohesive energy, equilibrium constants, bulk modulus, lattice elastic constants, vacancy-formation energy, etc.) or fitted to zero-temperature ab initio calculations of perfect crystalline structures.

It has also been widely discussed that EAMtype potentials are less accurate in describing the dynamics of systems being far from equilibrium, for instance, the melting phase transition. In particular, these potentials often struggle to reproduce the experimental values of melting temperature for bulk metals and yield the discrepancy up to several hundred degrees [5, 28-30]. This indicates the necessity to modify the exploited force fields in order to enable a more accurate description of systems' properties at elevated temperatures. An accurate description of both equilibrium and non-equilibrium properties of metal systems is important, e.g., for studying irradiationdriven phase and structural transformations of nanostructures [31, 32] or irradiation-induced chemistry underlying novel nanofabrication techniques [33, 34].

Different approaches to account for finitetemperature effects in classical force fields for metal systems have been discussed in literature. A method for re-parameterization of interaction potentials was proposed [35] to adjust the calculated melting temperature of materials without affecting mechanical properties to which the potentials were fitted. In that method, the melting temperature was calculated using a trial interatomic potential and the Gibbs–Duhem equation (which relates changes in the chemical potential of a system to changes in its temperature and pressure) was then solved to update the parameters of potentials. This method was applied [35] to re-parameterize an EAM-type potential for Al and improved the calculated bulk melting temperature without considerable change in other properties. A correction to a manybody force field for titanium proposed in Ref.

[36] included the contribution of thermal excitations of electronic degrees of freedom. In that approach, an EAM-type potential was augmented by an additional term (related to electronic entropy) that arises from the Sommerfeld theory of metals. According to that theory, there is a temperature-dependent contribution to the free energy of a metal system that depends also on the density of states at the Fermi energy. In Ref. [37], several parameterizations of EAM-type potentials for Ti describing defects, plasticity and melting were presented. These potentials fit well to either low- or high-temperature experimental data but could not describe both temperature regions simultaneously. On this basis, a temperature-dependent potential, being а combination of potentials operating better in different regions, was suggested to study the properties of Ti in a wide temperature range. The knowledge accumulated in these studies suggests that modifications of conventional EAM-type potentials are required in order to match the calculated non-equilibrium properties (the melting temperature in particular) of metal materials to experimental values.

In our previous work [38], we presented a modification of an EAM-type potential (considering a many-body Gupta potential [39] as an example). With that modification, both the melting temperature and the nearequilibrium properties of selected metal systems were reproduced. It was revealed that augmenting steepness of the interaction potential by enhancing its repulsive part leads to an increase of the melting temperature. This happens because a higher thermal energy is needed to reach the threshold of atomic vibration amplitudes at which the melting occurs. To that end, the original EAM-type potential was augmented by adding a linear term to the repulsive part [38]. The linear correction represented a minor change to the potential energy but led to a significant increase of the melting temperature. It was applied to study thermal, geometrical and energetic properties of magnesium, titanium, platinum and gold, yielding a good agreement with experimental results. In Ref. [40], this method was used to evaluate melting points of finite-size NiTi nanoalloys with different composition of Ni and Ti. These results were used to evaluate bulk melting temperatures of $Ni_{1-x}Ti_x$ alloys, which agreed with an experimental phase diagram for the NiTi material.

In this paper, the previously developed methodology is generalized in the form of a new modification of an EAM-type potential. This modification represents a linear function multiplied by a sigmoid function, which gradually tends to zero beyond a given distance. A general procedure for constructing this modification is outlined and its parameters are related to the parameters of the linear correction [38]. The modified EAM-type potential is used for MD simulations of melting of nanometer-sized nanoparticles made of silver, gold and titanium. Structural and energetic equilibrium properties of these systems, such as lattice constants, cohesive energy and vacancy formation energy are also analyzed. Our results demonstrate that the new modification is applicable for metals with both cubic and hexagonal crystalline lattices. To be consistent with our previous works [38, 40] the Gupta potential is considered as an example but we stress that the modification proposed can also be applied to other interatomic potentials of the EAM type, e.g., to Sutton-Chen [20] or Finnis–Sinclair [41] potentials.

EAM-type Gupta potential

Similar to other many-body potentials of the EAM type the Gupta potential is constructed as a sum of (i) a short-range repulsive term that stems from the repulsion between atomic cores and (ii) a long-range attractive term which imitates delocalization of the outer-shell electrons and is related to electron density at a given atomic site. The total energy of an N-atom system interacting via an EAM-type potential reads as

$$U = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i} V(r_{ij}) + \sum_{i=1}^{N} F_i(\rho_i), \qquad (1)$$

Where $V(r_{ij})$ is the short-range repulsive interaction between atoms *i* and *j* separated by the distance r_{ij} ; the attractive term F_i stands for the energy obtained by embedding atom *i* into the local electron density ρ_i provided by the remaining atoms of the system.

The functional form of $F_i(\rho_i)$ may vary in different EAM-type potentials [25] while the Gupta potential employs a specific form of this function,

$$F_i(\rho_i) \propto -\sqrt{\rho_i}$$
.

This functional form is based upon the second-moment approximation of the tightbinding model [42, 43], according to which the attractive many-body term is related to the energy of *d* valence electron band and expressed as a square root of ρ_i . The latter is constructed empirically as a linear superposition of electron charge densities of constituent atoms,

$$\rho_i = \sum_{j \neq i} \psi(r_{ij}).$$

Within the Gupta representation, the functions $V(r_{ij})$ and $\psi(r_{ij})$ are introduced in exponential forms so that the total potential energy U_{Gup} reads as follows:

$$U_{\text{Gup}} = \sum_{i=1}^{N} \left[\frac{1}{2} \sum_{j \neq i} A e^{-p \left(\frac{r_{ij}}{d} - 1\right)} - \sqrt{\sum_{j \neq i} \xi^{2} e^{-2q \left(\frac{r_{ij}}{d} - 1\right)}} \right],$$
(2)

where *d* is the first-neighbor distance; *p*, *q* are related to bulk elastic constants; ξ represents an effective orbital-overlap integral; *A* adjusts the cohesive energy.

The parameters for silver, gold and titanium used in this work were taken from Ref. [22].

Linear correction to EAM-type potentials

The EAM-type Gupta potential (2) corrected with the linear term U_{lin} introduced in Ref. [38] reads

$$U = U_{\text{Gup}} + U_{\text{lin}} \equiv$$
$$\equiv U_{\text{Gup}} + \frac{1}{2} \sum_{i,j=1}^{N} (Br_{ij} + C), \qquad (3)$$

where *B* and *C* are parameters.

The linear form was chosen to match the curvature of the modified potential energy profile in the vicinity of the equilibrium point (governed by the second derivative of potential energy U) to that of the original EAM-type potential.

As discussed in Ref. [38], the term Br_{ij} (B > 0) makes the potential energy profile steeper at interatomic distances exceeding the equilibrium point r_0 whilst also slightly changing the depth of the potential well at r_0 . The constant term C < 0 was therefore added to mitigate the latter effect. In Ref. [38], parameters B and C were obtained empirically for a specific cutoff distance r_c for titanium, gold, platinum and magnesium. As shown below, these parameters can be derived for any material and any r_c using the following analytical estimate.

The correction to an EAM-type potential should not change the cohesive energy of a bulk material to which the potential was fitted. Therefore, the change in the total potential energy due to a linear correction should be equal to zero. If we approximate the real crystalline structure of a metal with a uniform distribution of atoms with number density n_0 , this condition can be written as

$$\int_{r < r_c} n_0 \left(Br_{ij} + C \right) dV = 0,$$
 (4)

leading to the relation

$$C = -\frac{3}{4}Br_c.$$
 (5)

Fig. 1 shows (lines) the calculated dependence
$$C(B)$$
 for gold and titanium for different values of r_c . These parameters of the linear correction leave intact the cohesive energy of bulk metal systems. Bulk gold and



Fig. 1. C(B) dependence for Au (a) and Ti (b) for different cutoff values of r_c ; lines show the results obtained using Eq. (5); symbols show the results of structure optimization calculations which account for the realistic crystal structures (see the 'Results and discussion' section)



Fig. 2. The calculated radial distribution functions (RDFs) for 10-nm Au (a) and Ti (b) nanoparticles (composed of approximately 30,000 atoms). The cutoff values of r_c used are shown by dashed lines

silver have fcc crystal lattices and very similar lattice constants, so the results shown for gold also describe silver crystals. For each metal we consider three cutoff distances between 6 and 8 Å, corresponding to minima in the radial distribution function (see the vertical lines in Fig. 2). The indicated values of r were chosen following Ref. [22]. In that work, the parameters of the Gupta potential for the fcc metals were derived accounting for interatomic interactions up to the fifth-neighbor shell, while the suggested cutoff values for titanium and other hcp structures corresponded to inclusion of seven to eight shells of neighboring atoms.

The linear correction causes a small displacement Δr of atoms from their equilibrium positions defined by the original EAM-type potential. Expanding U in a Taylor series about the equilibrium atomic positions for the original potential and keeping only the first term of this expansion one evaluates a change in potential energy associated with Δr as

$$\Delta U = -F_{lin}\Delta r =$$

$$= -\frac{2\pi}{3} \left(\frac{4}{3}\right)^3 \frac{C^3}{B^2} n_0 \Delta r.$$
(6)

As it was demonstrated in our earlier work [38], augmenting steepness of the interatomic potential beyond the equilibrium point by enhancing the repulsive contribution of the force field leads to a rise of the melting point. It happens because an increased thermal energy is needed to reach the threshold of atomic vibration amplitudes at which the melting phase transition occurs. Knowing the experimental bulk melting temperature T_m^{exp} and the value predicted by the original Gupta potential, T_m^{Gup} ,

parameters *B* and *C* can be chosen such that an increase in the melting temperature will be equal to $\Delta T = T_m^{exp} - T_m^{Gup}$.

Eqs. (5) and (6) define, for any r_c , a combination of parameters *B*, *C* that reproduce experimental values of cohesive energy and melting temperature of bulk materials. These conditions were used to define *B* and *C* for the three metals studied.

Generalized modification of EAM-type potentials

In this section, we generalize the above described methodology and propose a new modification of an EAM-type potential. The modification should keep features of the linear correction, i.e., maintain its behavior in the vicinity of atomic equilibrium points and enhance the repulsive interactions with an increase of atomic displacements. We construct the modification in such a way that it contains a parameter describing the characteristic range of the potential thus eliminating the dependence of the potential on the choice of the cutoff distance. These conditions are fulfilled by multiplying U_{lin} by a sigmoid function which is equal to unity at small interatomic distances and asymptotically approaches zero beyond a given distance. The modified EAM-type Gupta potential then reads as

$$U = U_{Gup} + U_{mod} \equiv$$
$$\equiv U_{Gup} + \frac{1}{2} \sum_{i,j=1}^{N} \frac{\tilde{B}r_{ij} + \tilde{C}}{1 + e^{\lambda(r_{ij} - r_s)}}.$$
(7)

The parameters \tilde{B} and \tilde{C} have the same meaning as B and C in Eq. (3): \tilde{B} defines an additional force acting on the nearest atoms



Fig. 3. Plots of $U_{mod}(r)$ (7) for different values of the parameters (solid lines) and U_{lin} (a dashed gray line) vs. the interatomic distance r, and also the piecewise linear approximation $\overline{U}_{mod}(r)$ (8) (dotted curves, see the Appendix for details). The used procedure of deriving the parameter values is given in the text

and \tilde{C} adjusts the depth of the potential well in the vicinity of the equilibrium point where U = 0. The parameter λ describes the slope of U_{mod} at large interatomic distances, while r_s defines the sigmoid's midpoint and hence the range of this potential. Fig. 3 shows the potential U_{mod} for a pair of atoms as a function of interatomic distance r. Due to its sigmoidtype shape, $U_{mod}(r)$ asymptotically approaches zero and its range serves as a natural cutoff distance for this interaction.

For each pair of atoms, the potential U_{lin} grows monotonically with interatomic distance up to the cutoff r_c , and all atoms located within the sphere of radius r_c experience the same force exerted by a given atom. On the contrary, U_{mod} has a maximum at interatomic distances of about 5-8 Å depending on the choice of λ and r_{s} (see Fig. 3). Thus, the force exerted by an atom due to U_{mod} enhances interaction with several nearest atomic shells while the interaction with more distant atoms weakens. The strength of this interaction is governed by the steepness of the potential beyond its maximum, i.e., by the parameter λ . Therefore, the force acting on the nearest neighbors due to U_{mod} should exceed (by the absolute value) the force F_{lin} as its effect is compensated by weaker interactions with more distant atoms. Thus, for each pair of atoms interacting via $U_{mod}(r)$, the initial slope of the potential should be steeper than the slope of $U_{lin}(\mathbf{r})$, i.e., $\tilde{B} > B$.

To analytically derive parameters of the new modification, $U_{lin}(r)$ in Eqs. (4) and (6) was substituted with $\overline{U}_{mod}(r)$, a piecewise linear approximation of the sigmoid-type function $U_{mod}(r)$, see Eq. (8) in Appendix. Then, parameters of this function were expressed through the parameters *B* and *C* of the linear correction. As a last step of this procedure, $\overline{U}_{mod}(r)$ was fitted with $U_{mod}(r)$ to derive λ and r_s . Further technical details are given in the Appendix. The parameters of U_{mod} used for an analysis of melting temperature and near-equilibrium properties of silver, gold and titanium nanosystems are summarized in Table 1. Details of this analysis are presented below in the 'Results and Discussion' section.

The modification U_{mod} (7) is qualitatively similar to the well-known Dzugutov potential [45] which was developed to model glassforming liquid metals. The Dzugutov potential coincides with the Lennard-Jones potential at small interatomic distances but has a maximum beyond the equilibrium point. This enables the suppression of crystallization and enforces the emergence of icosahedral structures. The maximum of U_{mod} corresponds to the positions of more distant atoms (see Fig. 3 and the RDFs in Fig. 2). As a result, the modification U_{mod} does not affect crystal structure but leads to an increase in the melting temperature whilst slightly changing the near-equilibrium properties of metals.

Computational details

All simulations described in this work were conducted using the MBN Explorer software package [46]. We considered spherical nanoparticles with radii from 1 to 5 nm (ranging from 250 to 30,000 atoms) that were cut from ideal silver, gold and titanium crystals. The systems were constructed using the MBN Studio software [47].

Prior to the analysis of the structural and energetic parameters of each system, energy minimization calculations were performed using the velocity-quenching algorithm. The MD simulations of the melting process were performed using a large simulation box of $20 \times 20 \times 20$ nm in the NVT canonical ensemble. The temperature T was controlled by a Langevin thermostat with a damping time of 1 ps. The nanoparticles were heated up (starting from the initial temperature T_0 well below the expected melting temperatures, T_0 = 300 K for Ag and Au and 1000 K for Ti) with $\ddot{}$ a constant heat rate of 0.5 K/ps, which is within the range of typical values used for MD simulations of phase transitions. The total simulation time for each run was 3 ns. The time integration of the equations of motion was done using the velocity-Verlet algorithm [2] with an integration time step of 1 fs. In the calculations performed with the linear correction U_{lin} , the interatomic interactions were truncated at the cutoff radius r_c ranging from about 6 to 8 Å as shown in Fig. 2. In the case of the potential augmented with $U_{\rm mod}$, its range served as a natural cutoff distance, which varied between 8 and 9 Å.

The melting temperatures of nanoparticles were determined from the analysis of heat capacity

$$C_V = \left(\partial E / \partial T \right)_V$$

defined as a partial derivative of the internal energy of the system with respect to temperature at a given volume. A sharp maximum of C_{ν} was attributed to the nanoparticle melting and the position of the maximum was referred to as the nanoparticle's melting point. The bulk melting temperature T_{m}^{bulk} was estimated by extrapolating the obtained values to the $N \rightarrow \infty$ limit according to the Pawlow law [48, 49]

$$T_m^{bulk} = T_m + \gamma N^{-1/3}$$

with γ being the factor of proportionality.

Results and discussion

Fig. 1 shows the dependence C(B) that describes the parameters of the linear correction U_{lin} at different values of cutoff r_c . Dashed lines were obtained by means of Eq. (5) within the uniform density model (see the section 'Linear correction to EAM-type potentials'), while symbols show the results of structure optimization of gold and titanium systems with realistic crystal structures. In the case of structure optimization, the parameters B and C were chosen to match experimental cohesive energies [50]. The outcomes of the uniform density model are in good agreement with the results of optimization calculations. Table 2 summarizes the bulk cohesive energy for silver, gold and titanium, calculated with the linear correction as well as the experimental values and the results obtained by means of the original EAM-type Gupta potential.

Fig. 4 shows the melting temperature of bulk silver, gold and titanium calculated using the linear correction U_{lin} to the Gupta potential, Eq. (3), at different values of the parameter *B* and the cutoff r_c . The parameter *C* was defined according to Eq. (5). Symbols denote the results of MD simulations of finitesized nanoparticles melting, extrapolated to the bulk limit. The figure shows that the calculated melting temperature increases linearly with *B*.

Table 1

Parameters of the potential U_{mod}

Element	$ ilde{B}$, eV/Å	\tilde{C} , eV	$\lambda, { m \AA}^{-1}$	<i>r</i> , Å
Ag	0.009	-0.048	5.93	7.10
Au	0.026	-0.145	4.68	7.36
Ti	0.052	- 0.269	2.77	6.68

Notation: \tilde{B} is an additional force acting on the nearest atoms; \tilde{C} adjusts the depth of the potential well in the vicinity of the equilibrium point where U = 0; λ describes the slope of U_{mod} at large interatomic distances; r_s defines the sigmoid's midpoint.

These results can be used to evaluate

$$\Delta T = \Delta T_m^{lin}(B) - \Delta T_m^{Gup}.$$

As follows from Eq. (6),

$$\Delta U = k \Delta T \propto \Delta r,$$

where Δr stands for an increase in the amplitude of thermal vibrations of atoms with respect to the values predicted by the original Gupta potential.

The slope of $\Delta T(B)$ is therefore proportional to the distance by which the atoms should be additionally displaced from equilibrium positions to initiate the melting process at the temperature corresponding to the experimental value. For silver and gold $\Delta r \approx 0.09$ Å, which is about 3% of their nearest-neighbor distances. For titanium we observed the dependence of Δr on the cutoff distance. For smaller cutoff values, $r_c = 6.2$ Å and 6.8 Å, an increase in the amplitude of thermal vibrations is equal to 0.06 Å and it increases up to 0.09 Å for $r_c = 8.1$ Å. These results suggest that an increase in the amplitude of thermal vibrations by a few percent leads to a dramatic rise of the melting point. A much steeper slope of $\Delta T(B)$ for Ti at $r_c = 8.1$ Å suggests that more distant atoms located in a concentric shell between 7 and 8 Å make a significant contribution to the melting process and the original Gupta potential cannot account properly for this contribution.

Tables 2–4 summarize the results on structural and energetic properties of silver, gold and titanium nanocrystals obtained with the sigmoid-type modification U_{mod} (7). These results are compared to those obtained by means of the original EAM-type Gupta potential (2) and the linear correction U_{lin} (3). As mentioned above, the calculated bulk

As mentioned above, the calculated bulk cohesive energies are summarized in Table 2. Neither linear correction nor sigmoid-type modification significantly change the values predicted by the original Gupta potential; all these values are in good agreement with experimental data [50] with a relative discrepancy of less than 0.5%.

Table 2

Comparison	of	the	calculated	bulk	cohesive	energy	values
		wi	ith experin	ienta	l data		

	Bulk cohesive energy, eV per atom					
Element	$U_{ m Gup}$	$U_{ m Gup}^{} + U_{lin}^{}$	$U_{\rm Gup}^{} + U_{\scriptscriptstyle mod}^{}$	Experiment [50]		
Ag	2.96	2.96	2.97	2.96		
Au	3.78	3.77	3.78	3.78		
Ti	4.87	4.87	4.83	4.85		

Notation: U_{Gup} is the original Gupta potential, Eq. (2); $(U_{\text{Gup}} + U_{\text{lin}})$ is the one corrected by U_{lin} , Eq. (3); $(U_{\text{Gup}} + U_{\text{mod}})$ is the one corrected by the sigmoid-type modification U_{mod} , Eq. (7), proposed in this work.



Fig. 4. The calculated dependences of the melting temperature of bulk silver (*a*), gold (*b*) and titanium (*c*) on the parameter *B* at the different cutoff r_c values (symbols) as well as the least-squares fit to these results (solid lines). Experimental values from Ref. [50] are shown by dashed lines. The calculation procedure is given in the text. B = 0 corresponds to the original Gupta potential, Eq. (2)

Table 3 presents the vacancy-formation energy that is the amount of cohesive energy required to form a vacancy in a crystal. It is defined [62, 63] as

$$E_{vf} \equiv (N-1) \left(E_{N-1}^{coh} - E_N^{coh} \right) = \\ = E_{N-1} - \frac{N-1}{N} E_N,$$

where

$$E_N = N E_N^{con},$$
$$E_{N-1} = (N-1) E_{N-1}^{coh}$$

are the potential energies of systems containing N and (N-1) atoms, whereas E_{N}^{coh} and E_{N-1}^{coh} are the corresponding cohesive energies per atom. The calculated values (columns labeled as U_{Gup} ', $U_{Gup} + U_{lin}$ ' and $U_{Gup} + U_{mod}$ ') are compared with available experimental data and the results of DFT calculations and MD simulations employing different EAM-type potentials.

The values calculated with the original Gupta potential are consistent with some experimental and theoretical values reported in literature [22, 23, 52, 55, 57], whereas other works predicted either smaller or much larger values of E_{yf} . Note that the theoretical results reported in literature were obtained with

different EAM-type potentials (Finnis–Sinclair and Gupta potentials as well as a distinct potential introduced in Ref. [54]) as well as with different EAM and modified EAM (MEAM) potentials. The variety of potentials and parameterizations used has resulted in a large (up to 40 %) discrepancy between the calculated values of E_{vt} .

Calculations performed with the Gupta potential corrected by U_{lin} (see the column ' U_{Gup} + U_{lin} ') yield smaller values of E_{vf} as compared to the original Gupta potential, and the magnitude of the decrease depends on the parameter B. The values of E_{yf} listed in Table 3 were obtained for each metal using the B values that reproduce the experimental bulk melting temperatures (see Fig. 4). The figure shows that for $r_c \approx 8$ Å, Å the value of B for silver, 0.0016 eV/Å, is three times smaller than that for gold, 0.005 eV/Å, and five times smaller than for titanium, 0.008 eV/Å. As a result, the vacancy-formation energy for silver calculated by means of the linear correction is slightly (by about 5 %) smaller than the value predicted by the original Gupta potential. For gold and especially titanium, larger values of B should be used to reproduce the experimental bulk melting temperatures, which leads to a more pronounced decrease of $E_{\rm v}$. The magnitude of this discrepancy for titanium is within

Table 3

	Vacancy formation energy $E_{\rm vf}$, eV						
Element	I	$II \rightarrow II$		Experiment	Calculation		
	$O_{\rm Gup}$	$U_{\text{Gup}} + U_{\text{lin}}$	$U_{\text{Gup}} + U_{mod}$	Experiment	EAM-type	DFT	
Ag	0.94	0.90	0.91	0.99±0.06[52] 1.09±0.10 [53]	0.79[19] (Gupta) 0.88[22] (Gupta) 0.97 [23] (EAM) 1.10 [54]	_	
Au	0.72	0.58	0.81	0.62–0.67 [55] 0.70–1.10 [55]	0.60[19] (Gupta) 0.75[22] (Gupta) 1.03 [23] (EAM) 1.10 [54]	_	
Ti	1.49	1.22	1.44	1.55 [56]	1.43 [21] (FS) 1.49 [57] (EAM) 1.56[58] (Gupta) 1.78[59](MEAM) 1.79[28](MEAM)	1.97 [60] 2.14 [61]	

Comparison of the vacancy formation energy E_{vf} obtained in this paper with the published experimental and calculated data

Notation: U_{Gup} corresponds to the E_{vf} value calculated with the original EAM-type Gupta potential; $(U_{\text{Gup}}+U_{lin})$, $(U_{\text{Gup}}+U_{mod})$ correspond to the E_{vf} values done using the potential corrected by U_{lin} and the new modification U_{mod} ; EAM, MEAM – embedded-atom method and modified EAM [51]; DFT is the density functional theory; FS is the Finnis–Sinclair potential [41].

the uncertainty range of the existing theoretical data obtained by means of different EAM-type potentials (see Table 3). In MD simulations reported in literature [21, 28, 57–59] E_{vf} varies from about 1.4 to 1.8 eV while DFT calculations [60, 61] predicted even larger values up to 2.1 eV.

The sigmoid-type modification U_{mod} gives the results which are closer to the experimental values and the results of other MD simulations [21–23, 57] compared to the original Gupta potential and linear correction. This is due to the change in the asymptotic behavior of the original Gupta potential, i.e., the weakening of interatomic interactions at large distances.

Table 4 presents the equilibrium lattice constants for silver, gold and titanium calculated with U_{Gup} , $U_{\text{Gup}} + U_{\text{lin}}$ and $U_{\text{Gup}} + U_{\text{mod}}$. The force created by the linear correction causes a uniform strain on crystals, which become uniformly compressed. For silver and gold this effect is rather small (the relative change in the lattice parameters is less than 1 %) while the relative shortening of titanium crystals is about 2.5 %. This can also be attributed to a very steep linear correction (i.e., a large force) that should be used to reproduce the experimental bulk melting temperature of Ti. Note also that the geometry optimization of a Ti crystal using the original Gupta potential yields the structure which is elongated along the [0001] axis as compared to the experimental value (the calculated lattice parameter c = 4.75 Å vs. the experimental value of 4.68 Å). The geometry optimization by means of the linear correction results in a uniform compression of the crystal, which brings the parameter c in a better agreement with the experimental value.

The sigmoid-type modification U_{mod} has a small impact on the equilibrium lattice parameters, which almost coincide with those predicted by the original Gupta potential and agree reasonably well with the experimental results. Contrary to the linear correction, U_{mod} does not

Table 4

Element	Equilibrium lattice constant, Å					
Element	$U_{ m Gup}$	$U_{ m Gup} + U_{lin}$	$U_{_{ m Gup}} + U_{_{mod}}$	Experiment [50]		
Ag	4.07	4.05	4.07	4.09		
Au	4.06	4.03	4.09	4.08		
Ti (<i>a</i>)	2.91	2.83	2.89	2.95		
Ti (c)	4.75	4.63	4.77	4.68		

Comparison of the calculated equilibrium lattice constants with experimental data

Footnote. The presented results were calculated with the original Gupta potential (U_{Gup}) , as well as with the Gupta potential corrected by U_{lin} and the new modification U_{mad} . Two lattice parameters, a and c, are listed for titanium.



Fig. 5. Melting temperature of Ag (*a*), Au (*b*) and Ti (*c*) nanoparticles of diameter *D* calculated by 3 ways: using the original EAM-type Gupta potential (Eq. (2)), its linear correction U_{lin} (Eq. (3)) and the new modification U_{mod} (Eq. (7)); 3 values of r_c were considered (symbols). The extrapolation of the calculated numbers to the bulk limit was made (lines). Experimental values of bulk melting temperature are shown by stars

induce a strong compression of the Ti crystal and its lattice parameters obtained by means of U_{mod} are similar to those calculated with U_{Gup} . As discussed above, this is due to the functional form of U_{mod} wherein a positive contribution of U'_{mod} plays the role at small interatomic distances (which span over a few nearest atomic layers) while a negative contribution of U'_{mod} plays the role at larger values of *r*.

Fig. 5 shows the melting temperatures of finite-sized Ag, Au and Ti nanoparticles as functions of their inverse diameter D. For all these metals, the bulk melting temperature predicted by the original Gupta potential is significantly lower than the experimental values. The most illustrative example is titanium (see Fig. 5, c) whose melting temperature calculated with U_{Gup} is approximately 1380 K. It is more than 500 K lower than the experimental value of 1941 K (marked by a star symbol) which yields the relative discrepancy of about 30 %. A similar feature has been observed for gold and silver - the absolute discrepancy is smaller for these metals (about 330 and 100 K, respectively) while the relative discrepancy for gold is as large as 25 %. These results further justify the necessity of correcting the EAM-type potential to bring the calculated bulk melting temperatures in closer agreement with the experimental values. The modification U_{mod} produces a similar effect as the linear correction - it leads to an increase of nanoparticles' melting temperatures and, as a result, to an increase in bulk melting temperatures. The new modification improves the calculated bulk melting temperature for the three metals considered. Good agreement with the experimental values has been obtained for titanium and silver (the relative discrepancies from the experimental values are 0.8 and 1.5 %, respectively) while a somewhat larger discrepancy of about 6 % has been observed for gold. This is linked to the observation that the sigmoid-type modification increases the slope of the $T_{\rm m}(1/D)$ dependence for silver and titanium nanoparticles but it almost does not change the slope for gold nanoparticles. The utilized parameters of U_{mod} for gold have been chosen such that all the quantities considered in this work agree better with experimental data as compared to the original Gupta potential. An even better agreement might be achieved by performing a more detailed analysis of the multi-dimensional parameter surface of U_{mad} . A finer tuning of parameters should bring the calculated T_m^{uulk} for gold to a better agreement with experimental data.

Summary

We formulated a recipe for modification of classical embedded-atom method (EAM)-type potentials aiming at a quantitative description of both equilibrium and non-equilibrium properties of metal systems by means of molecular dynamics simulations. The modification suggested in this work asymptotically approaches zero at large interatomic distances and generalizes the previously developed linear correction [38]. A general procedure for constructing the modified EAM-type potential was outlined and the relation between parameters of the new modification and the linear correction was elaborated.

The procedure developed has been applied to analyze the melting temperature as well as lattice constants, cohesive energy and vacancy formation energy of nanosystems made of silver, gold and titanium. It was demonstrated that the modified potential leads to an increase in the melting temperature of the metals and to a better agreement with experimental values as compared to the uncorrected EAM-type potential. The new modification induces a small (on the order of a few per cent or less) change of the equilibrium properties but increases the bulk melting temperature by more than 30% as it is demonstrated for the case of titanium. We have considered the many-body Gupta potential as an example but the generality of the correction allows its application in combination with other potentials of the EAM type such as Sutton-Chen or Finnis-Sinclair potentials. The results presented for the metals with cubic and hexagonal crystalline lattices further confirm a wide range of applicability of the proposed modification.

Appendix

Derivation of parameters of U_{mad}

To analytically derive the parameters of the sigmoid-type potential $U_{mod}(r)$, the latter was approximated by a piecewise linear function:

$$\overline{U}_{\text{mod}}(r) = \begin{cases} B_1 r + C_1, & r < R_0 \\ B_2 r + C_2, & R_0 < r < R_2, \\ 0, & r > R_2 \end{cases}$$
(8)

where $B_1 > 0$ ($C_1 < 0$) and $B_2 < 0$ ($C_2 > 0$),

$$R_0 = -\frac{C_1 - C_2}{B_1 - B_2}$$

is the point of intersection of the two linear segments, and $R_2 = -C_2/B_2$ is the point where $\overline{U}_{mod}(r) = 0$ (see dotted curves in Fig. 3). After

substituting Eq. (8) into Eq. (4) and carrying out the integration one arrives at the condition:

$$\frac{(1-\gamma)^{4}}{(1-\beta)^{3}} = -\frac{\gamma^{4}}{\beta^{3}},$$
(9)

where $\beta = B_2/B_1$ and $\gamma = C_2/C_1$. Substituting Eq. (8) in Eq. (6) one derives the force F_{mod} due to the potential $\overline{U}_{mod}(r)$. This force should be equal to the force F_{lin} arising due to the linear correction at a given cutoff in order to increase the melting temperature by the same value. This can be expressed as

$$\left(\frac{4}{3}\right)^{3} \frac{C^{3}}{B^{2}} = \frac{C_{1}^{3}}{B_{1}^{2}} \left[\frac{\left(1-\gamma\right)^{3}}{\left(1-\beta\right)^{2}} + \frac{\gamma^{3}}{\beta^{2}}\right].$$
 (10)

The procedure for deriving the parameters of the sigmoid-type function U_{mad} (7) and its approximation \overline{U}_{mod} (8) can be summarized as follows:

(i) The parameters B and C of the linear correction are obtained as described in the section 'Linear correction to EAM-type potentials';

(*ii*) Fixing the point $R_1 = -C_1/B_1$ at which $U_{mod}(r) = 0$ (see Fig. 3), a scan over different values of B_1 and C_1 is performed;

(*iii*) β and γ are derived from the numerical solution of Eqs. (9) and (10), and the corresponding values of B_2 and C_2 are obtained;

(*iv*) Repeating steps (i)-(iii) for different combinations (B_1, C_1) one obtains a multidimensional parameter surface (B_1, C_1, B_2, C_2) ;

(v) Once $B_{1,2}$, $C_{1,2}$ are derived, the resulting piecewise function is fitted with the sigmoid-type function U_{mod} , Eq. (7), to obtain the parameters λ and $r_{.}$

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THE AUTHORS

VERKHOVTSEV Alexey V.

MBN Research Center at Frankfurt Innovation Center of Biotechnology 3 Altenhöferallee, Frankfurt am Main, 60438, Germany verkhovtsev@mbnexplorer.com

KOROL Andrei V.

MBN Research Center at Frankfurt Innovation Center of Biotechnology 3 Altenhöferallee, Frankfurt am Main, 60438, Germany korol@mbnexplorer.com

SUSHKO Gennady B.

MBN Research Center at Frankfurt Innovation Center of Biotechnology 3 Altenhöferallee, Frankfurt am Main, 60438, Germany sushko@mbnexplorer.com

SCHRAMM Stefan

Goethe University Frankfurt 1 Max-von-Laue St., Frankfurt am Main, 60438, Germany

SOLOV'YOV Andrey V.

MBN Research Center at Frankfurt Innovation Center of Biotechnology 3 Altenhöferallee, Frankfurt am Main, 60438, Germany solovyov@mbnresearch.com

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СВЕДЕНИЯ ОБ АВТОРАХ

Верховцев Алексей Валерьевич — *Ph.D.*, научный сотрудник Научно-исследовательского центра мезобионаносистем (MBN), г. Франкфурт-на-Майне, Германия.

60438, Германия, г. Франкфурт-на-Майне, Альтенхёфераллее, 3 verkhovtsev@mbnexplorer.com

КОРОЛЬ Андрей Владимирович — кандидат физико-математических наук, доцент, научный сотрудник Научно-исследовательского центра мезобионаносистем (MBN), г. Франкфурт-на-Майне, Германия.

60438, Германия, г. Франкфурт-на-Майне, Альтенхёфераллее, 3 korol@mbnexplorer.com

Сушко Геннадий Борисович — Ph.D., научный сотрудник Научно-исследовательского центра мезобионаносистем (MBN), г. Франкфурт-на-Майне, Германия.

60438, Германия, Франкфурт-на-Майне, Альтенхёфераллее, 3 sushko@mbnexplorer.com

ШРАММ Штефан – *Ph.D.*, профессор Центра научных вычислений Франкфуртского университета им. Гёте.

60438, Германия, Франкфурт-на-Майне, Макс-фон-Лауэ штрассе, 1

СОЛОВЬЁВ Андрей Владимирович — доктор физико-математических наук, профессор, ведущий научный сотрудник Научно-исследовательского центра мезобионаносистем (MBN), г. Франкфурт-на-Майне, Германия.

60438, Германия, г. Франкфурт-на-Майне, Альтенхёфераллее, 3 solovyov@mbnresearch.com
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THE DIFFUSION PROBLEM IN A RECTANGULAR CONTAINER WITH AN INTERNAL SOURCE: EXACT SOLUTIONS OBTAINED BY THE FAST EXPANSION METHOD

A.D. Chernyshov¹, D.S. Sajko¹, V.V. Goryainov², S.F. Kuznetsov¹, O.Yu. Nikiforova¹

¹ Voronezh State University of Engineering Technology, Voronezh, Russian Federation;

² Voronezh State Technical University, Voronezh, Russian Federation

The diffusion problem in a rectangular-shaped body with the Derichlet's boundary conditions and an internal substance source depending on the rectangle points' coordinates has been solved generally by the fast expansion method (FEM). The exact solution containing free parameters was obtained, and by changing them one could get many new exact solutions. Exact solutions to the problem with a constant internal source were shown as an example. From our analysis of the exact solutions it follows that the concentration and diffusion fluxes distributions should be symmetrical relative to the plane y = b/2, provided that the substance concentration in the corners of the rectangular area is equal to zero. An investigation into the difference in the diffusion fluxes along the coordinate axes showed that the constant internal source affected the difference in the nonsymmetrical fluxes, and the concentration of the substance in the area corners had no effect.

Keywords: exact solution, diffusion, internal source, rectangular shape, fast expansion method

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ТОЧНЫЕ РЕШЕНИЯ ЗАДАЧИ О ДИФФУЗИИ В ПРЯМОУГОЛЬНОЙ ЕМКОСТИ С ВНУТРЕННИМ ИСТОЧНИКОМ, ПОЛУЧЕННЫЕ МЕТОДОМ БЫСТРЫХ РАЗЛОЖЕНИЙ

А.Д. Чернышов¹, Д.С. Сайко¹, В.В. Горяйнов², С.Ф. Кузнецов¹, О.Ю. Никифорова¹

¹ Воронежский государственный университет инженерных технологий, г. Воронеж, Российская Федерация;

² Воронежский государственный технический университет, г. Воронеж, Российская Федерация

Методом быстрых разложений решается в общем виде задача диффузии в теле прямоугольной формы с граничными условиями -1го рода и внутренним источником вещества, зависящим от координат точек прямоугольника. Получено точное решение, содержащее свободные параметры, изменяя которые можно получить множество новых точных решений. В качестве примера показаны точные решения задачи с постоянным внутренним источником. Из анализа точных решений следует, что распределения концентрации и диффузионных потоков будут симметричны относительно плоскости y = b/2 при условии равенства нулю концентрации вещества в углах прямоугольной области. Изучение перепада диффузионных потоков вдоль координатных осей показало, что на перепад несимметричных потоков влияет постоянный внутренний источник и не влияет концентрация вещества в углах области.

Ключевые слова: точное решение, диффузия, внутренний источник, прямоугольная форма, быстрое разложение

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Introduction

Planar problems of diffusion can be solved by different methods, for example, the method of least-squares collocation with increased accuracy. A parametric dual spline consisting of two cubic splines was constructed in [1] in Cartesian coordinates to define a domain bounary approximately and exactly. Numerical analytical representation of the solution of two- and three-dimensional boundaryvalue problems was obtained in [2] using integral Fourier-Laplace transforms. Ref. [3] describes a method for constructing the exact solutions for equations of nonlinear diffusion in a one-dimensional coordinate space based on the special superposition principle. The approximate self-consistent method for solving the system of functional equations, obtained from spectral expansion of Euler correlation of the carrier medium, was proposed in [4] for problems of diffusion in continuous media. Finite-difference methods were used in [5-8]. Quadrature methods were applied in [9-11], while a method based on using the Haar wavelets was used in [12,13].

In this study we relied on the fast expansion method (FEM) [14] to obtain some exact solutions to the problem on diffusion in a rectangular body with first-kind boundary conditions and an internal source depending on the coordinates of the rectangle points.

Problem statement

Let us consider a diffusion problem where the body has a rectangular shape, Ω_{\Box} . If the concentration C(x,y) is unknown, the phenomenon of diffusion can be described using a second-order partial differential equation for the variables x, y with the given internal source F(x,y) (Poisson's equation):

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + F(x, y) = 0,$$

$$(x, y) \in \Omega_{\scriptscriptstyle \Box}, \ 0 \le x \le a, \ 0 \le y \le b.$$
(1)

Boundary conditions are given as

$$C\Big|_{x=0} = f_1(y), \ C\Big|_{y=0} = f_2(x),$$

$$C\Big|_{x=a} = f_3(y), \ C\Big|_{y=b} = f_4(x).$$
(2)

The solution of the problem on the distribution of substance concentration C(x,y) is represented by the simplest dependence from the theory of fast expansions [14–16] using the polynomials taking the form

$$P_{1}(x) = 1 - \frac{x}{a}, \quad P_{2}(x) = \frac{x}{a},$$

$$P_{3}(x) = \frac{x^{2}}{2} - \frac{x^{3}}{6a} - \frac{ax}{3}, \quad P_{4}(x) = \frac{x^{3}}{6a} - \frac{ax}{6},$$

$$P_{1}(y) = 1 - \frac{y}{b}, \quad P_{2}(y) = \frac{y}{b},$$

$$P_{3}(y) = \frac{y^{2}}{2} - \frac{y^{3}}{6b} - \frac{by}{3}, \quad P_{4}(y) = \frac{y^{3}}{6b} - \frac{by}{6},$$

$$(x, y) \in \Omega \ (0 \le x \le a, \ 0 \le y \le b).$$

The assumed exact solution C(x,y) can be formulated as the final expression used for fast decomposition in [14–16], i.e., consisting of the polynomial and the finite trigonometric parts:

$$C(x, y) = \sum_{i=1}^{4} A_i(y) P_i(x) + A_5(y) \sin \pi \frac{x}{a} + A_6(y) \sin 2\pi \frac{x}{a},$$

where

i

$$A_{i}(y) = \sum_{j=1}^{4} A_{i,j} P_{j}(y) + A_{i,5} \sin \pi \frac{y}{b} + A_{i,6} \sin 2\pi \frac{y}{b},$$

$$= 1 \div 6, \ 0 \le x \le a, \ 0 \le y \le b.$$
(3)

The form of expression (3) is attractive because a similar form can be used for highly accurate approximation of the broad class of smooth functions from the Sobolev–Liouville space, given in boundary conditions and as the internal source; these functions have certain practical value.

The functions included in boundary conditions (2) and the internal source F(x,y) of substance concentration can be written as finite sums, similar to dependence (3):

$$f_{1}(y) = \sum_{j=1}^{4} f_{1,j}P_{j}(y) +$$

$$+ f_{1,5} \sin \pi \frac{y}{b} + f_{1,6} \sin 2\pi \frac{y}{b},$$

$$f_{2}(x) = \sum_{j=1}^{4} f_{2,j}P_{j}(x) +$$

$$+ f_{2,5} \sin \pi \frac{x}{a} + f_{2,6} \sin 2\pi \frac{x}{a},$$

$$f_{3}(y) = \sum_{j=1}^{4} f_{3,j}P_{j}(y) +$$

$$+ f_{3,5} \sin \pi \frac{y}{b} + f_{3,6} \sin 2\pi \frac{y}{b},$$

$$f_{4}(x) = \sum_{j=1}^{4} f_{4,j}P_{j}(x) +$$

$$+ f_{4,5} \sin \pi \frac{x}{a} + f_{4,6} \sin 2\pi \frac{x}{a}.$$

$$F(x, y) = \sum_{i=1}^{4} \left(\sum_{j=1}^{4} F_{i,j}P_{j}(y) + \right) +$$

$$+ F_{i,5} \sin \pi \frac{y}{b} + F_{i,6} \sin 2\pi \frac{y}{b}\right)P_{i}(x)$$

$$+ \left(\sum_{j=1}^{4} F_{5,j}P_{j}(y) + F_{5,5} \sin \pi \frac{y}{b} + \right) +$$

$$+ F_{5,6} \sin 2\pi \frac{y}{b} \sin \pi \frac{x}{a} +$$

$$+ \left(\sum_{j=1}^{4} F_{6,j}P_{j}(y) + F_{6,5} \sin \pi \frac{y}{b} + \right) +$$

$$+ F_{6,6} \sin 2\pi \frac{y}{b} \sin 2\pi \frac{x}{a}.$$
(4)

The coefficients $f_{i,j}$ and $F_{i,j}$ in equalities (4) and (5) are assumed to be known. The coefficients $A_{i,j}$ from Eq. (3) are assumed to be unknown so far. They must be found by exactly satisfying boundary conditions (2) and differential equation (1). Solution (3) of boundary-value problem (1), (2) must satisfy the consistency conditions for boundary conditions (2) and differential equation (1) in the corners:

$$f_{1}(0) = f_{2}(0), \quad f_{2}(a) = f_{3}(0),$$

$$f_{3}(b) = f_{4}(a), \quad f_{1}(b) = f_{4}(0),$$

$$C_{xx}(0,0) + C_{yy}(0,0) + F(0,0) = 0,$$

$$C_{xx}(a,0) + C_{yy}(a,0) + F(a,0) = 0,$$

$$C_{xx}(0,b) + C_{yy}(0,b) + F(0,b) = 0,$$

$$C_{xx}(a,b) + C_{yy}(a,b) + F(a,b) = 0.$$
(6)

Conditions (6) follow because the concentration C(x,y) is independent of the direction of approach to the corners of the rectangle.

Consequently, we arrive to the following problem:

It is required to find such a solution to Eq. (1) with the given internal source in the form (5), which exactly satisfies boundary conditions (2) and consistency conditions (6).

Solution of the problem

First let us substitute the assumed exact solution of the problem in the form (3) into boundary conditions (2):

$$\sum_{j=1}^{4} f_{1,j}P_{j}(y) + f_{1,5}\sin\pi\frac{y}{b} +$$

$$f_{1,6}\sin 2\pi\frac{y}{b} = \sum_{j=1}^{4} A_{1,j}P_{j}(y) +$$

$$+A_{1,5}\sin\pi\frac{y}{b} + A_{1,6}\sin 2\pi\frac{y}{b} ,$$

$$\sum_{j=1}^{4} f_{2,j}P_{j}(x) + f_{2,5}\sin\pi\frac{x}{a} +$$

$$+f_{2,6}\sin 2\pi\frac{x}{a} = \sum_{i=1}^{4} A_{i,1}P_{i}(x) +$$

$$+A_{5,1}\sin\pi\frac{x}{a} + A_{6,1}\sin 2\pi\frac{x}{a} ,$$

$$\sum_{j=1}^{4} f_{3,j}P_{j}(y) + f_{3,5}\sin\pi\frac{y}{b} +$$

$$+f_{3,6}\sin 2\pi\frac{y}{b} = \sum_{j=1}^{4} A_{2,j}P_{j}(y) +$$

$$+A_{2,5}\sin\pi\frac{y}{b} + A_{2,6}\sin 2\pi\frac{y}{b} ,$$

$$\sum_{j=1}^{4} f_{4,j} P_j(x) + f_{4,5} \sin \pi \frac{x}{a} + f_{4,6} \sin 2\pi \frac{x}{a} = \sum_{i=1}^{4} A_{i,2} P_i(x) + f_{4,6} \sin 2\pi \frac{x}{a} + A_{6,2} \sin 2\pi \frac{x}{a}.$$
(7)

The obtained equalities (7) must hold true for $\forall (x, y) \in \Omega_{\Box}$ with respect to the unknowns $A_{i,i}$.

 $A_{i,j}$. Next, we substitute C(x,y) from expression (3) into differential equation (1):

$$\begin{split} &\sum_{i=1}^{4} \left(\sum_{j=1}^{4} A_{i,j} P_{j}\left(y\right) + A_{i,5} \sin \pi \frac{y}{b} + \right. \\ &+ A_{i,6} \sin 2\pi \frac{y}{b} \right) P_{i}''\left(x\right) - \\ &- \frac{\pi^{2}}{a^{2}} \left(\sum_{j=1}^{4} A_{5,j} P_{j}\left(y\right) + A_{5,5} \sin \pi \frac{y}{b} + \right. \\ &+ A_{5,6} \sin 2\pi \frac{y}{b} \right) \sin \pi \frac{x}{a} - \\ &- \frac{4\pi^{2}}{a^{2}} \left(\sum_{j=1}^{4} A_{6,j} P_{j}\left(y\right) + A_{6,5} \sin \pi \frac{y}{b} + \right. \\ &+ A_{6,6} \sin 2\pi \frac{y}{b} \right) \sin 2\pi \frac{x}{a} + \\ &+ \sum_{i=1}^{4} \left(\sum_{j=1}^{4} A_{i,j} P_{j}''\left(y\right) - A_{i,5} \frac{\pi^{2}}{b^{2}} \sin \pi \frac{y}{b} - \right. \\ &- A_{i,6} \frac{4\pi^{2}}{b^{2}} \sin 2\pi \frac{y}{b} \right) P_{i}\left(x\right) + \\ &+ \left(\sum_{j=1}^{4} A_{5,j} P_{j}''\left(y\right) - A_{5,5} \frac{\pi^{2}}{b^{2}} \sin \pi \frac{y}{b} - \right. \\ &- A_{5,6} \frac{4\pi^{2}}{b^{2}} \sin 2\pi \frac{y}{b} \right) \sin \pi \frac{x}{a} + \\ &+ \left(\sum_{j=1}^{4} A_{6,j} P_{j}''\left(y\right) - A_{6,5} \frac{\pi^{2}}{b^{2}} \sin \pi \frac{y}{b} - \right. \\ &- A_{6,6} \frac{4\pi^{2}}{b^{2}} \sin 2\pi \frac{y}{b} \right) \sin 2\pi \frac{x}{a} + \\ &+ \sum_{i=1}^{4} \left(\sum_{j=1}^{4} F_{i,j} P_{j}\left(y\right) + F_{i,5} \sin \pi \frac{y}{b} + \right. \end{split}$$

$$+F_{i,6}\sin 2\pi \frac{y}{b}P_{i}(x) +$$

$$+\left(\sum_{j=1}^{4}F_{5,j}P_{j}(y) + F_{5,5}\sin \pi \frac{y}{b} +$$

$$+F_{5,6}\sin 2\pi \frac{y}{b}\sin \pi \frac{x}{a} +$$

$$+\left(\sum_{j=1}^{4}F_{6,j}P_{j}(y) + F_{6,5}\sin \pi \frac{y}{b} +$$

$$+F_{6,6}\sin 2\pi \frac{y}{b}\sin 2\pi \frac{x}{a} = 0.$$
(8)

Eq. (8) must hold true for any

 $0 \le x \le a, \ 0 \le y \le b.$

The following functions are linearly independent in equalities (7) and (8):

$$P_{1}(x), P_{2}(x), P_{3}(x), P_{4}(x), P_{1}(y), P_{2}(y), P_{3}(y), P_{4}(y), \sin \pi \frac{x}{a}, \sin \pi \frac{y}{b},$$
(9)
$$\sin 2\pi \frac{x}{a}, \sin 2\pi \frac{y}{b}.$$

Functional system (7), (8) is reduced to a system of linear algebraic equations by equating the coefficients in Eqs. (7) and (8) on the left and on the right in front of linearly independent functions (9), taking into account the following equalities [14, 15]:

$$P_1'' = P_2'' = 0, P_3'' = P_1, P_4'' = P_2.$$

The resulting system of linear algebraic equations is overdetermined but it has a solution because consistency conditions (6) are satisfied. It follows from analysis of the algebraic system that consistency conditions (6) are satisfied automatically, since all algebraic relations obtained from (6) are included in the system of linear algebraic equations. It is necessary to solve 36 algebraic equations to find the unknowns $A_{i,j}$, while the rest of the equations are used to compose the relations between the coefficients

 $f_{i,i}, (i = 1 \div 4, j = 1 \div 6)$

and

$$F_{i,j}, (i = 1 \div 6, j = 1 \div 6).$$

Thus, the values of the coefficients $A_{i,j}$ are found from the following equalities:

 A_1

$$f_{1,k}, \ A_{2,k} = f_{3,k}, \ k = 1 \div 6,$$

$$A_{3,1} = f_{2,3}, \ A_{3,2} = f_{4,3},$$

$$A_{3,3} = -F_{1,3}, \ A_{3,4} = -F_{1,4},$$

$$A_{3,5} = \frac{\pi^2}{b^2} f_{1,5} - F_{1,5},$$

$$A_{3,6} = \frac{4\pi^2}{b^2} f_{1,6} - F_{1,6},$$

$$A_{4,1} = f_{2,4}, \ A_{4,2} = f_{4,4},$$

$$A_{4,3} = -F_{4,1}, \ A_{4,4} = -F_{2,4},$$

$$A_{4,5} = \frac{\pi^2}{b^2} f_{3,5} - F_{2,5},$$

$$A_{4,6} = \frac{4\pi^2}{b^2} f_{3,6} - F_{2,6},$$

$$A_{5,1} = f_{2,5}, \ A_{5,2} = f_{4,5},$$

$$A_{5,3} = \frac{\pi^2}{a^2} f_{2,5} - F_{5,1},$$

$$A_{5,5} = F_{5,5} / \left(\frac{\pi^2}{a^2} + \frac{\pi^2}{b^2}\right),$$

$$A_{5,6} = F_{5,6} / \left(\frac{\pi^2}{a^2} + \frac{4\pi^2}{b^2}\right),$$

$$A_{6,1} = f_{2,6}, \ A_{6,2} = f_{4,6},$$

$$A_{6,3} = \frac{4\pi^2}{a^2} f_{2,6} - F_{6,1},$$

$$A_{6,4} = \frac{4\pi^2}{a^2} f_{4,6} - F_{6,2},$$

$$A_{6,6} = F_{6,6} / \left(\frac{4\pi^2}{a^2} + \frac{4\pi^2}{b^2}\right).$$

$$(10)$$

Substituting the coefficients from equalities (10) into expression (3), we obtain an exact solution to the problem.

The following conditions should be satisfied for giving boundary conditions (2) and internal source (5)

$$f_{1,1} = f_{2,1}, \quad f_{2,2} = f_{3,1},$$

$$f_{3,2} = f_{4,2}, \quad f_{1,2} = f_{4,1},$$

$$F_{3,3} = F_{3,4} = F_{4,3} = F_{4,4} = 0.$$
(11)

$$f_{1,3} = -f_{2,3} - F_{1,1}, \quad f_{1,4} = -f_{4,3} - F_{1,2},$$

$$f_{3,3} = -f_{2,4} - F_{2,1}, \quad f_{3,4} = -f_{4,4} - F_{2,2}.$$

$$F_{1,3} = F_{3,1}, \quad F_{1,4} = F_{3,2},$$
(12)

f

$$F_{4,1} = F_{2,3}, \quad F_{2,4} = F_{4,2},$$

$$f_{1,5} = \frac{b^2}{\pi^2} \left(\frac{b^2}{\pi^2} F_{3,5} + F_{1,5} \right),$$

$$f_{1,6} = \frac{b^2}{4\pi^2} \left(\frac{b^2}{4\pi^2} F_{3,6} + F_{1,6} \right),$$

$$f_{2,5} = \frac{a^2}{\pi^2} \left(\frac{a^2}{\pi^2} F_{5,3} + F_{5,1} \right),$$

$$f_{2,6} = \frac{\dot{a}^2}{4\pi^2} \left(\frac{\dot{a}^2}{4\pi^2} F_{6,3} + F_{6,1} \right),$$

$$f_{3,5} = \frac{b^2}{\pi^2} \left(\frac{b^2}{\pi^2} F_{4,5} + F_{2,5} \right),$$

$$f_{4,6} = \frac{\dot{a}^2}{\pi^2} \left(\frac{\dot{a}^2}{4\pi^2} F_{5,4} + F_{5,2} \right),$$

$$f_{4,6} = \frac{\dot{a}^2}{4\pi^2} \left(\frac{\dot{a}^2}{4\pi^2} F_{6,4} + F_{6,2} \right).$$
(13)

Therefore, solution (10) holds when conditions (11)-(13) are satisfied.

Example of constructed exact solutions and their analysis

Let a constant internal source be present in a rectangular container. This version of the internal source can be obtained from expressions (5) and condition (12) provided that the equalities

$$F_1(y) = F_2(y),$$

$$F_3(y) = F_4(y) = F_5(y) = F_6(y) = 0.$$
(14)

hold true. The condition $F_1(y) = F_2(y)$ in equalities (14) implies the equality of the coefficients

$$F_{1,1} = F_{1,2} = F_{2,1} = F_{2,2} = Q, \tag{15}$$

while the remaining coefficients are simultaneously equal to zero:

$$F_{1,3} = F_{1,4} = F_{1,5} = F_{1,6} =$$

= $F_{2,3} = F_{2,4} = F_{2,5} = F_{2,6} = 0.$ (16)

Thus, if equalities (14)-(16) are satisfied, we have a constant internal source

=

$$F(x,y) = Q. \tag{17}$$

Let us write the boundary conditions satisified for source (17). For this purpose, in view of equalities (15), we rewrite equalities (12) in the form

$$f_{1,3} + f_{2,3} + Q = 0, \ f_{1,4} + f_{4,3} + Q = 0,$$

$$f_{2,4} + f_{3,3} + Q = 0, \ f_{4,4} + f_{3,4} + Q = 0.$$
 (18)

Suppose only the coefficients included in equalities (18) can be different from zero in Eqs. (4). Several types of boundary conditions are possible for this case: they correspond to different combinations of the values of the coefficients in equalities (18). Let

$$f_{1,3} = f_{1,4} = f_{2,4} = f_{4,4} = 0,$$

$$f_{2,3} = f_{4,3} = f_{3,3} = f_{3,4} = -Q.$$
(19)

Then, taking into account the values of the coefficients from equalities (19), boundary conditions (2) have the form

$$C|_{x=0} = 0, \ C|_{x=a} = -\frac{Q}{2}(y^2 - by),$$

$$C\Big|_{y=0} = C\Big|_{y=b} = -Q\left(\frac{x^2}{2} - \frac{x^3}{6a} - \frac{ax}{3}\right).$$
 (20)

Substituting the coefficients from equalities (16) and (19) into expressions (10), we obtain:

$$A_{2,3} = A_{2,4} = A_{3,1} = A_{3,2} = -Q.$$

After simplifications, the exact solution of Eq. (1), corresponding to conditions (20), with a constant internal source (17) takes the form

$$C(x, y) = -\frac{Q}{2} (y^{2} - by) \frac{x}{a} - Q\left(\frac{x^{2}}{2} - \frac{x^{3}}{6a} - \frac{ax}{3}\right).$$
(21)

Eq. (21) can be used to calculate substance concentration C(x,y) at any point in the rectangle. It follows from this equation that C(x,y) = 0 in the corners of the rectangle. The distribution C(x,y) for the case

$$Q = 4, a = 1 \text{ m}, b = 2 \text{ m}$$
 (22)

is shown in Fig. 1,*a*. Evidently, this distribution, calculated by Eq. (21), has a plane of symmetry passing through the section y = b/2. The highest concentration C(x,y) = 2 is at the point (*a*; *b*/2); the lowest one, C(x,y) = 0, is located in the corners of the domain and at the boundary x = 0 (this also follows from boundary conditions (20)). The maximum concentration difference is between the points of the curve obtained by section of the surface C(x,y)with the plane y = b/2, and is equal to

$$\Delta C(x,y) = C(a; b/2) - C(0; b/2) = 2.$$



Fig. 1. Distribution of substance concentration C(x,y), constructed by Eqs. (21) (*a*) and (25) (*b*)

Now let us consider the case when the concentrations of the substance in the corners of the domain are given along with the constant internal source (17).

The boundary conditions are written so that equalities (19) are satisfied and the coefficients $f_{i,j}$ included in conditions (11) are not equal to zero. Let us introduce the notations

$$f_{1,1} = f_{2,1} = C_1, \quad f_{2,2} = f_{3,1} = C_3,$$

$$f_{3,2} = f_{4,2} = C_4, \quad f_{1,2} = f_{4,1} = C_2.$$
(23)

In view of Eqs. (19) and (23), the boundary conditions can be written in the form

$$C|_{x=0} = C_{1}\left(1 - \frac{C}{b}\right) + C_{2}\frac{y}{b},$$

$$C|_{x=a} = C_{3}\left(1 - \frac{C}{b}\right) + C_{4}\frac{y}{b} - \frac{Q}{2}\left(y^{2} - by\right),$$

$$C|_{y=0} = C_{1}\left(1 - \frac{x}{a}\right) + C_{3}\frac{x}{a} - Q\left(\frac{x^{2}}{2} - \frac{x^{3}}{6a} - \frac{ax}{3}\right),$$

$$C|_{y=b} = C_{2}\left(1 - \frac{x}{a}\right) + C_{4}\frac{x}{a} - Q\left(\frac{x^{2}}{2} - \frac{x^{3}}{6a} - \frac{ax}{3}\right).$$
(24)

Using equalities (19) and (23), we find from Eqs. (10)

$$\begin{split} A_{1,1} &= C_1, A_{1,2} = C_1, \\ A_{2,1} &= C_3, A_{2,2} = C_4, \\ A_{2,3} &= A_{2,4} = A_{3,1} = A_{3,2} = -Q. \end{split}$$

Consequently, the exact solution of diffusion equation (1) with constant internal source (17), corresponding to boundary conditions (24), takes the form

$$C(x, y) = \left(C_{1}\left(1 - \frac{C}{b}\right) + C_{2}\frac{y}{b}\right)\left(1 - \frac{x}{a}\right) + \left(C_{3}\left(1 - \frac{C}{b}\right) + C_{4}\frac{y}{b}\frac{x}{a} - \frac{Q}{2}\left(y^{2} - by\right)\frac{x}{a} - Q\left(\frac{x^{2}}{2} - \frac{x^{3}}{6a} - \frac{ax}{3}\right).$$
(25)

The distribution of concentration C(x,y) for particular values of the parameters

$$Q = 4, C_1 = 1,$$

 $C_2 = 4, C_3 = 2, C_4 = 3,$ (26)
 $a = 1 \text{ m}, b = 2 \text{ m}.$

is shown in Fig. 1, *b*. Evidently, the distribution C(x,y) that is calculated by Eq. (25) has no planes of symmetry. The highest concentration C(x,y) = 4.5 is at the point (a; b/2), and the lowest, C(x,y) = 1, is at the point (0;0).

Substituting the values x = a/2 and y = b/2 into solution (25), we calculate the concentration value in the center of the domain:

$$C\left(\frac{a}{2}, \frac{b}{2}\right) =$$

= $\frac{C_1 + C_2 + C_3 + C_4}{4} + \frac{Q}{16}(a^2 + b^2).$

Let us calculate the diffusion fluxes of substance by the following equations [17]:

$$q_{x}(x, y) = -D \frac{\partial C(x, y)}{\partial x},$$

$$q_{y}(x, y) = -D \frac{\partial C(x, y)}{\partial y}.$$
(27)

where D is the diffusion coefficient.

Substituting the exact solution (21) into these formulas, we obtain:

$$q_x(x,y) =$$

$$= DQ\left(\frac{1}{2a}\left(y^2 - by\right) + \left(x - \frac{x^2}{2a} - \frac{a}{3}\right)\right),$$
⁽²⁸⁾

$$q_{y}(x,y) = DQ \frac{x}{2a}(2y-b).$$
 (29)

Substituting solution (25) into Eqs. (27), we obtain:

$$q_{x}(x,y) = \frac{D}{a} \left(C_{1} \left(1 - \frac{C}{b} \right) + C_{2} \frac{y}{b} \right) - \frac{D}{a} \left(C_{3} \left(1 - \frac{C}{b} \right) + C_{4} \frac{y}{b} \right) + (30) + DQ \left(\frac{1}{2a} \left(y^{2} - by \right) + \left(x - \frac{x^{2}}{2a} - \frac{a}{3} \right) \right);$$

$$q_{y}(x,y) = D\left(\frac{C_{1}}{b} - \frac{C_{2}}{b}\right)\left(1 - \frac{x}{a}\right) + D\left(\frac{C_{3}}{b} - \frac{C_{4}}{b}\right)\frac{x}{a} + DQ\frac{x}{2a}(2y - b).$$
(31)

The diffusion fluxes of substance shown in Fig. 2 are constructed by Eqs. (28) and (29) using the data from (22). The diffusion coefficient was equal to $D = 4 \cdot 10^{-6} \text{ m}^2/\text{s}$ in the calculations .

The data in Fig. 2 allow us to conclude that the diffusion flux $q_x(x,y)$ has the same plane of symmetry as the corresponding concentration distribution C(x,y) for diffusion under the action of only the internal source Q; that is, the plane of symmetry passes through the section y = b/2.

Given the ratio b/a = 1 - 4, the shapes taken by the distribution of substance concentration C(x,y) and the diffusion flux $q_x(x,y)$ in the rectangular domain are qualitatively similar to the distributions shown in Figs. 1 and 2. If the length of any of the sides (*a* or *b*) of the rectangle is ten or more times larger than the other, such a difference leads to a qualitative change in the distributions of substance concentration C(x,y)and diffusion flux $q_x(x,y)$, compared with the distributions shown in Figs. 1 and 2, *a*.

For example, if only the value of the variable y is changed in (26) from 2 to 10 meters, then the graphs C(x,y) and $q_x(x,y)$, constructed by Eqs. (25) and (28), have the form shown in Fig. 3.



Fig. 2. Graphical representation of diffusion fluxes of substance q(x,y) constructed by Eqs. (28) (*a*) and (29) (*b*); D = 4.10-6 m²/s



Fig. 3. Distributions of substance concentration C(x,y) (*a*) and diffusion fluxes of substance q(x,y) (*b*) at b/a = 10



Fig. 4. Distributions of substance concentration C(x,y) (*a*) and diffusion fluxes of substance q(x,y) (*b*) at b/a = 1/5

If only the value of the variable x is changed in (26) (for example, to 10 meters instead of 1), the distributions C(x,y) and $q_x(x,y)$, constructed by Eqs. (25) and (28), take the form shown in Fig. 4.

It can be seen from Figs. 3,*a* and 4,*a* that substance concentration in the corners of the domain is small compared with the maximum concentration, and the shape of the distribution C(x,y) constructed by Eq. (24) (see Fig. 3,*a*) is now qualitatively similar to the shape of distribution C(x,y) constructed by Eq. (21) (see Fig. 1,*a*).

Analysis of the data shown in Figs. 2, 3, *b* and 4, *b* indicates that it would be of interest to consider the difference in diffusion fluxes along the coordinate axes. As evident from Fig. 2, *a*, the flux difference between the boundaries x = 0 and x = a in any sections is

$$y = const (0 \le y \le b),$$

i.e., a constant value; it is found by the formula

$$\Delta q_x = q_x (0, y) \Big|_{y=\text{const}} - -q_x (a, y) \Big|_{y=\text{const}} = -\frac{DQa}{2}.$$
(32)

It can be seen from Fig. 2,*b* that the diffusion flux $q_y(x,y)$ takes the greatest value in the section x = a. The flux difference $q_y(x,y)$ at x = a between the boundaries y = 0 and y = b is found by the formula

$$\Delta q_{y} = q_{y}(a,0) - q_{y}(a,b) = -DQb. \quad (33)$$

Equalities (32) and (33) hold true both for symmetric diffusion fluxes $q_x(x,y)$ and $q_y(x,y)$ calculated by Eqs. (28) and (29), and for asymmetric ones calculated by Eqs. (30), (31). Thus, it follows from equalities (32) and (33) that the differences Δq_x and Δq_y of asymmetric fluxes $q_x(x,y)$ and $q_y(x,y)$ are affected by a constant internal source but not by the concentration of matter in the corners of the rectangle.

Conclusion

The examples presented confirm that the fast expansion method allows to obtain not only approximate solutions [18-20] but also exact ones. The analytical solution of the diffusion equation formulated in this study can be used to obtain exact solutions of this equation for different boundary conditions, for constant as well as variable internal sources. The coefficients of boundary conditions (2) and internal source (5) should be selected taking into account Eqs. (11)-(13).

It follows from analysis of the exact solutions obtained that if the substance concentrations in the corners of the rectangular domain equal zero, the distributions of the concentration C(x,y)and the diffusion fluxes $q_x(x,y)$ and $q_y(x,y)$ of the substance are symmetrical relative to the plane y = b/2. If the concentrations in the corners are not equal to zero, then the distributions C(x,y), $q_x(x,y)$ and $q_y(x,y)$ do not possess such symmetry.

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THE AUTHORS

CHERNYSHOV Alexander D.

Voronezh State University of Engineering Technology 19 Revolutsii Pr., Voronezh, 394000, Russian Federation chernyshovad@mail.ru

SAJKO Dmitrij S.

Voronezh State University of Engineering Technology 19 Revolutsii Pr., Voronezh, 394000, Russian Federation dmsajko@mail.ru

GORYAINOV Vitalij V.

Voronezh State Technical University 84, 20 let Oktyabrya St., Voronezh, 394006, Russian Federation gorvit77@mail.ru

KUZNETSOV Sergei F.

Voronezh State University of Engineering Technology 19 Revolutsii Pr., Voronezh, 394000, Russian Federation sfs134@mail.ru

NIKIFOROVA Olga Yu.

Voronezh State University of Engineering Technology 19 Revolutsii Pr., Voronezh, 394000, Russian Federation niki22@mail.ru

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СВЕДЕНИЯ ОБ АВТОРАХ

ЧЕРНЫШОВ Александр Данилович — доктор физико-математических наук, профессор кафедры высшей математики и информационных технологий Воронежского государственного университета инженерных технологий.

394000, Российская Федерация, г. Воронеж, пр. Революции, 19 chernyshovad@mail.ru

САЙКО Дмитрий Сергеевич — доктор физико-математических наук, профессор, заведующий кафедрой высшей математики и информационных технологий Воронежского государственного университета инженерных технологий.

394000, Российская Федерация, г. Воронеж, пр. Революции, 19 dmsajko@mail.ru

ГОРЯЙНОВ Виталий Валерьевич — кандидат физико-математических наук, доцент кафедры прикладной математики и механики Воронежского государственного технического университета. 394006, Российская Федерация, г. Воронеж, ул. 20-летия Октября, 84 gorvit77@mail.ru

КУЗНЕЦОВ Сергей Федорович — кандидат физико-математических наук, доцент кафедры высшей математики и информационных технологий Воронежского государственного университета инженерных технологий.

394000, Российская Федерация, г. Воронеж, пр. Революции, 19 sfs134@mail.ru

НИКИФОРОВА Ольга Юрьевна — старший преподаватель кафедры высшей математики и информационных технологий Воронежского государственного университета инженерных технологий. 394000, Российская Федерация, г. Воронеж, пр. Революции, 19 niki22@mail.ru DOI: 10.18721/JPM.13305 УДК 532.517

NUMERICAL MODELING OF AIR DISTRIBUTION IN A TEST ROOM WITH 2D SIDEWALL JET. I. Foundations for eddy-resolving approach application based on periodical formulation

M.A. Zasimova¹, N.G. Ivanov¹, D. Markov²

¹ Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation;

² Technical University of Sofia, Sofia, Bulgaria

The paper presents the methods and results of numerical modeling of turbulent airflow in a test room based on the vortex-resolving wall-modeled large eddy simulation approach. The room ventilation is provided by a plain air jet at Re = 5233. The jet is supplied from a slit placed at a side wall under the ceiling. The room geometry and airflow parameters correspond to the experimental benchmark test by Nielsen et al. (1978), but with the periodicity boundary conditions in the transverse direction. Calculations were carried out with the ANSYS Fluent software using fine grids consisting of up to $6x10^7$ cells. The paper presents detailed analysis of parametric computations aimed at the evaluation of numerical simulation adequacy. In particular, the grid dependency study was performed and the Kolmogorov scale was estimated.

Keywords: turbulent airflow, plain jet, Large Eddy Simulation, ventilation

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ЦИРКУЛЯЦИИ ВОЗДУХА В ПОМЕЩЕНИИ ПРИ ПОДАЧЕ ИЗ ПЛОСКОЙ ЩЕЛИ. І. Отработка применения вихреразрешающего подхода с использованием периодической постановки

М.А. Засимова¹, Н.Г. Иванов¹, Д. Марков²

¹ Санкт-Петербургский политехнический университет Петра Великого,

Санкт-Петербург, Российская Федерация;

² Софийский технический университет, София, Болгария

Представлены методика и результаты численного моделирования турбулентного течения воздуха в тестовом помещении на основе вихреразрешающего подхода – метода моделирования крупных вихрей с пристенным моделированием. Вентиляция помещения осуществляется плоской воздушной струей, подаваемой из расположенного под потолком на торцевой стенке щелевого отверстия, при значении числа Рейнольдса Re = 5233. Геометрия помещения и параметры течения соответствуют классическому тестовому эксперименту (Nielsen et al., 1978), однако задача ставилась как периодическая, что справедливо для помещения, сильно вытянутого в поперечном направлении. Расчеты в программном пакете ANSYS Fluent выполнены с использованием весьма подробных сеток размерностью до $6 \cdot 10^7$ ячеек. Подробно описаны результаты методических расчетов, направленных на оценку адекватности выполненного численного моделирования, в частности проведен анализ сеточной зависимости и дана оценка колмогоровского масштаба для рассматриваемого течения.

Ключевые слова: турбулентное течение, плоская струя, метод моделирования крупных вихрей, вентиляция

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Introduction

One of the challenges posed in design and modernization of buildings is configuring the heating, ventilation and air conditioning (HVAC) systems controlling the microclimate. Comfort and safety are ensured in the living quarters by maintaining the parameters of the air (air velocity, temperature, concentration of harmful impurities, etc.) within the required range, which largely depends on the air supply scheme for the ventilation system. In this regard, improving the accuracy of assessing the quality of the air provided by the ventilation system is an issue that is steadily gaining importance.

Methods of computational fluid dynamics allowing to carry out three-dimensional simulation of turbulent jet flows have been increasingly popular in the recent years. Approaches that estimate the flow parameters based on numerically solving the steady/ unsteady Reynolds-averaged Navier-Stokes equations (RANS/URANS) have become widely popular in engineering practice. The RANS/URANS approaches were employed, for example, for designing and/or modernizing the ventilation systems for a swimming pool [1], an ice rink [2], a university assembly hall of historical and architectural value [3], the interior of St. Isaac's Cathedral in St. Petersburg [4].

Methods of computational fluid dynamics turn out to be even more important for developing life support systems than ventilation systems for buildings, since almost every proposed solution is unique. An example of solving such problems are the computations of ventilation for crew and passenger cabins of aircraft [5, 6]. Over the past two decades, the RANS/URANS approaches have been used to assess the performance and efficiency of life support systems for spacecraft. In particular, calculations of the atmosphere at the International Space Station (ISS) were carried out under standard conditions [7], as well as after using a carbon dioxide fire extinguisher in the US Orbital Segment of the ISS [8].

Despite examples of successful solutions to applied ventilation problems, the accuracy of the calculation results for air distribution in rooms obtained by the RANS/URANS approaches remains an open question. The degree of uncertainty in the results of RANS/ URANS calculations can be estimated either by direct comparison of the calculated results with the data of a physical experiment, or by comparing the RANS/URANS results with the data obtained by more accurate eddy-resolving approaches to describing turbulent flows.

Direct Numerical Simulation (DNS) from first principles can be used as an eddy-resolving Full Navier-Stokes equations approach. are solved within the DNS approach, which allows to describe all scales of turbulence if applied correctly. It is well known that the DNS approach requires huge computational costs and its application is limited to very moderate values of the Reynolds number. An alternative for numerical studies with manageable computational costs is the Large Eddy Simulation method (LES). The LES approach involves solving filtered Navier-Stokes equations, allowing to describe the behavior of large eddies in combination with semi-empirical simulation of small-scale eddies. The LES method not only makes it possible to carry out fundamental studies, including those aimed at assessing the accuracy of RANS simulation, but is also gaining ground for solving applied problems [9], including in modeling ventilation flows characterized by relatively moderate Reynolds numbers, and also, in most cases, fairly mild requirements for near-wall resolution.

Different studies modeled HVAC systems using the LES approach. Simulation of air exchange by the LES approach was first presented in [10], considering the ventilation in a test room of a simple shape, with experimental data available [11]. A more complex problem of flow in a relatively cluttered room equipped with a displacement ventilation system is solved in [12]. Ref. [13]

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presents air distribution estimates carried out by LES for the Columbus orbital module, which is part of the ISS, equipped with a multi-jet ventilation system; the calculation results were also compared with experimental data. Later, the LES approach was used to determine the parameters of air exchange in a university lecture hall [14] and in the premises of a residential building [15].

The practical application of the LES approach needs to further refined by solving test problems. This study describes and tests the procedure for applying the Wall-Modeled LES approach (WMLES). The well-known test problem of ventilation flow in a room where a plain air jet is supplied from a slit located under the ceiling [11] was chosen as the object of research. Detailed experimental data are available for this test on the distributions of the velocity components and their fluctuations, measured using Laser Doppler Anemometry (LDA). The test room in [11] was a rectangular parallelepiped with a square cross section; however, in this study, we formulated a three-dimensional problem with periodic conditions imposed in the transverse direction, which is to say that the side walls were excluded from consideration.

This statement makes it possible to correctly reproduce the flow structure only in the central part of the room, without affecting the three-dimensional structure of secondary flows. The clear advantage of such a "quasitwo-dimensional" simplified statement was that it made it possible to carry out a series of parametric calculations, considerably optimizing the computational costs.

We present the results of systematic calculations, and recommendations for applying the WMLES method developed based on these results.

The sidewall effect is considered in the second part of this study, published as a separate paper [16], providing a detailed comparison of the calculation results in a complete statement, without assuming periodic flow [11].

Problem statement

Room geometry. The air flow in a rectangular region is considered (Fig. 1). The coordinate system is chosen so that x is the longitudinal, y the vertical, and z the transverse direction. The origin of the coordinate system is at the corner of the room. The height of the room, taken as a length scale, is H = 3 m. The length of the room is L = 9 m, so L/H = 3. The room is assumed to be infinite in the lateral z direction, while calculations are carried out for three values of the width W of the computational domain, so that W/H is taken equal to 1/6, 1/3 and 1. Air is supplied to the room through an inlet slit with the height of $h_{in} = 0.056H = 0.168$ m and the width of W; this slit is located directly under the ceiling on one of the side walls. The outlet slit



Fig. 1. The geometry of the computational domain for the aspect ratio of the room W/H = 1

located near the floor on the opposite wall has a height of $h_{out} = 0.16H = 0.48$ m and a width of W. A channel with a length of 0.5H adjacent to the slit is included in the computational domain to prevent the formation of return currents at the outlet boundary of the domain.

Physical parameters of the environment and boundary conditions. Isothermal motion of air described by the model of incompressible fluid with constant physical properties is considered: the density $\rho = 1.23 \text{ kg/m}^3$, the dynamic viscosity $\mu = 1.79 \cdot 10^{-5} \text{ Pa} \cdot \text{s}$.

Air is supplied to the entrance to the room at a mean flow velocity equal to $V_{in} = 0.455$ m/s. The Reynolds number computed from the height of the inlet slit is $\text{Re} = \rho h_{in} V_{in} / \mu = 5233$. An auxiliary problem of air flow in a flat channel with a height of h_{in} , also based on the WMLES method was solved before imposing the boundary conditions at the inlet. The transverse dimensions of the computational domain in this case correspond to the selected value of W/H. The velocity distributions in the section $x/h_{in} = 18$ from the entrance to the channel served as the velocity profiles at the entrance to the room (a uniform profile was given at the entrance to the channel), extracted from the time-averaged solution. Additional calculations were carried out for the case with the transverse size W/H=1/6, giving a uniform velocity profile, as well as the inlet profile extracted from the solution to the problem of flow in the channel in the section $x/h_{\rm m} = 60$ at the entrance to the room.

Periodic boundary conditions were imposed at the lateral boundaries along the z direction. Soft boundary conditions were imposed at the outlet boundary. The remaining boundaries of the computational domain were solid walls on which the no-slip conditions were imposed.

Turbulence simulation. Turbulent air flow was simulated using the eddy-resolving WMLES approach, which is based on solving the filtered Navier–Stokes equations (see, for example, [9]). The instantaneous variables f are replaced by the sum of the filtered and subgrid-scale variables:

$$F = \tilde{f} + f'.$$

The value of \tilde{f} is determined by the expression

$$\tilde{f}(x,t) = \int_{Vol} G(x - x', \Delta) f(x', t) dx'^3, \quad (1)$$

where $G(x - x', \Delta)$ is the filter function determining the size and structure of smallscale turbulence (for example, a box filter); x is the coordinate of the point under consideration, Δ is the characteristic filter size (filter width). Eddies whose size is smaller than the filter width are not resolved.

The filtered Navier–Stokes equations for incompressible fluid with constant physical properties can be written in the following form:

$$\begin{cases} \nabla \cdot \mathbf{V} = 0; \\ \frac{\partial \mathbf{V}}{\partial t} + \nabla \cdot (\mathbf{V}\mathbf{V}) = \\ = -\frac{1}{\rho} \nabla \cdot p + 2\nu (\nabla \cdot \underline{S}) - \nabla \cdot \underline{\tau}^{SGS}, \end{cases}$$
(2)

where **V** is the velocity vector with the components (V_x, V_y, V_z) ; <u>S</u> is the strain rate tensor; $\underline{\tau}_{SGS}$ is the term resulting from spatial filtering of the equations.

The generalized Boussinesq hypothesis is used to determine the subgrid-scale stresses:

$$\tau_{ij}^{SGS} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\nu_{SGS}S_{ij}, \qquad (3)$$

where v_{SGS} , m^2/s , is the subgrid-scale turbulent viscosity to be found using some subgrid model.

The classical subgrid-scale model is the algebraic Smagorinsky model, proposed back in 1963 [17]. Based on dimensional analysis, the subgrid-scale viscosity in this model is expressed in terms of filter size and the magnitude of the strain-rate tensor:

$$v_{SGS} = (C_S \Delta)^2 S,$$

where $C_s = 0.2$ is the empirical Smagorinsky constant.

The computational grid acts as the filter in practical implementations of the LES approach, with Δ usually defined as the cube root of the volume of the grid cell.

The WMLES S-Omega approach was used in our calculations; its practical implementation is based on the data given in [18]. Compared with the classical Smagorinsky model, the subgrid-scale viscosity is determined here using a modified linear subgrid scale, a damping factor (similar to the Van Driest factor in the Prandtl model for the RANS approach), and the difference $|S - \Omega|$ instead of the magnitude of the strain-rate tensor S:

$$\nu_{SGS} = \min\left\{\left(\kappa d_{w}\right)^{2}, \left(C_{S}\Delta\right)^{2}\right\} \times \\ \times \left|S - \Omega\right| \left(1 - \exp\left\{\left(-y^{+}/25\right)^{3}\right\}\right),$$
(4)

where $C_s = 0.2$ is the empirical Smagorinsky constant; S, s⁻¹, Ω , s⁻¹, are the magnitudes of strain rate and vorticity tensors

$$S = (2S_{ij}S_{ij})^{0.5}, \Omega = (2\Omega_{ij}\Omega_{ij})^{0.5};$$

 $\kappa = 0.41$ is the Kármán constant; d_w , m, is the distance to the nearest wall, y^+ is the normalized distance from the center of the first near-wall cell to the wall ($y^+ = d_w u_x/v$, while $u_\tau = (\tau_w/\rho)^{0.5}$, m/s, is the dynamic velocity, τ_w , Pa, is the shear stress on the wall).

The filter size Δ included in expression (4), defining the linear subgrid scale, is determined by the formula

$$\Delta = \min \left\{ \max(C_{w}d_{w}, C_{w}\Delta_{\max}, \Delta_{wn}), \Delta_{\max} \right\},$$
(5)

where Δ_{\max} , m, is the maximum grid cell size (found as the maximum edge length for an orthogonal hexagon); Δ_{wn} , m, is the grid step along the normal to the wall; $C_w = 0.15$ is an empirical constant.

Since only averaged values were extracted from the solution of the auxiliary problem on air flow in a flat channel to impose the inlet boundary conditions, one of the available synthetic turbulence generators, the Vortex Method, was used to determine the instantaneous fluctuation characteristics (turbulent content) in the inlet section [19]. When the synthetic turbulence generator is activated, it is required to determine the turbulence intensity at the inlet boundary. The value I = 4% was taken in our calculations.

Computational aspects of the problem. Numerical modeling was carried out in the ANSYS Fluent 16.2* general-purpose hydrodynamic code, with discretization of the governing equations by the finite volume method. The parameters selected for the computational algorithm provided spatial and temporal discretization with second-order accuracy. The central differencing scheme was used for approximating the convective terms in the equation of motion.

The non-iterative algorithm corresponding to time advancement by the method of fractional steps (NITA) was used. The time step Δt , equal to 0.006 s, was chosen so that the maximum value of the Courant number on the finest grid was less than unity in all cells of the computational domain. The computations showed that increasing the time step from 0.006 to 0.010 s does not affect the averaged characteristics of the flow; however, NITA had to be abandoned when the local Courant number turned out to be greater than unity. The reason for this is that it proved impossible to ensure the time evolution of the solution by the method of fractional steps, as the residuals began to grow indefinitely. The development of unsteady flow was controlled by placing specific monitoring points in the computational domain, allowing to detect the transition to a statistically steady flow regime.

Quasi-structured unrefined uniform grids with identical cubic cells were built in the ICEM CFD generator for the computations. The number of cells was varied from 3 to 58 million. The data on the grids used in the computations are given in Table 1.

The main series of computations for analyzing the grid dependence of the solution was performed for the narrowest region with W/H= 1/6. The coarsest (initial) mesh consisted of 3 million cells, where the size of each cubic cell was $\Delta = 16.8$ mm. Finer grids were generated by gradually increasing the dimension of the initial grid by $\sqrt{2}$, 2, and $2\sqrt{2}$ times in each direction. Thus, the total number of cells for four successively refined grids was 3, 8, 23 and 58 million cells (see Table 1, from the 1st to the 4th grids).

The average normalized distance y^+ from the center of the first near-wall cell to the wall of the initial grid with a total dimension of 3 million cells does not exceed unity, while the maximum values located near the inlet slit reach $y^+ = 20$.

The computations were carried out using the resources of the Polytechnic Supercomputer Center (http://scc.spbstu.ru). The problems were run on the Polytechnic RSC Tornado cluster with a peak performance of 943 tera-flops. The cluster contains 668 dual-processor nodes (Intel (R) Xeon (R) E5 2697v3), each node containing 14 cores. A problem was run on a maximum of 512 parallel cores, while it took at least three weeks of real time (258,000 core hours) to accumulate unsteady statistics.

Computational results and discussion

Assessment of the relationship between resolved and simulated turbulence. The validity of applying the eddy-resolving approach was established by estimating the ratio of the resolved to the simulated components of the turbulent energy spectrum. The value of subgrid-scale (SGS) viscosity reflecting the contribution of the simulated turbulence can be used for this

^{*} ANSYS Inc. ANSYS Fluent 16.2 User's Guide, 2015.

Parameter values of computational grids used

Table 1

Daramatar	Notation	Parameter value for grid					
Farameter	Notation	1st	2nd	3rd	4th	5th	6th
Relative length of computational domain along <i>z</i> axis	W/H	1/6					1
	N_{x}	536	751	1070	1446	1070	751
Number of partitions along coordinate axis	N_y	179	252	354	482	354	252
	N_z	30	43	59	80	119	250
Total number of cells (rounded), million	$N_x \times N_y \times N_z$	3	8	23	58	46	48
Cell size, mm	Δ	16.8	12.0	8.4	6.2	8.4	12.0
×10 ³	Δ/H	5.6	4.0	2.8	2.1	2.8	4.0

estimation to some extent. Fig. 2, a-d shows the ratios of instantaneous fields of SGS to molecular viscosity, in several sections of the room. The computational results are given for the baseline (narrowest) computational domain with W/H = 1/6 (on a grid of 8 million cells) and for the case with the ratio W/H=1. The mean value of relative SGS viscosity for the entire computational domain is approximately equal to 3, while the maximum value does not exceed 7. Notably, the distributions of v_{SGS}/v for different widths of the computational domain differ qualitatively at small x (see Fig. 2,c): the spatial distribution of v_{SGS}/v for the ratio W/H =1 indicates a large transverse scale of turbulent eddies compared with the longitudinal scale; such eddies cannot develop when W/H=1/6because periodic conditions are imposed; the dependence of the solution on the transverse size of the computational domain is discussed below.

The SGS turbulent kinetic energy simulated can be estimated by the following formula [20]:

$$k_{\rm SGS} = 2C\Delta^2 |S|^2,$$

where C = 0.1.

Fig. 2, *e* shows the distribution of the instantaneous field of subgrid-scale turbulent kinetic energy k_{SGS} in a ratio to the mean resolved turbulent kinetic energy $\langle k \rangle$, defined as

$$\langle k \rangle = [\langle (V_x')^2 \rangle + \langle (V_y')^2 \rangle + \langle (V_z')^2 \rangle]/2.$$

The contribution of subgrid-scale kinetic energy to the total kinetic energy, equal to $\langle k \rangle + k_{SGS}$, is less than 3% in the jet region. The contribution of subgrid-scale kinetic energy to the total kinetic energy is even smaller in the backflow region, characterized by low velocities, and does not exceed 1% on average. In general, it can be concluded that the fraction of simulated turbulence is small, and the main contribution is made by resolved turbulence.



Fig. 2. Fields of ratios of SGS to molecular viscosity in sections z = 0.25 m (a), y = 1.5 m (b), x= 3.0 m (c) and x= 6.0 m (d); (e) is the field of subgrid-scale turbulent kinetic to resolved turbulent kinetic energy, in the section z = 0.25 m (the W/H values are shown)

Estimation of the Kolmogorov scale. The Kolmogorov scale η (m) is an important characteristic in simulation of turbulent flows, reflecting the characteristic size of the minimum eddies where kinetic energy dissipates due to the action of viscous friction forces. This scale determines the minimum requirements to the spatial resolution in direct numerical simulation, which must fully resolve the entire turbulent energy spectrum. The magnitude of the Kolmogorov scale is found by the formula

$$\eta = \left(\frac{v^3}{\varepsilon}\right)^{1/4},\tag{6}$$

where ε , m^2/s^3 , is the dissipation rate of turbulent kinetic energy per unit mass; v, m^2/s , is the kinematic viscosity.

The local values of the Kolmogorov scale for a near-ceiling jet take their minimum values in the region of the near-wall boundary layer in the initial zone of jet propagation. However, the degree of eddy resolution in the region of the near-wall boundary layer is not explicitly considered within our study; below we confine ourselves to discussing the quality of predicting wall friction by comparing solutions obtained on different grids. Quantitative estimates of the Kolmogorov scale were primarily carried out for the mixing layer whose degree of resolution is extremely important for adequately predicting the structure of the ventilation flow. Estimates of n are carried out using the computed data for the baseline (narrowest) computational domain with W/H= 1/6, while two different methods are used to determine the local dissipation rate of turbulent kinetic energy.

Method I for estimating ε . This method for determining ε to subsequently estimate the magnitude of the Kolmogorov scale η relies on the data from an additional steady RANS computation. A quasi-structured grid with the dimension of 141,000 cells clustered in the region of the mixing layer and to the walls of the room, so that the value of y^+ was less than unity (a grid-independent solution is taken for this grid). A uniform velocity distribution $(V_{in} = 0.455 \text{ m/s})$ was set at the inlet boundary. A semiempirical RNG k- ε turbulence model was used to close the RANS equations, allowing to directly extract the field ε from the obtained numerical solution.

As it turned out, there are pronounced differences in the flow structures predicted by the RANS and WMLES computations in the baseline computational domain at W/H = 1/6. This is confirmed by comparing the fields of the mean velocity magnitude obtained by the given approaches (Fig. 3, *a* and *b*). As revealed below, the reason for the differences in the flow structure is that the results of WMLES computations at W/H = 1/6 largely depend on the size of the computational domain in the transverse direction. The distribution of η , computed from such a 'mismatched' distribution of ϵ , is shown in Fig. 3,*c*.

In addition, an auxiliary 2D RANS problem was solved, where a 'frozen' velocity field, extracted from the WMLES computation, was given, considering the mean field in the central section of the room, z= 0.25 m (see Fig. 3,b). The equations of motion were not solved in the 'frozen' statement; only the turbulence characteristics were computed (also using the



Fig. 3. Fields of mean velocity modulus magnitude, computed by RANS (*a*) and WMLES (*b*) models; RANS computations of Kolmogorov scale distributions, obtained from the ε fields, corresponding to two different flow patterns (*c*,*d*);

The dashed line in Fig. 3, b marks a part of the section for data analysis in the mixing layer

RNG *k*- ε model). The field of ε obtained by this method was also used to calculate the field of η (see Fig. 3,*d*).

It can be seen from Fig. 3, c that the local value of the Kolmogorov scale in the distribution of η , computed from the field of ε corresponding to the combined RANS computations of the distributions of velocity and turbulent characteristics, varies from $\eta_{min} = 0.42$ mm in the region of the jet mixing layer up to $\eta_{max} = 13.3$ mm in the region of low-velocity flow (see Fig. 3, c, bottom left corner). The distribution of the Kolmogorov scale constructed from the field of ε corresponding to the 'frozen' WMLES velocity field is shown in Fig. 3,d. In this case, the distribution of local values of η differed considerably from the picture shown in Fig. 3, *c* but the minimum value practically did not change: $\eta_{min} = 0.43$ mm; the localization of the region of small values of η did not change either, while the maximum value of η in this

case was $\eta_{max} = 34$ mm. Thus, the dimension of the grid for direct numerical simulation of the flow in the region W/H=1/6 on a uniform grid of cubic elements with a linear size η_{min} should be at least 182 billion cells. A grid with the total dimension of at least 1100 billion cells will be required for DNS computations in the region W/H=1, described in the experimental study [11]; in this case, the time step value should not exceed 10^{-3} s to ensure the Courant number values less than unity. Importantly, these estimates do not take into account the decrease in η in the boundary layer of the near-wall jet, so grids of even higher dimensions are required to perform DNS computations in reality.

The results of the estimates are summarized in Table 2, listing the ratios of the linear size of the cell in the computational grid to the local minimum and maximum values of the Kolmogorov scale for the four cases considered.

Method II for estimating ε . This method for determining ε directly uses the data obtained by the LES approach based on interpreting the equation for kinetic turbulent energy:

$$\frac{\partial k}{\partial t} + \overline{V_j} \frac{\partial k}{\partial x_j} + \frac{\partial}{\partial x_j} \overline{V'_j k} =$$
$$= -\frac{1}{\rho} \frac{\partial}{\partial x_j} \delta_{jk} \left(\overline{V_k p} \right) +$$
(7)

$$+\nu\frac{\partial^2 k}{\partial x_j^2}-\overline{V_j'V_k'}\frac{\partial \overline{V_k}}{\partial x_j}-\nu\frac{\partial V_k'}{\partial x_j}\frac{\partial V_k'}{\partial x_j},$$

where the last term is exactly the expression for its dissipation rate,

$$\varepsilon = v \frac{\partial V_k'}{\partial x_j} \frac{\partial V_k'}{\partial x_j}.$$
 (8)

The DNS approach allows to fully resolve the turbulent energy spectrum; therefore, if the dissipation rate is calculated directly by Eq. (8), it is determined exactly. The dissipation rate has a maximum in the high-frequency part of the energy spectrum, and the high-frequency part of the spectrum is simulated by the SGS viscosity in the LES method, so the value of the resolved dissipation rate calculated by Eq. (8) is underestimated compared to the exact value of ε . The value of ε increases in LES computations of successively refined grids that provide a better resolution of the high-frequency region of the spectrum Accordingly, the values of η decrease, approaching the exact value.

The estimate of η , obtained by directly calculating ε using Eq. (8), is illustrated in Fig. 4, *a,b*, where the isolines correspond to the distributions for the ratio of the linear cell size in the grids, consisting of 8 and 58 million cells, to the local values of the Kolmogorov scale. The corresponding minimum values η_{min} for different grids are given in Table 2: the value of the Kolmogorov scale decreases by 33% as the grid is refined from 3 to 58 million cells (the size of cubic elements decreases by almost 3 times).

The dissipation rate of turbulent kinetic energy can be also estimated from the data of LES computations according to the method proposed in [22]; this procedure has already been successfully applied in [23], considering the problem of jet flow. According to the data in [22], instead of directly estimating the value of ε from the LES data, all the other terms in Eq. (7) can be calculated, yielding an indirect but more accurate estimate of ε (the sum of all calculated terms should be substituted into equation (6) to find η). The value of the Kolmogorov scale obtained in this way should not change substantially with the change in the dimension of the computational grid.

To estimate η in the mixing layer, it is sufficient to calculate only one component in the generation term entering into Eq. (7), which makes the dominant contribution to generating turbulence in this region:

$$\overline{V_{y}V_{x}}\frac{\partial \overline{V_{x}}}{\partial y} = \left(\overline{V_{y}V_{x}} - \overline{V_{y}}\ \overline{V_{x}}\right)\frac{\partial \overline{V_{x}}}{\partial y}.$$
 (9)

Table 2

Grid Number	Quantity	Calculated value				
Ond Number	Qualitity	Ι	II	III	IV	
$(\Delta = 16.8 \text{ mm})$	η_{min} , mm	0.42	0.43	1.41	0.56	
	η_{max}, mm	13.3	34.0	8.7	_	
	$\Delta\!/\eta_{\rm min}$	40	39	12	30	
	$\Delta\!/\eta_{max}$	1.3	0.5	1.9	_	
$2nd \\ (\Delta = 12.0 \text{ mm})$	η_{min} , mm	0.42	0.43	1.27	0.63	
	$\eta_{_{max}}, mm$	13.3	34.0	9.0	_	
	$\Delta\!/\eta_{\rm min}$	29	28	9	19	
	$\Delta\!/\eta_{max}$	0.90	0.35	1.30	—	
$3rd \\ (\Delta = 8.4 \text{ mm})$	η_{min} , mm	0.42	0.43	1.14	0.64	
	η_{max}, mm	13.3	34.0	9.8	_	
	$\Delta\!/\eta_{\rm min}$	20	20	7	13	
	$\Delta\!/\eta_{max}$	0.60	0.25	0.90	_	
$4th \\ (\Delta = 6.2 \text{ mm})$	η_{min} , mm	0.42	0.43	1.06	0.64	
	η_{max}, mm	13.3	34.0	9.2	_	
	$\Delta\!/\eta_{\rm min}$	15	14	6	10	
	$\Delta\!/\eta_{max}$	0.50	0.18	0.70	—	

Values of Kolmogorov scale estimated by methods I–IV

Notes. 1. About the methods: I, II determined the ratios of the cell size Δ to the minimum (η_{min}) and maximum (η_{max}) values of the local Kolmogorov scale (KS), calculated from the RANS computations of the velocity field and turbulence characteristics (I), and in the 'frozen' WMLES velocity field (II); III, IV constructed the KS by the dissipation rate resolved in the LES computation (8) (III), as well as according to the dissipation rate estimated based on expression (9) (IV).

2. The numbering of the grids corresponds to Table 1.



Fig. 4. Distribution of ratio of linear cell size to Kolmogorov scale, computed directly by the estimate of ε based on the data from LES computations (a,b), and by the estimate based on expression (9) (c,d). Data are given for the jet region.

The dimension of the grids was 8 million (a,b) and 58 million (c,d) cells



Fig. 5. Distributions of skin friction coefficient along the upper (a) and lower (b) walls; velocity profiles along the lines A-A and B-B (c).
The dimensions of the grids used, million cells: 3, 8, 23 (long, medium and short dashes, respectively) and 58 (solid line)

Calculating term (9) from the data of WMLES computations allowed to obtain one more estimate of ε and, accordingly, the Kolmogorov scale. The distributions of the ratios of linear cell sizes in the grids consisting of 8 and 58 million cells to the local values of the field of η computed in this way are shown in Fig. 4, c, d, respectively. The computed minimum values η_{min} for different grids are given in the last column of Table 2: they practically do not vary from grid to grid, tending to η_{min} = 0.64 mm as the grid is refined. In this case, a computational grid with the dimension of 51 billion cells is required to carry out valid DNS computations for W/H = 1/6 (306 billion cells for W/H = 1).

Dependence of the solution on the grid parameters. A series of parametric computations estimating the degree to which the inlet boundary conditions affected the solution was also carried out for the computational domain W/H= 1/6. Fig. 5, a, b shows the time-averaged distributions of the skin friction coefficient C_f along the midsection of the upper and lower walls (with no additional spatial averaging). Apparently, the quantitative prediction of the skin friction coefficient depends on the degree of spatial resolution, especially on the upper wall. A monotonic increase in friction is observed as the grid is refined. The differences between the solutions obtained on the initial (3 million cells) and on the first refined (8 million cells) grids reach 15%; with grid dependence grows with further refinement. Some qualitative influence of the spatial resolution on the predicted flow structure is also observed, as evidenced by the local differences in friction distributions. For example, the near-wall jet separates in the vicinity of the upper wall at x > 7 m, generating a recirculation zone (see Fig. 5,a). The position of the separation point depends on the dimension of the computational grid: separation on the coarsest grid occurs approximately 1 m closer to the entrance compared with the grid with the most refined spatial resolution. The positions of the points on the bottom wall where the flow separates and reattaches also depend on the grid to some extent (see Fig. 5,b).

Fig. 5, c shows the distributions of the averaged longitudinal velocity along the vertical lines located in the mid-section: A-A with x/H = 1.0 and B-B with x/H = 2.0 (shown with in Fig. 1 with a dashed line). The dependence of the velocities in the jet on the spatial resolution can be observed: the finer the grid, the higher the maximum velocity in the jet, both in section A-A (region I) and in section B-B (region III). Some grid dependence is also visible in the backflow region (section B-B, region II).

The results of computations on the grids consisting of 23 and 58 million cells are close



Fig. 6. Averaged flow structure (longitudinal velocity along lines *A*-*A* and *B*-*B*) depending on different velocity profiles at the inlet (*a*), and on using a synthetic turbulence generator (the data obtained when the generator was turned off is shown with long dashes) for the same inlet profile $x/h_{in} = 18$ (*b*); (*a*) corresponds to the inlet velocity profiles: uniform (short dashes),

at $x/h_{in} = 18$ and 60 (solid and dash-dotted lines, respectively)

to each other both in velocity profiles and in the friction distributions. Thus, the solution can be interpreted as almost grid-independent for a grid with the dimension of 23 million cells. The grid dependence of the solution is more pronounced for cells with a linear size of 12 mm (a grid of 8 million cells); however, it was decided to use these cells with increasing transverse size of the computational domain. If a finer grid with a linear cell size of 8 mm were used in the computations for W/H= 1, it would consist of approximately 140 million cells, which was unacceptable with the available computing resources.

Influence of inlet boundary conditions. A series of parametric computations estimating the degree to which the inlet boundary conditions affected the solution was also carried out for the computational domain W/H= 1/6 (a grid with the dimension of 8 million cells). Three different velocity profiles were considered (homogeneous profile and profiles extracted from the solution of the problem on the flow in a channel in a section 18 and 60 calibers from the entrance to the channel). An additional alternative without a synthetic turbulence generator was calculated for a profile taken in a cross section of 18 calibers.

The influence of the inlet boundary conditions is illustrated in Fig. 6, showing the distributions of the averaged longitudinal velocity component along the same vertical lines A-A and B-B located in the mid-section. The dependence of the averaged flow structure on the velocity profile at the inlet is illustrated in Fig. 6,a (all distributions given here were obtained using a synthetic turbulence generator). Evidently, the velocity in the jet is somewhat higher when a well-developed profile is given at the inlet: the differences in the section A-A (region I) are about 10%, stratification of the velocity distributions is also pronounced downstream. The backflow is also characterized by a lower intensity for a uniform profile (see Fig. 6, a, section *B-B*, region II). Note that the two solutions obtained for two inlet velocity distributions different from a uniform profile are very close to each other.

A comparison of the velocity distributions obtained for the same inlet profile with and without a synthetic turbulence generator is shown in Fig. 6, b. It can be seen that the velocity in the jet core turns out to be somewhat lower in the case when the turbulence generator is not used, and the degree of the generator's influence approximately corresponds to the transition from a uniform to a well-developed profile. However, using a synthetic turbulence generator has little effect on the description of the general air circulation in the room, including the level of velocities in the backflow zone.



Fig. 7. Fields of mean velocity magnitude in the longitudinal mid-section, obtained for two statements of the problem: periodic (a-c) and full, with side walls [16] (d). Values of W/H are shown



Fig. 8. Computed (lines) and experimental [11] (symbols) profiles of mean longitudinal velocity in four sections, obtained in a full statement with side walls [16] (solid lines) and in a periodic setting (other lines) at different values of W/H:
1/6 (short dashes), 1/3 (long dashes) and 1 (dash dotted line)

Influence of the length of the computational domain in the transverse direction. It is a well-known situation in simulation of periodic flows using eddy-resolving approaches that the solution can be significantly affected by the insufficient length of the computational domain in the periodic direction. A series of computations was carried out to investigate the effect of this parameter in the given problem; the relative width of the computational domain was taken equal to W/H = 1/6 (the standard case, for which the study of the grid dependence and the influence of boundary conditions at the inlet is presented above), W/H = 1/3, and 1.

The structure of the averaged flow obtained in a periodic statement for the three indicated values of W/H is shown in Fig. 7, a-c; Fig. 7, d shows the flow structure computed in the full statement, taking into account the side walls [16]. Evidently, a two-vortex flow pattern is observed at W/H = 1/6 and 1/3: an intense secondary flow occupies only the right half of the computational domain, while a less intense secondary eddy with the opposite direction of rotation evolves in the left half. Increasing the dimension of the computational domain in the periodic direction changes the pattern of the averaged flow: a pair of large eddies transforms into a single one, occupying almost the entire computational domain (see Fig. 7,*c*). Note that the flow structure obtained in the periodic statement at W/H = 1 practically coincides with the flow pattern in the mid-section (see Fig. 7, *d*), computed in the full statement, with side walls.

The influence of the length of the computational domain in the periodic direction is also illustrated by the velocity profiles shown in Fig. 8 in comparison with the experimental data [11]. The lines located here in the

mid-section were shown above by the dashed line in Fig. 1: *A*-*A* and *B*-*B* are vertical lines; *C*-*C* and *D*-*D* are horizontal lines with y/H = 0.972 and 0.028, respectively.

It can be seen from Fig. 8 that the profiles obtained for W/H = 1 in the periodic and full statements coincide almost completely. These computations adequately reproduce the flow pattern that was observed experimentally [11] (the quantitative differences between the computational results in the full statement and the experimental data obtained for the backflow region are discussed in [16]). It should be concluded that the flow structure for $W/H \ge 1$ is reproduced correctly for the region that is infinite in the z direction. The periodic conditions significantly affect the shape and length of the eddies in the transverse direction for a computational domain of a smaller length, and a certain anisotropy is observed. Eddy structures that are large-scale in the transverse direction are observed at W/H=1in the instantaneous fields of SGS viscosity given above (see Fig. 2, c, d). It is impossible to reproduce such eddies in the numerical solution in simulations with a computational domain of a smaller transverse size, which leads to noticeable changes in the averaged fields.

Even though the structure of the averaged flow depends on the size of the computational domain in the standard case with W/H=1/6, it reflects all the characteristic features of the given flow, namely: the propagation of a near-wall turbulent jet, the development of a mixing layer and the formation of large eddy structures governing the flow as a whole. Thus, the computational results on the influence of the grid and the inlet boundary conditions obtained at W/H=1/6 can be extended to all of the situations considered.

Conclusion

Eddy-resolving WMLES approach was used in this study for numerical simulation of turbulent air flow in a room ventilated by a 2D air jet supplied from a slit located under the ceiling with the Reynolds number $Re = 5 \cdot 10^3$. The problem was posed in a periodic statement describing a quasi-two-dimensional flow in a room strongly elongated in the transverse direction. The calculations were carried out in the ANSYS Fluent general-purpose CFD code, providing second-order spatial and temporal discretization.

The dependence of the solution on the grid was analyzed in a series of calculations performed on grids with the linear size of a cubic cell ranging from 6 to 16 mm; a baseline grid with a linear cell size of 12 mm was found acceptable. Estimates of the Kolmogorov scale revealed that the minimum values of the Kolmogorov scale in the mixing layer are locally about 20 times smaller than the linear cell size for the standard grid.

We have found that using a synthetic turbulence generator for imposing the inlet boundary conditions has practically no effect on the description of the general air circulation in the room, including the level of velocities in the backflow zone.

We have established that the length of the computational domain in the transverse direction noticeably affects the calculation results if $W/H \le 1$. In case of calculations in the region with the length $W/H \ge 1$, the averaged structure of a quasi-two-dimensional flow is reproduced correctly in a room elongated in the transverse direction.

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THE AUTHORS

ZASIMOVA Marina A.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation zasimova_ma@spbstu.ru

IVANOV Nikolay G.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation ivanov_ng@spbstu.ru

MARKOV Detelin

Technical University of Sofia 8 Kliment Ohridsky boulevard, Sofia, 1000, Bulgaria detmar@tu-sofia.bg

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СВЕДЕНИЯ ОБ АВТОРАХ

ЗАСИМОВА Марина Александровна — ассистент Высшей школы прикладной математики и вычислительной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 zasimova_ma@spbstu.ru

ИВАНОВ Николай Георгиевич — кандидат физико-математических наук, доцент Высшей школы прикладной математики и вычислительной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 ivanov_ng@spbstu.ru

МАРКОВ Детелин – *PhD, доцент Софийского технического университета, г. София, Болгария.* 1000, Болгария, г. София, бульвар Климента Орхидского, 8 detmar@tu-sofia.bg

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NUMERICAL MODELING OF AIR DISTRIBUTION IN A TEST ROOM WITH 2D SIDEWALL JET. II. LES-computations for the room with finite width

M.A. Zasimova¹, N.G. Ivanov¹, D. Markov²

¹ Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation;

² Technical University of Sofia, Sofia, Bulgaria

The paper presents the results of numerical modeling of turbulent airflow in a test room based on the vortex-resolving wall-modeled large eddy simulation approach. The room ventilation is provided by a plain air jet at Re = 5233. The jet is supplied from a slit placed at a side wall under the ceiling. The problem formulation reproduces the test experiment conditions (Nielsen et al., 1978, 1990) as completely as possible. Two configuration with various air supply slit width are considered. Calculations are carried out with the ANSYS Fluent software using the grid consisting of 48 million cells. The paper demonstrates that in the near-wall jet zone the computational results agree well with the experimental data, but visible disagreement is obtained in the recirculation flow region (occupied zone) with relatively low velocities.

Keywords: turbulent airflow, plain jet, large eddy simulation, ventilation

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ЦИРКУЛЯЦИИ ВОЗДУХА В ПОМЕЩЕНИИ ПРИ ПОДАЧЕ ИЗ ПЛОСКОЙ ЩЕЛИ. II. LES-расчеты для помещения конечной ширинЫ

М.А. Засимова¹, Н.Г. Иванов¹, Д. Марков²

¹ Санкт-Петербургский политехнический университет Петра Великого, Санкт-Петербург, Российская Федерация;

² Софийский технический университет, София, Болгария

Представлены результаты численного моделирования турбулентного течения воздуха в тестовом помещении на основе вихреразрешающего подхода — метода моделирования крупных вихрей с пристенным моделированием. Вентиляция помещения осуществляется плоской воздушной струей, подаваемой из расположенного под потолком на торцевой стенке щелевого отверстия, при Re = 5233. Задача ставилась в постановке, максимально полно воспроизводящей условия тестовых экспериментов (Nielsen et al., 1978, 1990). Рассмотрены две геометрические конфигурации, отличающиеся шириной входного отверстия. Расчеты в программном пакете ANSYS Fluent выполнены с использованием сетки размерностью 48 млн. ячеек. Показано, что результаты расчетов хорошо согласуются с экспериментальными данными в пристенной струе, однако наблюдается заметное рассогласование результатов расчетов и эксперимента в зоне возвратного течения (обитаемой зоне), характеризующейся малыми скоростями.

Ключевые слова: турбулентное течение, плоская струя, метод моделирования крупных вихрей, вентиляция

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Introduction

A crucial factor in developing and optimizing heating, ventilation and air conditioning (HVAC) systems for residential, public and industrial buildings is organizing the air exchange ensuring comfortable microclimate for humans. The most popular methods used for simulation of air exchange are based on integral estimates and balance ratios corresponding to various conditions of supply air distribution [1]. These methods integrate empirical approaches and can be only adjusted to a specific type of flow (propagation of a free submerged jet, propagation of a near-wall jet, etc.). For this reason, balance computational methods do not always yield complete and quantitatively reliable data even for integral flow parameters in real conditions, for example, for rooms with complex geometry. Furthermore, air in applied problems is typically supplied to a room using various types of diffusers, and it is difficult to describe the characteristics of diffusers in computational methods. A complete picture of the flow, including data on the mean and local characteristics of the flow, can be gained using more accurate approaches to describing the turbulent motion of air.

Data on the spatial structure of the flow, typical for ventilation problems, which is important for substantiating design decisions, can be obtained by numerical modeling of multidimensional fluid dynamics problems. One of the most common approaches to numerical modeling of turbulent flows is solving steady/ unsteady Reynolds-averaged Navier-Stokes equations (often referred to as RANS/URANS in literature) [2], closed by a semi-empirical turbulence model. Notably, the available studies on free jet flows suggest that two-parameter k- ε turbulence models [3], as well as Sekundov's model [4] with one differential equation return satisfactory results; however, validation of RANS data for simulation of complex jet flows remains a pivotal challenge.

Eddy-resolving approaches are methods for predicting the parameters of turbulent flows, have high accuracy, making it possible to obtain not only averaged but also instantaneous fields of physical quantities. The classical eddy-resolving approaches include, first of all, the direct numerical simulation method (DNS) based on directly solving the full Navier–Stokes equations. Another eddy-resolving approach is Large Eddy Simulation (LES), solving the filtered Navier–Stokes equations, which allows to resolve large eddies but requires semi-empirical modeling of small-scale eddies.

Eddy-resolving approaches have extremely high computational costs; however, the LES approach takes less computational resources compared to DNS, especially if there is no goal to resolve the near-wall regions and the simulation is limited to applying techniques based on the RANS approach. Hybrid RANS-LES approaches, including Wall Modeled LES (WMLES) have seen rapid advances over the past two decades. For example, eddy-resolving approaches are described in [5, 6].

The degree of uncertainty for the eddy-resolving LES and RANS-LES models, as well as for other approaches to modeling turbulence including some empiricism can be estimated by solving test problems for which reliable and well-described experimental data are available.

This study presents the results of validation computations for the well-known test problem of ventilation flow in a room where an air jet is supplied from a slit located under the ceiling [7, 8]. A series of laboratory experiments described in [7, 8] was aimed at studying turbulent air flow in the model of a ventilated room. Laser Doppler anemometry (LDA) was used for measuring the velocity fields and fluctuation characteristics with controlled accuracy. The measurement data are well documented: they are represented graphically in [7, 8] and available as a database at http://www. cfd-benchmarks.com/.

This paper continues the investigation in [9], where technique involving the WMLES approach was tested for computations in a simplified periodic statement. In contrast to [9], we consider the full statement of the problem, including the side walls and most accurately reproducing the experimental conditions.

Studies with numerical simulation of experiment in [7]

Table

No.	Authors	Year	Country	Method	Code	Computational Grid		
2D problem statement								
[10]	Heikkinen, Piira	1991	Finland	RANS (k-ε)	WISH	$\begin{array}{c} 28 \times 17, \\ 45 \times 26 \end{array}$		
[11]	Vogl, Renz	1991	Germany	RANS $(k-\varepsilon)$	Fluent	56 × 62		
[12]	Skalicky, Morgenstern, Auge, Hanel, Rosler	1992	Germany	RANS (k-ε)	Psiom2D ResCUE	$64 \times 32,$ 128×64		
[14]	Chen	1995	USA	$\begin{array}{c} \text{RANS} (k\text{-}\varepsilon) \\ k\text{-}\varepsilon \text{ RNG} \end{array}$	PHOENICS	$50 \times 45, 100 \times 70$		
[15]	Chen	1996	USA	RANS (k-ɛ; RSTM –IP, –GY, –QI)	PHOENICS	50 × 45		
[16]	Peng, Davidson, Holmberg	1996	Sweden	RANS (LRN k-ε)	CALC-BFC	50 × 47, 102 × 132		
[19]	Bennetsen	1999	Denmark	RANS (k - ε , k - ω , ASM, DSM)	CFX 4.2	$72 \times 48, \\144 \times 96$		
[20]	Voight	2001	Denmark	RANS (<i>k</i> -ε, RNG, LS; <i>k</i> -ω, SST)	EllipSys	$192 \times 128, 288 \times 192$		
[23]	Mora, Gadgil, Wurtz	2003	USA, France	RANS (<i>k</i> -ε) Zonal models: PL, PL-SDF, SD-SDF	SPARK Star CD	$10 \times 10, \\ 40 \times 40$		
[25]	Rong, Nielsen	2008	Denmark	RANS (k-ε; k-ω, BSL, SST)	CFX 11.0	4,736, 18,944, 28,800 cells		
[26]	Dreau, Heiselberg, Nielsen	2013	Denmark	RANS (<i>k</i> -ε) low-Re, realizable; <i>k</i> -ω, SST)	CFX 11.0 Star-CCM+	4,068, 4,793, 16,658 cells		
[29]	Yuce, Pulat	2018	Turkey	RANS $(k-\varepsilon; k-\omega)$	Fluent 16.2	4,000–43,100 cells		
	-		3D problem	with periodic conditi	on			
[13]	Rosler, Hanel	1993	Germany	RANS (k-ε)	ResCUE	$\begin{array}{c} 64 \times 28 \times 4, \\ 128 \times 48 \times 4 \end{array}$		
[20]	Voight	2001	Denmark	RANS (k-ε LS, k-ω, k-ω BSLREV)	EllipSys	$96 \times 64 \times 16$		
[27]	Ivanov, Zasimova	2018	Russia	WMLES S-Omega	Fluent 16.2	751×252×250		
			3D p	roblem statement				
[17]	Davidson, Nielsen	1996	Sweden Denmark	LES (Smagorinsky, dynamic Germano)	SLAP	$72 \times 42 \times 52, \\102 \times 52 \times 52$		
[18]	Davidson	1996	Sweden	RANS (<i>k</i> -ε), LES (Smagorinsky, dynamic Germano)	CALC-BFC	$72 \times 42 \times 52, \\ 102 \times 52 \times 52$		
[19]	Bennetsen	1999	Denmark	RANS (k-ε, RNG; k-ω, ASM, DSM), LES (MS, Smagorinsky, dynamic Germano	CFX 4.2 LESROOM	96 \times 64 \times 32, 84 \times 72 \times 72 (RANS) 64 \times 64 \times 32, 96 \times 64 \times 64 (LES)		

No.	Authors	Year	Country	Method	Code	Computational Grid
[20]	Voight	2001	Denmark	RANS (k-ε LS, k-ω BSLREV), LES (Mixed Scale, Smagorinsky,	EllipSys	$96 \times 64 \times 16 (RANS) 72 \times 48 \times 36, 96 \times 64 \times 48 (LES)$
[21]	Jiang, Chen	2001		LES (Smagorinsky,		
[22]	Jiang, Mingde, Chen	2003	USA	Filtered Dynamic, Small-Scale model)	PHOENICS	$\begin{array}{c} 66 \times 18 \times 34, \\ 66 \times 34 \times 34 \end{array}$
[24]	Ivanov	2005	Belgium Russia	RANS (k-ε) LS; SA)	SINF, FINE	$\begin{array}{c} 37 \times 41 \times 29, \\ 73 \times 81 \times 57 \end{array}$
[27] [28]	Ivanov, Zasimova	2018	Russia	WMLES S-Omega	Fluent 16.2	751×252×250
[30]	Van Hoof, Blocken	2019	Belgium	RANS	Fluent 15.0	212,160– 1,697,280 cells

Continued

Notations: RSTM is the Reynolds Stress Models [6], LRN is the Low Reynolds Number correction, BSL is Baseline revised, LS is the Launder Sharma k- ϵ model, ASM is the Algebraic Stress Model, DSM is the Differential Reynolds Stress Model.

Since experimental data in [7] were first published, multiple attempts have been made to reproduce the qualitative picture of the flow and quantitative data on the velocity profiles using the methods of computational fluid dynamics. Aside from the actual experimental data, the CFD Benchmarks website contains the best known computational data obtained by various scientific groups from 1991 to 2013 for the conditions corresponding to the test [7]. Notably, no results of numerical simulation are available in literature for the conditions of the experiment described in [8] with a smaller width of the inlet slit.

The table contains brief information about the studies [10-30] giving the results of numerical modeling of air exchange in a room model close to the data in [7]. The calculations were carried out in two-dimensional, quasi-two-dimensional (imposing periodic conditions in the transverse direction) and three-dimensional statements. These studies describe in detail the computational results, establishing the influence of turbulence models and various numerical parameters on the obtained solution.

The table provides data on the general dimensions of the computational grids used in numerical computations described in [10–30]. Naturally, the dimensions of the grids gradually increase over time: for example, the coarse computational grid used in computations in 1991 consisted of 100 control volumes, while the finest grid consists of approximately $4.8 \cdot 10^7$ cells (2018).

It is evident from the data in the table that the model problem was numerically solved both using the RANS approach, closed by semiempirical turbulence models (such as $k-\varepsilon$, $k-\omega$, $k-\omega$ SST, etc.), and using the eddy-resolving LES approach in combination with different subgridscale models. Until recently, only three research groups (Davidson et al. [17, 18], Bennetsen [19], Voight [20]) performed computations for the model problem [7] using the LES approach; however, the computational grids were very rough by modern standards (with dimensions of less than half a million cells). Importantly, it is now clear [9] that such grids do not allow to describe the behavior of three-dimensional turbulent structures with a sufficient degree of accuracy for the given problem.

Generalizing the results of numerical simulation available in literature for the experimental conditions in [7], we can conclude that the general picture obtained for the averaged flow agrees with the experiment but the local characteristics turn out to be inaccurate. It is now possible to run accurate numerical simulations of turbulent flows on fairly refined grids (with dimensions up to 10^7-10^8 cells) based on different eddy-resolving approaches, including WMLES.

This study presents the results of numerical simulation of turbulent airflow in a closed room using the eddy-resolving WMLES approach for the conditions approximating the experiments in [7, 8].

Problem statement

Room geometry. We considered airflow in a room shaped as a rectangular parallelepiped with the dimensions $3H \times H \times H$. The room is shown schematically in Fig.1, *a*, the origin of the coordinate system is located in the bottom corner of the room. The height of the room H = 3 m was taken as the length scale.

The inlet to the computational domain was located on the side wall of the room, under the ceiling; this inlet was an air slit with the width w_{in} and the height $h_{in} = 0.056H = 0.168$ m. In accordance with different experimental conditions in [7, 8], two geometric configurations with different inlet widths were considered.

In the first scenario, the slit width coincided with the room width, $w_{in} = H$; this statement of the problem corresponds to the experimental conditions in [7].

In the second scenario, the width of the slit was halved and was equal to $w_{in} = 0.5H$, the slit was located in the center relative to the side walls of the room (see Fig. 1,*a*); this statement corresponds to the experimental conditions in [8].

A rectangular exhaust slit with the width H and the height $h_{out} = 0.16H = 0.48$ m was located on the opposite side wall, near the floor, discharging air from the room. An outlet ventilation duct shaped as a rectangular parallelepiped with the dimensions

 $0.50H \times 0.16H \times 1.0H$ was installed adjacent to the slit in order to prevent backflow generated on the surface of the exhaust slit.

The experimental data from [7, 8] are available along the lines marked with dashes in Fig. 1,*a*. Vertical lines *A*-*A* are located at x = 1.0H, and *BB* at x = 2.0H; horizontal lines *C*-*C* are located at y = 0.972H (at a distance $h_{in}/2$ from the ceiling, which corresponds to the midsection of the inlet slit), and *D*-*D* at y = 0.028H (at a distance $h_{in}/2$ from the floor). The subscripts '1' correspond to the central section of the room (z = 0.5H), and '2' to the lateral section (z = 0.1H).

Notably, the laboratory experiments in [7, 8] were carried out in a scaled-down model of the room to reduce the errors in measuring the velocity: the width and height of the model were the same and were H = 0.0893 m, and the length was 0.268 m. However, the descriptions in [7, 8] and in subsequent numerical studies were given for the data scaled to full-size conditions.

Boundary conditions. The problem is considered in the isothermal approximation, which corresponds to the experimental conditions, where a uniform temperature field was maintained in the room. A model of incompressible fluid with constant physical properties was used to describe isothermal motion of air: density $\rho = 1.23$ kg/m³, dynamic viscosity $\mu = 1.79 \cdot 10^5$ Pa·s.



Fig. 1. Geometric model of the room (*a*). Experimental data are available along the additional lines shown; the lines and the symbols correspond, respectively to computed and experimental distributions of longitudinal velocity at the entrance to the room along two axes (*b*, *c*) for the scenario with $w_{in} = 3$ m; sections at z = 3.000 m (*b*) and y = 2.916 m (*c*) are shown

Air is supplied to the entrance to the room at an average velocity equal to $V_{in} = 0.455$ m/s (this value corresponds to a volumetric flow rate of 825 m³/h for the first scenario with a wide inlet slit). The Reynolds number computed from the height of the inlet slit is Re = $\rho h_{in} V_{in}/\mu = 5.23 \cdot 10^3$.

The experimental velocity distributions in the inlet section along the central longitudinal and transverse lines are shown by symbols in Figs. 1, b, c. We should note that the inlet ventilation duct is not described in [7, 8], which is to say that no data was provided for how the inlet velocity field was generated.

The inlet velocity profiles were extracted from an additional WMLES solution to the corresponding problem of airflow in a straight ventilation duct with the dimensions $L_{duct} \times h_{in} \times w_{in}$. The duct length was taken equal to $L_{duct} = 2.0H$ = 6 m, and its cross section corresponded to the inlet slit with the dimensions $h_{in} \times w_{in}$.

Soft boundary conditions were imposed at the exit boundary of the computational domain. The remaining boundaries of the computational domain were solid walls where no-slip conditions were imposed.

Mathematical model. Turbulent air flow was simulated using the eddy-resolving WMLES approach, which is based on solving the filtered Navier–Stokes equations (see, for example, [31]). By applying the filtering procedure, the instantaneous variables f in the Navier–Stokes equations are replaced by the sum of filtered and subgrid-scale variables $f = \tilde{f} + f$. The quantity \tilde{f} is determined by the expression

$$\tilde{f}(x,t) = \int_{Vol} G(x-x',\Delta) f(x',t) dx^{3}, \quad (1)$$

where $G(x - x', \Delta)$ is the filtering function determining the size and structure of small-scale turbulence (for example, a box filter); *x*, m, is the coordinate of the given point, Δ , m, is the characteristic size of the filter (filter width).

Eddies whose size is smaller than the filter width are not resolved.

The filtered equations for incompressible fluid with constant physical properties can be written in the following form:

$$\begin{cases} \nabla \cdot \mathbf{V} = 0; \\ \frac{\partial \mathbf{V}}{\partial t} + \nabla \cdot (\mathbf{V}\mathbf{V}) = \\ = -\frac{1}{\rho} \nabla \cdot p + 2\nu (\nabla \cdot \underline{S}) - \nabla \cdot \underline{\tau}^{SGS}, \end{cases}$$
(2)

where **V** is the velocity vector with the components (V_x, V_y, V_z) ; <u>S</u> is the strain rate tensor; $\underline{\tau}_{SGS}$ is the term resulting from spatial filtering of the equations.

The generalized Boussinesq hypothesis is used to determine the subgrid-scale stresses:

$$\tau_{ij}^{SGS} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2\nu_{SGS} S_{ij}, \qquad (3)$$

where v_{SGS} is the subgrid-scale turbulent viscosity to be determined using some semi-empirical subgrid model.

The WMLES S-Omega approach implemented based on the data in [32] was used in the computations. Compared with the standard Smagorinsky model, the subgrid-scale viscosity is determined using a modified linear subgrid scale, a damping factor (similar to the Van Driest factor in the Prandtl model for the RANS approach), and the difference $|S - \Omega|$ instead of the magnitude of the strain-rate tensor S:

$$\mathbf{v}_{SGS} = \min\left\{\left(\hat{e}d_{w}\right)^{2}, \left(C_{S}\Delta\right)^{2}\right\} \times \left|S-\Omega\right| \times \left(1-\exp\left\{\left(-y^{+}/25\right)^{3}\right\}\right),$$
(4)

where $C_s = 0.2$ is the empirical Smagorinsky constant; *S*, s⁻¹, Ω , s⁻¹, are the magnitudes of strain rate and vorticity tensors

$$(S = (2S_{ij}S_{ij})^{0.5}, \Omega = (2\Omega_{ij}\Omega_{ij})^{0.5});$$

 $\kappa = 0.41$ is the Kármán constant; d_w , m, is the distance to the nearest wall, y^+ is the normalized distance from the center of the first wall cell to the wall.

The quantity Δ is determined by the formula

$$\Delta = \min \left\{ \max(C_w d_w, C_w \Delta_{\max}, \Delta_{wn}), \Delta_{\max} \right\},$$
(5)

where Δ_{\max} , m, is the maximum grid cell size (found as the maximum edge length for an orthogonal hexagon); Δ_{wn} , m, is the grid step along the normal to the wall; $C_w = 0.15$ is an empirical constant.

Since only averaged values were extracted from the solution of the auxiliary problem on air flow in a flat channel to impose the inlet boundary conditions, one of the available synthetic turbulence generators, the Vortex Method [33], was used to determine the instantaneous fluctuation characteristics (turbulent content) in the inlet section. With the synthetic turbulence generator engaged, it is required to determine



Fig. 2. Instantaneous velocity fields in vertical sections z = 0.3 m, 1.5 m and 2.7 m of the room model (*a*); fields of mean velocity magnitude in sections z = 1.5 m (*b*), x = 3.0 m (*c*) and x = 6.0 m (*d*)

the turbulence intensity at the inlet boundary; the value I = 4% was given.

Computational aspects of the problem. Numerical modeling was carried out in the ANSYS Fluent 16.2* general-purpose hydrodynamic code, with discretization of the governing equations by the finite volume method. A uniform grid consisting of cubic elements and built in the ICEM CFD generator was used. The grid dimension was approximately 48 million cells ($751 \times 252 \times 250$), while the linear size of the cell was $\Delta = 12$ mm.

The parameters selected for the computational provided spatial algorithm and temporal discretization with second-order accuracy. The central differencing scheme was used for approximating the convective terms in the equation of motion. The non-iterative algorithm corresponding to time advancement by the method of fractional steps (NITA) was used. The time step Δt , equal to 0.01 s, was chosen so that the maximum value of the Courant number in the computational domain was less than unity. Additional computations confirmed that a decrease in the time step to 0.006 s does not affect the averaged flow characteristics. The rationale for the choice of the grid and other aspects related to applying the LES method are considered in the first part of this study [9], considering a periodic problem with no influence from the side walls.

The development of unsteady flow was controlled by placing monitoring points in different positions in the room, allowing to detect the transition to a statistically steady flow regime. Notably, the fluctuation characteristics of the flow are highly sensitive to the length of the averaging interval. Samples from 1500 s (150,000 time steps) to 3,000 s were computed to accumulate representative statistics. The averaged characteristics computed over shorter averaging periods turned out to be significantly dependent on the sample.

The computations were carried out using the resources of the Polytechnic Supercomputer Center (http://www.scc.spbstu.ru). The problems were run on the Polytechnic RSC Tornado cluster with a peak performance of 943 teraflops. The cluster contains 668 dual-processor nodes (Intel (R) Xeon (R) E5 2697v3), each node containing 14 cores. A problem was run on a maximum of 512 parallel cores, while it took at least three weeks of real time (258,000 core hours) to accumulate unsteady statistics.

Computational results and discussion

Description of the flow structure (scenario 1, $w_{in} = H$). The structure of the flow in the room is illustrated in Fig. 2, showing the instantaneous, i.e.,

$$V = (V_x^2 + V_y^2 + V_z^2)^{0.5},$$

and averaged, i.e.,

$$V_m = (\langle V_x \rangle^2 + \langle V_y \rangle^2 + \langle V_z \rangle^2)^{0.5},$$

fields of the velocity magnitude for the first computational scenario, with the width of the inlet slit coinciding with the width of the room ($w_{in} = H$), in several sections of the room. The symbols $\langle ... \rangle$ here and below refer to time averaging.

A near-wall turbulent jet of air develops near the ceiling (the upper regions of the fields in Fig. 2), which is practically symmetric

^{*} ANSYS Inc. ANSYS Fluent 16.2 User's Guide, 2015.

relative to the midsection of the room. As the jet propagates from the inlet slit to the opposite side wall, the velocities approximately halve (from $V_{in} = 0.455$ to 0.200 m/s). Colliding with the wall opposite to the entrance, the jet turns around, and a secondary low-velocity flow is generated in the bottom of the room, characterized by velocities less than 0.1 m/s.

As follows from the flow patterns in the cross sections (see Fig. 2, c, d), the flow in most of the room is uniform along the transverse z-direction, even though the cross section of the room is a square (W/H = 1). Pronounced deviations from the two-dimensional (planar) structure of the flow are observed near the side walls of the room, as well as in the region of lower velocities of recirculation flow. Thus, a simplified statement of the problem with the periodic condition imposed makes it possible to predict the structure of the flow; however, as established in [9], the periodic computational domain has to sufficiently extended in the transverse direction for this purpose, i.e., $W/H \ge 1$.

The pattern of the flow in the midsection (see Fig. 2, b) indicates that two regions with substantially different scales are observed in the room: the jet flow zone, i.e., the region where an intense near-ceiling jet develops, with characteristically high air velocities, and the occupied zone with low-velocity circulation flow, which is where fresh air is supplied to people in the room in real-world conditions. It is rather difficult to describe such a flow by numerical modeling because the flows evolving in different areas of the room have different scales.

The data obtained at the monitoring points located in the jet flow zone also point to multiscale flow (point A with coordinates 3.0, 2.8 and 1.5 m) and recirculation flow (point *B* with coordinates 3.0, 0.4 and 1.5 m); Fig. 3, *a* shows the evolution of the longitudinal velocity component at these points.

High-frequency fluctuations are observed in the jet flow zone, with their amplitude comparable to the mean velocity ($\langle V_x \rangle = 0.29$ m/s for the point *A*, and the value of the maximum deviation from this average equals 0.27 m/s). The characteristic time scale of the fluctuations at the point *A* is less than 5 s. The relative amplitude of the fluctuations is much higher in the region of lower velocities; the characteristic time scale of low-frequency oscillations also turns out to be an order of magnitude higher than in the jet flow zone, for example, it is about 150 s at the point *B*.

Fig. 3, *b* shows the frequency dependence of the power spectral density (PSD), calculated from the *x*-velocity component (see Fig. 3, *a*), which was obtained using the formula

$$PSD = 2A_{Ur}^{2}\Delta t,$$

where A_{Ux} is the amplitude of harmonic components in the Fourier transform.

A straight line added to the graph reflects the decrease in the spectrum by the Kolmogorov law (denoted as the "-5/3 law"). This law states that the frequency power spectrum exhibits universal behavior in the inertial range $E \sim k^{-5/3}$, where *E* is the spectral power density of kinetic energy, *k* is the wavenumber. A region where the Kolmogorov law is satisfied can be observed on the spectral curves plotted from the data at the points *A* and *B*. The graphs also show that the energy spectra of fluctuations are filled for more than two decades, which indicates that the given flow is described by a regime with developed turbulence.



Fig. 3. Time history of *x*-velocity components at two monitoring points: point *A* with coordinates (3.0, 2.8 and 1.5 m) and point *B* (3.0, 0.4 and 1.5 m) (*a*); energy spectra of velocity fluctuations at these points


Fig. 4. Computed (solid lines) and experimental (squares) velocity profiles; profiles of velocity fluctuations (dashed lines and triangles, respectively) in several sections of the geometric model of the room (see Fig. 1,a)

Comparison with experimental data (scenario 1, $w_{in} = H$). Fig. 4 shows the profiles of the time-averaged x-velocity component $\langle V_x \rangle$, and its root-mean-square deviations from the mean value $(\langle V_{x}'^{2} \rangle)^{0.5}$ in eight sections (lines) of the room (see Fig. 1, *a* for the locations of sections). The graphs summarize the data obtained in the course of this numerical simulation and experimental data given in [7]. The top of Fig. 4 shows graphs along the lines drawn in the central section of the room, the bottom shows lines in the lateral section. It is evident from the graphs that the flow in the room is quasitwo-dimensional in a wide range of transverse coordinates (as noted above); the profiles of velocity and its fluctuations in the central and lateral sections are identical both qualitatively and quantitatively.

The results of numerical computations are in good agreement with the experimental data in the region of the near-ceiling jet. At the same time, there is a disagreement between the computational and experimental results in the backflow zone. The computed profiles of velocity and its fluctuations in vertical sections (lines *A*-*A* and *B*-*B*) adequately reproduce the experimental data; there is some discrepancy in the results in the vicinity of the room's floor at y < 1 (see Fig. 4,*a*,*b*). A certain disagreement between the computed and experimental results can also be observed from the data for velocity and its fluctuations in the horizontal sections of the room located in the backflow zone (lines C-C in Fig. 4, c, d), where local maxima of the velocity appear. Conversely, the computations are in good agreement with the experiment along the horizontal lines D-D (see Fig. 4, e, f).

results Comparing the with the data obtained earlier by other authors, numerically simulating the experimental conditions in [7] (see Table 1), we can conclude that the results of these studies are in better agreement with the experimental data [7] both in terms of velocity profiles and fluctuation characteristics. This is particularly pronounced in the jet flow zone (sections D-D in Fig. 4, e, f), for which quantitative agreement of the computational and experimental data was obtained in this study, and the position of the point where the jet separates from the top wall was predicted accurately. Our computations predict more intense flow than was observed in the experiment for the region of secondary flow (sections C-C in Fig. 4, c, d): the values of velocity and its fluctuations prove to be overestimated by the computational data. All studies published previously by other authors pointed to a significant disagreement between the computations and the experiment in the backflow zone with relatively low velocities.



Fig. 5. Instant isosurfaces of Q criterion, colored by velocity magnitude; constructed for two computational scenarios: $w_{in} = H(a)$ and 0.5H (b)



Fig. 6. Computed (solid lines) and experimental [8] (symbols) profiles of longitudinal velocity component in sections A-A and B-B for scenario 2, $w_{in} = 0.5H$

Characteristics of the flow with decreasing width of the inlet slit (scenario 2, $w_{in} = 0.5H$). Fig. 5 shows the characteristics of the flow for scenario 2, where the width of the inlet slit is half the width of the computational domain; the flow structures in both scenarios are compared. The figure shows three-dimensional isosurfaces of the Q criterion taking the form Q = 0.5 $(\Omega^2 - S^2)$, where Q has a value equal to 0.1 s⁻²; the colors of the isosurfaces correspond to the values of the velocity magnitude. As the width of the inlet slit is halved, additional mixing layers evolve in the transverse (z) direction; their development is noticeable in the nearceiling zone in the corners of the room: the averaged flow exhibits a fundamentally threedimensional nature here. The differences in the patterns of jet propagation are smoothed out away from the entrance; the numerical solutions demonstrate practically the same distributions of the Q criterion in the region where the jet ineracts with the opposite side wall.

On the whole, it can be concluded that the global structure of the flow is identical for the two scenarios differing by the width of the inlet slit, except for the region in the vicinity of the entrance.

Fig. 6 compares the time-averaged profiles of the x velocity components obtained in the computations with the experimental data from [8] along the vertical lines AA and B-B (note that only a very limited set of experimental data is available for the problem with the smaller widths of the inlet slit). Fig. 6, a shows the distributions along the lines in the central section, with z = 1.5 m; Fig. 6, b shows the distributions along the lines in the lateral section, with z = 0.3 m (this value of the transverse coordinate is already outside the inlet slit). The graphs confirm that the computational results are in complete agreement with the experimental data in the near wake (lines A-A). Differences between the computed and experimental velocity profiles in the area of the room located closer to the exit (lines B-B), especially in the lateral section. The reasons for disagreement may stem both from the drawbacks of the numerical simulation technique and from the uncertainty of the experimental data given in [8]. We should note that the computations revealed a strong sensitivity of the averaged flow characteristics to the duration of the sample used for averaging: independence from the averaging interval was achieved in the computations (for the samples exceeding 1500 s).

The computations indicate that using a sufficiently long sample for averaging is of fundamental importance for an averaged flow with a substantially three-dimensional pattern, characteristic for scenario 2. There is no information about the averaging technique (including the duration of the samples) used in the experiments in [7, 8]. It is also known that the errors in velocity measurements can sharply increase in the region of low-velocity flow: specifically, a greater disagreement between the computational and experimental data is observed in this region.

Conclusion

The eddy-resolving WMLES approach was used in this study for numerical simulation of turbulent air flow in a room with a square cross-section ventilated by a plain air jet supplied from a slit located under the ceiling; the Reynolds number $Re = 10.5^3$. The problem was formulated in a statement that most fully reproduced the conditions of the test experiment. Two geometric configurations were

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4. **Guliaev A.N., Kozlov V.E., Sekundov A.N.,** A universal one-equation model for turbulent viscosity, Fluid Dynamics. 28 (4) (1993) 485–494. considered, differing by the width of the inlet slit. The computations were carried out in the ANSYS Fluent general-purpose CFD code, providing second-order spatial and temporal discretization.

Despite the geometric simplicity, the flow evolving in the room combines many factors that complicate the simulations:

a plain near-wall jet develops under the ceiling of the room;

after turning around, the descending jet flows onto the lower wall;

the side walls play a certain role, forming the three-dimensional structure of the averaged flow.

We have established that the computational results are in good agreement with the experimental data in the near-wall jet, however, there is a noticeable discrepancy between the computational results and the experiment in the backflow zone (occupied zone), which is characterized by relatively low velocities.

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THE AUTHORS

ZASIMOVA Marina A.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation zasimova_ma@spbstu.ru

IVANOV Nikolay G.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation ivanov_ng@spbstu.ru

MARKOV Detelin

Technical University of Sofia 8 Kliment Ohridsky boulevard, Sofia, 1000, Bulgaria detmar@tu-sofia.bg

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СВЕДЕНИЯ ОБ АВТОРАХ

ЗАСИМОВА Марина Александровна — ассистент Высшей школы прикладной математики и вычислительной физики Санкт-Петербургского политехнического университета Петра Великого. 195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 zasimova_ma@spbstu.ru

ИВАНОВ Николай Георгиевич — кандидат физико-математических наук, доцент Высшей школы прикладной математики и вычислительной физики Санкт-Петербургского политехнического университета Петра Великого.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 ivanov_ng@spbstu.ru

МАРКОВ Детелин — *PhD, доцент Софийского технического университета.* 1000, Болгария, г. София, бульвар Климента Орхидского, 8 detmar@tu-sofia.bg

EXPERIMENTAL TECHNIQUE AND DEVICES

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AN ALGORITHM OF THE INITIAL APPROXIMATION FORMATION IN THE IONOSPHERIC TOMOGRAPHY PROBLEM WITH INTER-SATELLITE DATA REGISTRATION

P.N. Nikolaev

Samara National Research University, Samara, Russian Federation

In the paper, an original approach to the formation of the initial approximation in the ionospheric tomography problem with inter-satellite registration of total electron content is presented. The direct Radon transform of the electron density (ED)'s orbital profile is proposed to approximate using convolution of the function of latitudinal distribution of ED's maximum in the profile with the kernel function. This approximation makes it possible to estimate the latitude distribution of the ED maximum from the total electron content measurements by the deconvolution procedure. An analytical expression of the convolution kernel was obtained. Based on the proposed approach, two variants of formation of the initial approximation which used different prior information, namely, on the solar activity index and on the height of the ionization maximum in the profile, were considered. An accuracy of the mentioned formation was analyzed by the results of statistical simulation, and it was compared with the previously known approach where both the height of the ionization maximum in the profile of the ionization maximum in the profile of the height of the ionization where both the height of the ionization maximum in the profile and ED at this height were known.

Keywords: satellite monitoring, ionospheric tomography, initial estimation, statistical modeling

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АЛГОРИТМ ФОРМИРОВАНИЯ НАЧАЛЬНОГО ПРИБЛИЖЕНИЯ В ЗАДАЧЕ ТОМОГРАФИИ ИОНОСФЕРЫ ПРИ МЕЖСПУТНИКОВОЙ СХЕМЕ РЕГИСТРАЦИИ ДАННЫХ

П.Н. Николаев

Самарский национальный исследовательский университет имени академика С.П. Королева, г. Самара, Российская Федерация

В работе представлен оригинальный подход к формированию начального приближения в задаче томографии ионосферы при межспутниковой схеме регистрации данных полного электронного содержания (ПЭС). Предлагается аппроксимировать прямое преобразование Радона орбитального профиля электронной концентрации (ЭК) ионосферы сверткой функции широтного распределения максимума ЭК в профиле с функцией ядра. Такая аппроксимация позволяет оценить широтное распределение максимума ЭК по данным измерения ПЭС методом деконволюции. Получено аналитическое выражение функции ядра свертки. На основе предложенного подхода рассмотрены два варианта формирования начального приближения, использующие разную априорную информацию: об индексе солнечной активности и о высоте максимума ионизации в профиле. Проанализирована точность указанного формирования по результатам статистического моделирования, проведено сравнение с известным подходом, когда известны как высота максимума ионизации в профиле, так и концентрация на этой высоте.

Ключевые слова: спутниковый мониторинг, томография ионосферы, начальное приближение; статистическое моделирование

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Introduction

Methods for studying the ionosphere, aimed at remote sensing in a wide range of positions of transceiving systems, have seen increasing use in recent years. These systems make it possible to reconstruct the ionospheric structures based on computer tomography algorithms. Monitoring of the ionospheric electron density (ED) assesses the total electron content (TEC), which is a linear integral of the ED along the path of electromagnetic wave propagation, expressed in TECU units (Total Electron Content Units, 1 TECU = 10^{16} electrons·m⁻²).

The linear integral of the distribution function f(x,y) along the straight line located at a distance *l* from the origin and making an angle θ with the positive direction of the axis *OX* corresponds to the Radon transform at the point (l,θ) :

$$\left[\tilde{R}f\right](l,\theta) = p(l,\theta) =$$
$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y) \delta(x\cos\theta + y\sin\theta - l) dxdy.$$

The solution to the tomographic problem consists in finding the estimate $f^*(x,y)$ of the function f(x,y) from a set of integral characteristics obtained from all possible angles, and assumes that the exact value of $p(l,\theta)$ is known for all l and θ .

The problem of radio tomography (RT) of the ionosphere is typically confined to solving systems of linear equations (SLE) [1]. In this case, the solution of the SLE is a complex computational problem, since the matrix of the SLE (projection operator) contains about $10^{6}-10^{7}$ elements, even though it is sparse. An approach to solving the problem of ionospheric tomography was proposed in [2, 3] for an inter-satellite scheme for recording TEC data using a convolution algorithm.

The problem of ionospheric RT via satellites involves a small number of angles for obtaining

the integral characteristic. Even though the positions of transceiver systems cover a wide range, whether it is a chain of ground receiving stations [4, 5] or proposals for space-based receivers and transmitters [6, 7], the obtained angles are still insufficient to satisfy the condition for the unique solution, and the inverse tomography problem is incorrect.

An initial approximation should be used to formulate the tomography problem correctly, corresponding to the distribution and values of the estimated parameters with some degree of confidence. For example, an IRI model (International Reference Ionosphere) and the Chapman distribution are used in [8-12] to construct the initial approximation for a chain of ground stations.

The initial approximation in [7, 13], where receivers and transmitters were used on the satellites of the ionospheric tomography system, was set in the entire reconstructed region to a constant value of $4 \cdot 10^{11}$ electrons·m⁻³, which is the averaged value of the reference ED for all heights and latitudes in reconstructed region. However, because the ED of the equatorial ionosphere is higher than that of the mid-latitude and polar zones, and also because the system alternates between the illuminated and shadowed regions of the orbit due to the change between day and night, the accuracy with which such an initial approximation can be given is about 80-90%.

Ref. [13] compared the quality of ED reconstruction by a constellation of five satellites for an initial approximation given by a constant and for initial approximations obtained from the IRI-2007 ionospheric model [14], differing from the reference by 5, 10, 20 and 30% on average. The initial approximation based on the IRI ionospheric model yielded a better result compared with the initial approximation taken as constant.

In this study, we propose an original approach to rapidly formulating the initial



Fig. 1. Scheme of radio path with perigee altitude $h_{track} = 225$ km; the dots indicate the location of two satellites in one circular orbit (dashed line)

approximation whose accuracy value is intermediate between the accuracy values provided by the approaches considered above.

The proposed approach has a number of advantages:

simpler mathematical implementation than the IRI-2007 model;

less input data required.

As a result, the satellites are supposed to have great autonomy (there is no need to transmit a large amount of input data to the satellite, such as ionospheric index, magnetic index, and solar activity indices).

This approach is applicable to obtaining integral characteristics by transceivers of a constellation of satellites located in the same orbital plane.

The accuracy of the initial approximation for the ionospheric ED profile is determined by numerical simulation, solving the forward and inverse problems.

The forward problem consists in obtaining the TEC for a given ED distribution in the orbital plane for a given radio path.

The inverse problem consists in reconstructing the ED distribution in the orbital plane from the available set of TEC measurements, with an initial approximation generated for this purpose. The generated initial approximation is compared with the given distribution.

The accuracy of the initial approximation was estimated in our study, as in [1, 7, 11], using the norms in the spaces l^2 and l^∞ :

$$\delta(l^2) = \frac{\sqrt{\sum_i (F_i - \tilde{F}_i)^2}}{\sqrt{\sum_i F_i^2}},$$

$$\delta(l^{\infty}) = \frac{\max_{i} \left| F_{i} - \tilde{F}_{i} \right|}{\max_{i} \left| F_{i} \right|}$$

where F and \tilde{F} are the model distribution and the generated initial approximation, respectively; *i* is the number of a pixel in the distribution.

The norm $\delta(\vec{P})$ is the root mean square establishing a large difference in the values of F and \tilde{F} in a small region of the distribution. The norm $\delta(\vec{P})$ corresponds to the difference between F and \tilde{F} in the worst case.

Problem statement

Consider two satellites located in the same circular orbit; one satellite serves as a transmitter, and the other as a receiver (Fig. 1). The satellites are located so that the perigee altitude of their radio path is below the maximum ED in the orbital profile. This number of satellites is sufficient to form an initial approximation by the proposed algorithm.

The height distribution of ED close to the Chapman distribution [9, 10] was taken as baseline:

$$N_{e}(h, N_{m}, H_{m}) =$$

$$= N_{m} \cdot \exp\left(1 - \frac{h - H_{m}}{\sigma} - \exp\left(-\frac{h - H_{m}}{\sigma}\right)\right), \quad (1)$$

where N_m is the maximum value of ED N_e in the height profile; h is the altitude above sea level; H_m is the height of the maximum ED above sea level; σ is the scale parameter.

Algorithm for forming the initial approximation for the distribution of electron density in the ionosphere

Consider a circular polar orbit with an altitude of $h_{orb} = 1000$ km and an inclination of $i = 90^{\circ}$. The satellites are located in orbit in such a way that the angular distance between them is equal to $\Delta \phi = 54^{\circ}$, which corresponds to the satellites the farthest away from each other in orbit, from the constellation considered in [13] intended for solving the tomography problem in the altitude range of 200- 500 km. The chosen angular position of the satellites allows to form a radio path between them with a pericenter altitude $h_{track} = 225$ km. This radio path is certain to cross the ED maximum layer at two points; therefore, the TEC measured in this radio path is the largest among other TECs measured in the radio paths of the constellation [13].

The radio path between two satellites located in the same orbit (Fig. 1) is described in the polar coordinate system (CS) by the equation of the straight line

$$r(\varphi) = \frac{l}{\cos(\varphi - \theta)},$$

where *l* is the length of the perpendicular dropped to the straight radio path from the origin, $l = R_{Earth} + h_{track}$; θ is the the angle between the positive direction of the axis *OXorb* and the direction of this perpendicular; R_{Earth} is the average radius of the Earth, $R_{Earth} = 6371.136$ km.

The height of the maximum ED H_m in the formula (1) depends on the latitude φ (this is due to the changing day and night conditions of the formation of the ionospheric profile), as well as on the zenith angle of the Sun [15]. To use expression (1) and carry out further analytical calculations for the segment of the orbit where the radio path is determined, we



Fig. 2. Convolution kernel g(z)

assumed that the height of the maximum ED H_m is the average in the segment $\Delta \varphi = 54^{\circ}$:

$$\langle H_m \rangle = \frac{1}{2\pi} \int_{\varphi_1}^{\varphi_2} H_m(\varphi) d\varphi,$$

where φ_1 , φ_2 are the angular coordinates of the first and second satellite, respectively.

The measurements can cover more than 20° in latitude for RT using a chain of ground stations. Given this value of the latitudinal angular distance, it is acceptable to use the initial approximation (1) with a constant height of the ED maximum, as established in [11, 12]. Since the angular distance between two intersections of the ED maximum by the radio path was taken about 20° in this study, it seems reasonable to assume that the height of the ED maximum H_m is constant in the segment $\Delta \varphi = 54^\circ$.

Thus, the distribution of ED (1) in the orbital plane of the transmitter and receiver in the segment $\Delta \phi$ is expressed as follows in the polar SC:

$$N_{e}(r, \varphi) = N_{m}(\varphi) \times \exp\left(1 - \frac{r - R_{m}}{\sigma} - \exp\left(-\frac{r - R_{m}}{\sigma}\right)\right), \quad (2)$$

where φ is the angular coordinate in the polar SC; $r = R_{\text{Earth}} + h$ is the radial coordinate in the polar CS; $Rm = R_{\text{Earth}} + \langle H_m \rangle$.

The linear integral from $N_e(r,\varphi)$ along the radio line *L* is curvilinear in the polar SC:

$$p(l, \theta) = \int_{L} N_e(r, \varphi) dl =$$
$$= \int_{\varphi_1}^{\varphi_2} N_e(r(\varphi), \varphi) \cdot \sqrt{r^2 + \left(\frac{dr}{d\varphi}\right)^2} d\varphi,$$

where the equation of the radio path for a small angle $\varphi - \theta$ has the form

$$r(\varphi) = \frac{l}{\cos(\varphi - \theta)} \approx l \left(1 + \frac{1}{2} (\varphi - \theta)^2 \right).$$

Thus, $p(l,\theta)$ is written as the integral of the convolution for the function N_m and the kernel g (Fig. 2) with respect to the parameter θ :

$$p(l,\theta) = (N_m * g)(\theta) =$$
$$= \int_{\varphi_1}^{\varphi_2} N_m(\varphi) \cdot g(\varphi - \theta) d\varphi,$$

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where

$$g(z) = l \cdot (1 + z^{2}) \cdot$$
$$\cdot \exp\left(1 - \frac{1}{\sigma} \cdot (l - R_{m}) - \frac{l}{2\sigma}z^{2} - \exp\left(-\frac{1}{\sigma} \cdot (l - R_{m}) - \frac{l}{2\sigma}z^{2}\right)\right).$$

The expression for $p(l,\theta)$ makes a transition to infinite limits with respect to the angle φ :

$$p(l,\theta) = \int_{-\infty}^{+\infty} N_m(\varphi) \cdot g(\varphi - \theta) d\varphi,$$

since $g(\varphi - \theta)$ decays exponentially for $\varphi \rightarrow \varphi_1$, φ_2 (Fig. 2).

Since the expression for the convolution integral is known, the latitudinal ED profile $N_m(\varphi)$ can be estimated using the deconvolution method [16]:

$$\hat{N}_{m}(\varphi) =$$

$$= F^{-1}\left(\frac{G^{*}(f)}{\left|G(f)\right|^{2} + \alpha\left\langle\left|G(f)\right|^{2}\right\rangle} \cdot P(f)\right) = (3)$$

$$= F^{-1}\left(W(f) \cdot P(f)\right) = (w * p)(\varphi),$$

where G(f), W(f), P(f) are the Fourier images for g, w and p, respectively; $G^*(f)$ is the conjugate Fourier transform for g; α is the regularization parameter; $\langle |G(f)|^2 \rangle$ is the average value of the energy spectrum G(f).

Substituting expression (3) into Eq. (2), the expression for modeling the initial approximation takes the form

$$N_{e}(h, \varphi) = (w * p)(\varphi) \cdot \exp\left(1 - \frac{h - H_{m}}{\sigma} - \exp\left(-\frac{h - H_{m}}{\sigma}\right)\right).$$
(4)

The resulting expression is the product of the latitudinal ionospheric profile $(w \cdot p)(\varphi)$ and the height profile

$$\exp\left(1-\frac{h-H_m}{\sigma}-\exp\left(-\frac{h-H_m}{\sigma}\right)\right),\,$$

from which it follows that the latitude and height profiles can be found separately.

If the latitudinal profile can be found by Eq. (3), then the height profile can be formed

under different assumptions, which will affect the final accuracy of the initial approximation.

Thus, expression (4) can serve as a basis for formulating two versions of the algorithm for generating the initial ED approximation.

Version 1. The height is taken as an average over the orbit $H_m = \langle H_m \rangle$. Then,

$$N_{e}(h, \varphi) = (w * p)(\varphi) \cdot \exp\left(1 - \frac{h - \langle H_{m} \rangle}{\sigma} - \exp\left(-\frac{h - \langle H_{m} \rangle}{\sigma}\right)\right).$$
(5)

Version 2. The height H_m is known a priori. Then,

$$N_{e}(h, \varphi) = (w * p)(\varphi) \cdot \exp\left(1 - \frac{h - H_{m \ apr}}{\sigma} - \exp\left(-\frac{h - H_{m \ apr}}{\sigma}\right)\right).$$
(6)

The efficiency of the proposed versions can be estimated numerically by using the stochastic approach and comparing the result of the algorithm with the simulated distribution.

Results and discussion

Estimating the accuracy of the initial approximation based on the results of statistical modeling. Let us compare the two proposed versions for forming the initial approximation of the ionospheric ED profile in the plane of the satellite orbit with one known parameter. Three possible cases are possible here (cases *II* and *III* correspond to versions 1 and 2).

Case I. The initial approximation is formed by Eq. (1), when the parameters N_m and H_m are given a priori (this method was considered in [11, 12]);

Case II. The initial approximation is formed by Eq. (5), when $H_m = \langle H_m \rangle$;

Case III. The initial approximation is formed by Eq. (6), when H_m is known a priori.

We assessed the accuracy of all three cases of forming the initial approximation by statistical modeling of the ED distribution in the plane of the polar orbit (10,000 numerical experiments) for different indices of solar activity, months, Greenwich Mean Time, and geographic longitudes. Consider a circular polar orbit of two satellites with an altitude $h_{orb} = 1000$ km and an inclination $i = 90^{\circ}$. The angular distance between the satellites is considered to be constant, equal to $\Delta \varphi = 54^{\circ}$, which corresponds to the perigee altitude of their radio path $h_{track} = 200$ km. As the satellites were moving in orbit, the TEC was recorded every 0.5°.





The ED distribution was given using the NeQuick ionospheric model [17]:

vertical size of image element was 12.5 km; horizontal size of image element was 50 km. The rest of the parameters of the model

were distributed by a uniform law:

solar activity index $F_{10.7} \in [63.7; 193] \cdot 10^{-22}$ W·m⁻²·Hz⁻¹;

month $m \in [1; 12];$

GMT time $t \in [0:00; 24:00]$ UTC;

geographic latitude (longitude of the ascending node of the orbit) $\lambda \in (0; 360]^{\circ}$.

The spread in the parameters of the NeQuick model determines the spread in the errors of the initial approximation. The scale parameter σ was chosen taking into account the solar activity index *F* 10.7 ranging from 84 to 93 km.

The results of modeling by the algorithm for forming the initial approximation for the first case (10,000 simulations of the ED distribution were carried out) are shown in Fig. 3. The mean errors in this series of numerical experiments in the metrics l^2 and l^{∞} are $\delta(l^2) = 0.23$ and $\delta(l^{\infty}) = 0.27$, respectively. This result is the upper estimate of the accuracy of the initial approximation among the three considered cases, since the parameters N_m and H_m were taken to be known a priori.

Fig. 4,*a* shows an example of one of 10,000 implementations of the ED distribution, formed by the NeQuick model for the following conditions:

solar activity index $F_{10.7} = 127.6 \cdot 10^{-22}$ W·m⁻²·Hz⁻¹;

month: October

GMT t = 10:00;

geographic latitude (longitude of the ascending node of the orbit) $\lambda = 50^{\circ}$.



Fig. 4. Ionospheric ED distributions in the plane of the polar orbit in latitude-altitude coordinates: *a* is the model distribution; *b* is the initial approximation generated by Eq. (1) with the known N_m and H_m ; *c* is the absolute value of the residual



Fig. 5. Latitudinal ED profiles: initial $N_m(\varphi)_{H_m} = H_m(\varphi)$ (*a*); $N_m(\varphi)_{H_m} = \langle H_m \rangle$, taken for mean height (*b*); $\hat{N}_m(\varphi)$, calculated by Eq. (3) (*c*)

Figs. 4, b, c show the initial approximation formed for case I, and the absolute value of the residual between the model and the distribution generated for this implementation.

The latitudinal ED profile $\hat{N}_m(\varphi)$ was estimated in the simulation for cases II and III (see above) using Eq. (3) (Fig. 5,*c*) for the model distribution (Fig. 4,*a*). The value of the regularization parameter α in Eq. (3) was selected based on the minimization criterion for the residual:

$$d = \left\| \hat{N}_{m \alpha} - N_{m} \right\|_{1} \to \min$$

For comparison, Fig. 5,*a* shows the initial latitudinal profile $N_m(\varphi)_{H_m} = H_m(\varphi)$ of the model distribution, and Fig. 5,*b* the latitudinal profile of the model distribution for the mean height $N_m(\varphi)_{H_m} = \langle H_m \rangle$.

The difference between the profile in Fig. 5, a and the profiles in Figs. 5, b, c in the

metrics l^2 and l^{∞} is given in Table 1. It can be seen from the results obtained that the values of the latitudinal profile $N_m(\varphi)_{H_m} = \langle H_m \rangle$ for the mean height $\langle H_m \rangle$ can be used as values for the latitudinal profile $N_m(\varphi)_{H_m} = H_m(\varphi)$. This is used to generate the initial approximation for case III, where the values of $\hat{N}_m(\varphi)$ are given at a priori known heights H_m .

The solar activity index $F_{10.7}$ determines the shape of the ED profile and the height of the maximum in it [15]; therefore, the mean height of the ED maximum can be approximately described by a linear dependence

$$\langle H_m \rangle (F_{10,7}) = a \cdot F_{10,7} + b \pm \Delta \langle H_m \rangle,$$

where $a = 0.65 \cdot 10^{16} \text{ km}^3 \cdot \text{Hz}^{-1} \cdot \text{W}^{-1}$; b = 243.4 km; $\Delta \langle H_m \rangle = 18.7 \text{ km}$ is the spread in mean height depending on seasonal and diurnal effects for P = 0.95.

Table 1

Error δ Metric $N_m(\phi)_{H_m} = \langle H_m \rangle$ $\hat{N_m}(\phi)$ l^2 0.100.16 l^{∞} 0.190.23

Comparison of deviations δ of latitudinal profiles (in two metrics) from true latitudinal profile, obtained by two methods

Notations: $N_m(\varphi)_{H_m} = \langle H_m \rangle$, $\hat{N}_m(\varphi)$ are the latitudinal profiles: taken for the mean height and calculated by Eq. (3). The true latitudinal profile is $N_m(\varphi)_{H_m} = H_m(\varphi)$.



Fig. 6. Histograms of errors of initial approximation in metrics $l^2(a)$ and $l^{\infty}(b)$ for case II, and $l^2(c)$ и $l^{\infty}(d)$ for case III



Fig. 7. Distributions of ionospheric ED in the plane of the polar orbit in latitude-altitude coordinates, obtained in the initial approximations by Eq. (4) for two values of the height: mean $\langle H_m \rangle$ (*a*) and known a priori H_m (*c*); the corresponding absolute values of the residuals are also given for cases with $\langle H_m \rangle$ (*b*) and H_m (*d*)

Table 2

Errors in generating the initial approximation in two metrics for the three considered cases for model distribution (see Fig. 4,a)

	Error δ			
Metric	<i>N</i> _m and <i>H</i> _m are known	$N_m = \hat{N}_m(\varphi),$ H_m is known	$N_m = \hat{N}_m(\boldsymbol{\varphi}), \ H_m = \langle H_m \rangle$	
l^2	0.18	0.31	0.30	
l ∞	0.18	0.30	0.25	

If the seasonal and diurnal effects in the ionosphere are not taken into account, then the term $\Delta \langle H_m \rangle$ can be discarded, defining $\langle H_m \rangle$ in the second version of the algorithm as $\langle H_m \rangle = a \cdot F_{10.7} + b$.

Fig. 6 shows histograms for the distribution of errors in the initial approximation in the metrics l^2 and l^∞ , generated for cases II and III for 10,000 numerical experiments. Fig. 7 shows the generated initial approximation and the absolute value of the residual between the model and the generated distributions for cases II and III for the implementation in Fig. 4,*a*.

Table 2 shows the errors in the initial approximation for the three considered cases of the model distribution (see Fig. 4,*a*). Cases II and III yield approximately the same accuracy, despite a noticeable visual difference (see Figs. 7, *a*, *c*).

According to the results of statistical modeling (Fig. 6), case II has mean errors of the initial approximation $\delta(l^2) = 0.39$ and $\delta(l^{\infty}) = 0.42$. The accuracy achieved is sufficient for obtaining a satisfactory solution to the tomographic problem, where the errors do not exceed the errors for the initial approximation [13] taken as a constant (the accuracy of the solution to the tomographic problem $\delta(l^2) = 0.35$ and $\delta(l^{\infty}) = 0.40$ for a reconstruction step of 50 km with respect to altitude). The accuracy of the initial approximation is higher for case III than for case II: $\delta(l^2) = 0.29$ and $\delta(l^{\infty}) = 0.33$, making this case similar to the initial approximation formed by the IRI-2007 model in [13] for obtaining the integral characteristics by transceiver devices of a constellation of satellites. Both versions of the algorithm (cases II and III) for generating the initial approximation are fast and can be implemented on board the satellite.

Reconstruction of ionospheric ED distribution. The quality with which the initial approximation was generated was assessed by tomographic reconstruction of the ED distribution using the approach proposed in [2, 3]. The configuration of satellites in low orbit, described in [3], was used as a scheme for detecting TEC: three satellites with transmitters and two with receivers, whose radio paths cover



Fig. 8. Histograms for errors in reconstructing the ED profile for three cases of initial approximation in two metrics: l^2 (*a*, *c*, *e*) and l^{∞} (*b*, *d*, *f*); cases I (*a*, *b*), II (*c*, *d*), III (*e*, *f*) were considered (see explanations in the text)



Fig. 9. Reconstruction of ionospheric ED distribution in the plane of polar orbit in latitude-altitude coordinates for three cases of initial approximation: I (a), II (c), III (e); the corresponding absolute values of the residuals for cases I (b), II (d), III (f) are also given

the altitude range from 200 to 500 km with a step of 50 km. The tomography problem was solved in this altitude range.

Fig. 8 shows the histograms for the distribution of errors in the reconstruction of the ED profile in the metrics l^2 and l^{∞} , obtained for three cases of the initial approximation (Eqs. (2), (5), (6)) for 10,000 numerical experiments. Case I, when N_m and H_m are given a priori, yields the reconstruction result with the most

accurate characteristics (see Fig. 8, *a*, *b*) among all three cases of the initial approximations based on the Chapman distribution. Fig. 9 shows the reconstructed ED distributions for cases II and III of of the initial approximation. Reconstruction errors $\delta(l^2)$ and $\delta(l^{\infty})$ for the corresponding cases are given in Table 3.

It can be seen from Fig. 9, c, d and e, f, corresponding to Cases II ($N_m = \hat{N}_m(\varphi)$, $H_m = \langle H_m \rangle$) and III ($N_m = \hat{N}_m(\varphi)$, H_m is known) of

Table 3

Comparison of errors in reconstructing the ED profile in two metrics for the three considered cases of the initial approximation for model distribution (see Fig. 4,a)

	Error δ		
Metric	<i>N</i> ^{<i>m</i>} and <i>H</i> ^{<i>m</i>} are known	$N_m = \hat{N}_m(\varphi),$ H_m is known	$N_m = \hat{N}_m(\boldsymbol{\varphi}), \\ H_m = \langle H_m \rangle$
l^2	0.08	0.13	0.12
l^{∞}	0.11	0.18	0.16

the initial approximation, that the reconstructions obtained have a similar form and differ only slightly by the number of artifacts; in this case, the errors are mainly due to the errors in reconstructing the latitudinal profile $\hat{N}_m(\varphi)$. In turn, the artifacts obtained at an altitude of 200 km are due to the systematic reconstruction error [2, 3]. The height of the ED maximum in Case II $(N_m = \hat{N}_m(\varphi), H_m = \langle H_m \rangle), H_m$, was reconstructed with satisfactory accuracy, despite the assumption that $H_m = \langle H_m \rangle$, and for this reason, this method (Case II) is preferable to Case III ($N_m = \hat{N}_m(\varphi)$, H_m is known), primarily because the reconstruction errors in the initial approximation for this case are smaller (see Fig. 8, c-f).

Conclusion

We have developed a numerical algorithm for generating the initial approximation of the ED profile, using it to solve the problem of ionospheric radio tomography by a low-orbit satellite constellation. The initial approximation generated by the algorithm is based on the Chapman distribution and is represented as a product of two factors responsible for the latitude and height distributions.

We have obtained an approximate analytical dependence of the latitudinal ED profile on the measured TEC data for an intersatellite detection scheme in the plane of the polar orbit.

We have confirmed that the latitudinal profile can be assessed by merely two satellites spaced apart in the orbit in such a way that the perigee altitude of their radio path is lower than the height of the ED maximum in the orbital profile.

We have found that the latitudinal

distribution makes the greatest contribution to the final ED estimate.

Statistical modeling revealed that the errors in generating the initial approximation of the orbital ionospheric ED profile by TEC measurements, lie in the range from 20 to 55%in the metric l^2 (the errors in reconstructing the ED profile in the metric l^2 lie in the range from 8 to 20%), while the errors in generating the initial approximation by the NeQuick and IRI-2007 models reach 30% (the errors in reconstructing the ED profile in the metric l^2 lie in the range from 11 to 20%), and the errors in generating the initial approximation given by a constant value corresponding to the mean ED level reach 90% (the errors reconstructing the ED profile in the metric l^2 lie in the range from 35 to 40%).

The developed algorithm makes it possible to use real TEC measurements to generate the initial approximation, thus accounting for the short-term disturbances in the ionosphere, which are not directly accounted for with the NeQuick and IRI-2007 models.

In addition, the proposed algorithm has a simpler mathematical implementation than these models and requires less input data, allowing to solve the problem of generating the initial approximation on board a satellite.

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THE AUTHOR

NIKOLAEV Petr N.

Samara National Research University 34 Moskovskoye Ave., Samara, 443086, Russian Federation nikolaev.pn@ssau.ru

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СВЕДЕНИЯ ОБ АВТОРЕ

НИКОЛАЕВ Петр Николаевич — кандидат физико-математических наук, ассистент межвузовской кафедры космических исследований Самарского национального исследовательского университета имени академика С.П. Королева, г. Самара, Российская Федерация.

443086. Российская Федерация, г. Самара, Московское шоссе, 34 nikolaev.pn@ssau.ru

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THE EFFECT OF LARGE-SCALE DISTURBANCES ON THE LAMINAR-TURBULENT TRANSITION IN A FREE-CONVECTIVE LAYER ON A VERTICAL SURFACE: AN EXPERIMENTAL STUDY

Yu.S. Chumakov, E.F. Khrapunov, A.D. Malykh

Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation

The results of an experimental study of a free convective boundary layer on a vertical heated surface are presented in this paper. Particular attention has been paid to investigation of the laminar-turbulent transition zone and determination of the zone boundaries. The main goal of the present work was to find the opportunity of the transition processes' control by using various large-scale obstacles located in the region of the laminar section of the boundary layer. A vertical aluminum plate 90 cm wide and 4.95 m high served as a free-convection flow generator. Based on the obtained results, it is safe to state that there is a possibility of a significant reduction in the length of the transition zone through the use of large-scale obstacles. This way permits the beginning of the region with developed turbulent heat transfer to be moved nearer to the front edge of the surface. Thus, these obstacles can be considered as passive elements for controlling the heat transfer intensity.

Keywords: natural convection, laminar-turbulent transition, heat transfer, natural convective boundary layer, experimental study

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ЭКСПЕРИМЕНТАЛЬНОЕ ИССЛЕДОВАНИЕ ВЛИЯНИЯ КРУПНОМАСШТАБНЫХ ВОЗМУЩЕНИЙ НА ЛАМИНАРНО-ТУРБУЛЕНТНЫЙ ПЕРЕХОД В СВОБОДНОКОНВЕКТИВНОМ СЛОЕ НА ВЕРТИКАЛЬНОЙ ПОВЕРХНОСТИ

Ю.С. Чумаков, Е.Ф. Храпунов, А.Д. Малых

Санкт-Петербургский политехнический университет Петра Великого, Санкт-Петербург, Российская Федерация

В работе описываются результаты экспериментального исследования свободноконвективного пограничного слоя на вертикальной нагретой поверхности, причем особое внимание уделяется изучению зоны ламинарно-турбулентного перехода, определению границ этой зоны. Основная цель данного исследования найти возможность управления процессами перехода, воздействуя на них различными крупномасштабными препятствиями, расположенными в области ламинарного участка пограничного слоя. Генератором свободноконвективного потока служила вертикальная алюминиевая пластина шириной 90 см и высотой 4,95 м. На основании полученных результатов можно с уверенностью утверждать, что с помощью крупномасштабных препятствий удается заметно сократить протяженность зоны перехода и тем самым приблизить начало области с развитым турбулентным теплообменом к передней кромке поверхности. Таким образом, препятствия можно рассматривать как пассивные элементы для управления интенсивностью теплообмена.

Ключевые слова: свободная конвекция, ламинарно-турбулентный переход, теплообмен, свободноконвективный пограничный слой, экспериментальное исследование

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Introduction

Numerous studies have considered the development of forced convective boundary layers under the influence of different types of external factors. In particular, it was discovered that external disturbances with low intensity have little effect on the transient processes in the boundary layer. Large-scale three-dimensional obstacles (the socalled macro-roughness elements) placed in the laminar region of the boundary layer can serve to achieve sharp acceleration in the development of unsteady processes and transition to turbulence in the near-wall layer. Such macro-roughnesses are widely used to control the laminar-turbulent transition (LTT) in forced convective flows, for example, for obtaining relatively thick boundary layers in landscape wind tunnels to simulate the flow of the surface boundary layer around different objects [1].

While sufficient experience in numerical and physical simulation of methods for controlling LTT with macroroughness elements has been accumulated for forced convective flows, very few studies deal with free convective flows. For example, the results of direct numerical simulation of turbulence developing in a free-convective layer in the wake of macro-obstacles have been given so far only in [2], and we were unable to uncover any results of physical simulation. However, it is natural to assume that the LTT region (whose length in the absence of disturbances is two to three times greater than the length of the laminar region) can be substantially reduced by generating the appropriate conditions for sudden 'trigger' excitation of turbulence in the boundary layer [3-5]. In turn, the length of the turbulent heat transfer region and therefore the intensity of heat transfer in general can be increased by reducing the length of the LTT region.

This paper reports on the results of experimental study of the LTT region in a freeconvective boundary layer near a vertical heated plate with a cross-row of large-scale 3D obstacles disturbing the initially laminar layer arranged on the surface. The measurement data obtained in for a flat plate are also given for comparison.

Problem statement

Our main goal consisted in exploring the possibility of controlling the transition processes in a free-convective boundary layer using different large-scale obstacles located in the laminar region of the boundary layer.

Two types of plates with a thickness of 8 mm were used as obstacles: with a rectangular section of 32×18 mm, and with a trapezoidal section with a height of 18 mm, where the lower base was 32 mm long and the upper one 16 mm long. The obstacles were glued to the plate across the vertical axis at a distance of 200 mm from the lower edge of the plate with a pitch of 32 mm. Fig. 1 shows a schematic representation of the plates, and a photograph of the obstacles installed on the heated surface.

The height of the obstacles H was chosen by estimating the thickness of the undisturbed laminar boundary layer in the region where the obstacle was supposed to be installed. The thickness of the boundary layer δ (m) can be estimated by the well-known semi-empirical formula [6] for air:

$$\delta = 4.23 \left(\frac{v^2 \cdot X}{g \cdot \beta \cdot \Delta T \cdot \Pr} \right)^{1/4}, \qquad (1)$$

where v, m²/s, is the kinematic coefficient of viscosity; X, m, is the axial coordinate; g, m/s², is the acceleration of gravity; β , K⁻¹, is the coefficient of thermal expansion of the medium; $\Delta T = T_w - T_\infty$, K, is the characteristic temperature difference (T_w, T_∞) are the temperature of the plate surface and the temperature at the outer edge of the boundary layer, respectively); Pr is the Prandtl number.

When X = 200 mm, the layer thickness is $\delta = 13$ mm, and the ratio of the obstacle height *H* to the layer thickness is $H/\delta = 1.4$, i.e., the obstacle protrudes slightly beyond the boundary layer. Notably, all temperaturedependent parameters in this formula and further in the text depend on the thermal conditions described below, including the characteristic temperature difference ΔT .

Brief description of the experimental test bench and measurement methods

Free convective flow was generated by a vertical aluminum plate with a width of 90 cm and a height of 4.95 m. A total of 25 heaters (not shown in Fig. 1) were mounted on the back side of the plate; they were controlled by an electronic system capable of maintaining the given temperature conditions for a long time. Different laws for heating the surface along its height and, in particular, constant surface temperature were simulated by setting a specific regime for each of the 25 sections. Because the plate was very high, all three flow regimes, i.e., laminar, transitional, and fully developed turbulent could be simulated up to the Grashof number $Gr = 4.5 \cdot 10^{11}$. A detailed description of the experimental testbed is given in [5, 7].

Averaged and fluctuation components of the temperature and the axial component of the velocity vector were measured. All measurements were made using a resistance thermometer and a hot-wire anemometer (TA).

The measuring probe consists of two sensors where tungsten wires with a diameter of 5 μ m and a length of 3–4 mm are used as sensitive elements. The wires of both sensors are located parallel to each other, spaced 2 mm apart, and parallel to the surface; the lower sensor (upstream with respect to the flow) measures the current temperature, and the upper sensor (after processing of the initial data) measures the current velocity.

It is known that if the velocity in nonisothermal flow is measured by thermal anemometry, the anemometer readings should be interpreted taking into account the temperature values. The given flow is characterized by low mean velocities and a high level of fluctuations, so the current velocities are typically measured by the method of thermal compensation by mean temperature, which can yield inaccurate velocity measurements.

We used the thermal compensation method described in [8] in this study. Without dwelling on a detailed description of this method, let us only note that unlike other methods of thermal compensation by mean temperature, the TA reading corresponding to the current velocity at a given point in space is interpreted taking into account the current temperature at the same point.

All measurements were carried out at a constant surface temperature $T_w = 60 \pm 0.5^{\circ}$ C, while the air temperature at the outer edge of the boundary layer T_{∞} varied from 24 to 26°C during the entire experimental period.

A coordinate device was used to move the sensor within the boundary layer, providing an accuracy of movement of about 1 mm along the vertical (axial) coordinate X and of about 1 μ m along the coordinate Y normal to the surface (i.e., across the boundary layer); movement along the normal coordinate was carried out remotely, in automatic mode. The coordinate system used is shown in Fig. 1.

Flow parameters were measured fully automatically in each section of the boundary layer.

The measurement sequence is described as follows.

1. Probe is moved (with an accuracy of 1 mm) in the selected section along the axial coordinate X (see Fig. 1).

2. The probe is automatically brought to the surface until touching it.



Fig. 1. Schemes of trapezoidal (*a*) and rectangular (*b*) elements; photograph of heated plate (*c*) showing its face (*I*) and trapezoidal elements serving as obstacles (*2*). The distances in the figure are given in mm

3. After movement stops, the probe is moved away from the surface at a distance of 0.6 mm (with an accuracy of 1 μ m).

4. The probe is ready to perform measurements in automatic mode along the normal coordinate Y with the given pitch.

5. Readings are taken from both sensors of the probe at each point almost simultaneously (with an interval of 10^{-5} s); such measurements are repeated with a given frequency (100 Hz). Typically, 2,000 samples of reading pairs were taken; thus, the time of one measurement was 20 s.

After appropriate data processing, we obtained a record of the current values of temperature and velocity at a given point. Then, after performing the averaging operation, we calculated the mean values of velocity, temperature and fluctuation intensity.

Comparative analysis of the results

The influence of obstacles on the laminarturbulent transition was studied by comparing the results of measuring the averaged and fluctuation characteristics of temperature and velocity fields in the near-wall region of the boundary layer. The results of a detailed study on the free-convection boundary layer without disturbances are given in [3-5,9,10]. These studies describe the main characteristics of LTT, in particular, the local peaks appearing for mean velocity and its fluctuation intensity, as well as the intensity of temperature fluctuations at the end of the transition region.

It was assumed in earlier studies that the axial coordinate X of the maximum values of fluctuation intensity can be considered the beginning of a fully developed turbulent boundary layer. However, analysis of the fields of current values of temperature and velocity indicates that the intermittency factor in the region of maximum values of fluctuation intensity is approximately 0.65-0.75, which only points towards increasing intensity of the transition process. In fact, it can be assumed that the LTT has ended and the flow in the boundary layer has passed into a fully developed turbulent regime only downstream relative to the coordinate of the maximum, when the fluctuation intensity decreases slightly decreases and almost does not change with an increase in the axial coordinate. The intermittency factor reaches 0.80 - 0.95 in this region.

The main conclusions obtained in previous studies [3-5,9,10], served as the basis for selecting criteria for assessing the length of

the LTT region and detecting the beginning of the fully developed turbulent regime in a freeconvection boundary layer.

All results for the flow without disturbances introduced (case B1) are shown by circles in the graphs below; the results for rectangular obstacles (case B2), by squares, and for the results of trapezoidal obstacles (case B3) by triangles.

The maximum values of the following dimensionless characteristics of the flow were analyzed:

temperature fluctuation intensities, IT_{m} ,

$$IT_m = \left(\sqrt{t^2} / \Delta T\right)_{\max}, \qquad (2)$$

where T_m , K, is the maximum temperature in a given section of the boundary layer; t, K, is the fluctuation component of the current temperature;

velocity fluctuation intensities, IU_m,

$$IU_{m} = \left(\sqrt{u^{2}}/U_{b}\right)_{\max},$$
 (3)

where U_m , m/s, is the maximum velocity in a given section of the boundary layer; u, m/s, is the fluctuation component of the current axial velocity; U_b m/s, is the buoyancy velocity, determined by the relation $U_b = (g\beta\Delta Tv)^{1/3}$;

termined by the relation $U_b = (g\beta\Delta Tv)^{1/3}$; dimensionless mean velocity U_m/U_b in the given section along the coordinate X.

It was not our intention to measure the full distributions of the characteristics of the boundary layer. Only the near-wall part of the distribution was measured, and this was sufficient to objectively assess the maximum values of the given characteristics in this section along the axial coordinate X.

Fig. 2 shows the distributions of the maximum values of temperature fluctuation intensity IT_m with respect to the local Grashof number, as well as along the dimensional coordinate X for the three given cases of obstacles. The thermophysical properties of air for calculating the Grashof number were taken at a mean temperature equal to $(T_w + T_x)/2$. The exception was the value of the thermal expansion coefficient, which was estimated at external temperature. The Grashof number is determined by the relation

$$\operatorname{Gr}_{x} = \frac{g \cdot \beta \cdot \Delta T \cdot X^{3}}{v^{2}}.$$
 (4)



Fig. 2. Maximum values of temperature fluctuation intensity IT_m in the section across the layer depending on local Grashof number Gr_x for three cases of obstacles (the curve numbers correspond to the case numbers)

Analysis of the data obtained for case B1 made it possible to discover the following features:

a smooth increase in the fluctuation intensity IT_m up to the maximum value at $X \approx$ 1000 mm, $Gr_x \approx 4.9 \cdot 10^9$;

a slight subsequent decrease in IT_m ; starting from $X \approx 1200 \text{ mm} (\text{Gr}_x \approx 8.4 \cdot 10^9)$, the values of IT_m practically do not change.

Analysis of the results obtained for cases B2 and B3 allows us to draw the following conclusions:

the growth rate of IT_m is about 20% higher for case B2, than the corresponding velocity for case B3 up to $X \approx 450 \text{ mm} (\text{Gr}_x \approx 4.4 \cdot 10^8)$. Then, starting from $X \approx 500 \text{ mm} (\text{Gr}_x \approx 6.1 \\ 10^8)$, the fluctuation values IT_m observed for B3 sharply increase and reach the maximum value at $X \approx 550 \text{ mm} (\text{Gr}_x \approx 8.1 \cdot 10^8)$. In turn, the fluctuations IT_m reach their maximum value only at $X \approx 750 \text{ mm} (\text{Gr}_x \approx 2.0 \cdot 10^9)$ for B2;

the values of the temperature fluctuation intensity for B2 and B3 approach each other with a further increase in the values of the coordinate X (local Grashof number), and, starting from $X \approx 1200$ mm (Gr_x $\approx 8.4 \cdot 10^9$) are combined with IT_m for B1, reaching an almost constant value.

Fig. 3 shows the distributions of the maximum values of velocity fluctuations IU_m along the plate for the three given cases. The following was established from analysis of the data presented:



Fig. 3. Maximum values of velocity fluctuation intensity IU_m in the section across the layer depending on local Grashof number Gr_x for three cases of obstacles (the curve numbers correspond to the case numbers)



Fig. 4. Maximum values of dimensionless mean velocity U_m/U_b in the section across the layer depending on local Grashof number Gr_x for three cases of obstacles (the curve numbers correspond to the case numbers)



Fig. 5. Dependences of Nusselt number on Grashof number for three cases of obstacles (the first numbers of the curves correspond to the numbers of the cases); segments of curves 4-6 are additionally shown:

(4) $\operatorname{Nu}_{x}^{lam} = 0.83 \operatorname{Gr}_{x}^{0.22}$; (5) $\operatorname{Nu}_{x} = 0.05 \operatorname{Gr}_{x}^{0.37}$; (6) $\operatorname{Nu}_{x} = 0.09 \operatorname{Gr}_{x}^{0.34}$

starting from $X \approx 300 \text{ mm} (\text{Gr}_x \approx 1.3 \cdot 10^8)$, the fluctuation intensity IU_m for both cases with disturbances (B2 and B3) considerably exceeds the fluctuation intensity IU_m for the case without disturbances. Moreover, a rapid increase in the intensity IU_m is observed for B2, and the maximum values of IU_m are reached at $X=500 \text{ mm} (\text{Gr}_x \approx 6.1 \cdot 10^8)$;

the intensities IU_m increase almost equally up to $X \approx 650 \text{ mm} (\text{Gr}_x \approx 1.3 \cdot 10^9)$ for B3 and B1, then IU_m for B3 begins to decrease, and the fluctuation intensity for B1 increases, reaching a maximum value at $X \approx 950 \text{ mm}$ (Gr_x $\approx 4.2 \cdot 10^9$);

the intensities IU_m approach each other for all three cases with a further increase in the values of the coordinate X (local Grashof number), reaching identical values at $X \approx 1400 \text{ mm} (\text{Gr}_{x} \approx 1.3 \cdot 10^{10}).$

Fig. 4 shows the distributions of the maximum values of the dimensionless mean velocity U_m/U_b with respect to the Grashof number. The following was established from analysis of the data presented:

the values of the maximum velocity U_m/U_b at the beginning of the boundary layer $(X \approx 300 \text{ mm or } \text{Gr}_x \approx 1.3 \ 10^8)$ for the three cases were distributed in accordance with resistances to the developing flow from the disturbances (obstacles). For example, case B3 has the greatest resistance, for which the value of velocity U_m/U_b increases monotonically

throughout the entire section observed. At the same time, the velocities U_m/U_b for cases B2 and B1 increase almost identically up to the coordinate $X \approx 400$ mm (Gr_x $\approx 3.1 \cdot 10^8$). After that the velocity U_m/U_b for case B2 still deviates from the values for B1, starting to slow down and merging with the curve for B3 at a distance $X \approx 900$ mm (Gr_x $\approx 3.5 \cdot 10^9$).

as expected, the velocity U_m/U_b for B1 steadily reaches the maximum value at $X \approx 850 \text{ mm} (\text{Gr}_x \approx 2.3 \cdot 10^9)$ and then, slowly decreasing, merges with the curves for the two other cases at $X \approx 1200 \text{ mm} (\text{Gr}_x \approx 8.4 \cdot 10^9)$.

Before we can analyze the results obtained for heat transfer, let us briefly describe the procedure for determining the local heat transfer coefficient α (W/(m². K)) and, ultimately, the Nusselt number Nu_x, expressed as

$$Nu_x = \frac{\alpha \cdot X}{\lambda},$$
 (5)

where λ , W/(m·K), is the thermal conductivity.

The procedure is based on the technique proposed in [3–5]. According to this technique, there is a thin heat-conducting layer near the wall, where the distribution of the averaged temperature linearly depends on the normal coordinate Y. Based on this, the heat flux q_w from the surface can be represented in the following form:

$$q_{w} = -\lambda \cdot \left(\partial T / \partial Y\right) \Big|_{w} = \alpha \cdot \Delta T.$$
 (6)

Consequently, the local heat transfer coefficient α can be easily calculated if the derivative is determined graphically from the experimental temperature distribution.

The degree to which the disturbances influence the process of transition from

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laminar to turbulent flow is well observed from the variation in heat transfer in this region. Fig. 5 shows the dependences of the Nusselt number Nu_x on the local Grashof number Gr_x for the case without disturbances (B1) and two cases with disturbances (B2 and B3).

Two regions are distinctly observed for B1: laminar and turbulent regions of the boundary layer with the corresponding laws of heat transfer:

$$Nu_{r}^{lam} = 0.83Gr_{r}^{0.22}; Nu_{r}^{turb} = 0.07Gr_{r}^{0.35}.$$

Additionally, notice the fairly extended LTT region (Gr_x ϵ (2 - 10)·10⁹). A complete absence of a laminar region is observed for both cases upstream after the obstacles. Moreover, a region with the laws of heat transfer characteristic for a turbulent flow regime begins almost immediately after the obstacles. For example, this ratio is Nu_x = 0.05·Gr_x^{0.37} for the case B2, and Nu_x = 0.09·Gr_x^{0.34} for the case B3.

Conclusion

Based on the data presented in the paper, we can claim with confidence that largescale obstacles can be used to substantially reduce the length of the transition region in free-convective boundary layers, moving the beginning of the region with fully developed turbulent heat transfer closer to the leading edge of the streamlined surface. In terms of practical application, obstacles of this kind can serve as passive elements for controlling the intensity of heat transfer.

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THE AUTHORS

CHUMAKOV Yuriy S.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation chymakov@yahoo.com

KHRAPUNOV Evgeniy F.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation hrapunov.evgenii@yandex.ru

MALYKH Anastasiya D.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation anfatneva@yandex.ru

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СВЕДЕНИЯ ОБ АВТОРАХ

ЧУМАКОВ Юрий Сергеевич — доктор физико-математических наук, профессор Высшей школы прикладной математики и вычислительной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация. 195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29

195251, Россииская Федерация, г. Санкт-Петербург, Политехническая chymakov@yahoo.com

ХРАПУНОВ Евгений Федорович — аспирант Высшей школы прикладной математики и вычислительной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 hrapunov.evgenii@yandex.ru

МАЛЫХ Анастасия Денисовна — студентка магистратуры Высшей школы прикладной математики и вычислительной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 anfatneva@yandex.ru

BIOPHYSICS AND MEDICAL PHYSICS

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A NOVEL PHYSICO-MATHEMATICAL TECHNIQUE OF ANALYZING THE QUANTITATIVE ELECTROENCEPHALOGRAMS: DEVELOPMENT AND APPLICATION

M.E. Sobolev¹, A.L. Gorelik², O.L. Vlasova¹

¹ Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation;

² V.M. Bekhterev National Medical Research Center for Psychiatry and Neurology,

St. Petersburg, Russian Federation

The article presents a physical and mathematical model developed by the authors. The model allows analyzing the amplitude-frequency characteristic (AFC) of electroencephalograms (EEG) of a human brain. The proposed method of EEG processing, in contrast to the previously used one, is based on approximating the AFC by an equation that contains a set of coefficients. This method is convenient for comparing data obtained from different subjects and, as found, has diagnostic significance. Previously, only the frequency / amplitude ratio or its inverse was used for evaluations. The results achieved indicate the possibility of differentiating patients of various neuropsychic profiles according to the values of the parametric indicators obtained by approximating the EEG amplitude-frequency response.

Keywords: quantitative EEG, amplitude-frequency characteristic, EEG mathematical analysis, schizophrenia, dementia

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РАЗРАБОТКА И ПРИМЕНЕНИЕ НОВОГО ФИЗИКО-МАТЕМАТИЧЕСКОГО МЕТОДА АНАЛИЗА КОЛИЧЕСТВЕННЫХ ЭЛЕКТРОЭНЦЕФАЛОГРАММ

М.Е. Соболев¹, А.Л. Горелик², О.Л. Власова¹

¹Санкт-Петербургский политехнический университет Петра Великого, Санкт-Петербург, Российская Федерация;

² Национальный медицинский исследовательский центр психиатрии и неврологии им. В. М. Бехтерева, Санкт-Петербург, Российская Федерация

В статье представлена разработанная авторами физико-математическая модель, позволяющая анализировать амплитудно-частотную характеристику (АЧХ) электроэнцефалограмм (ЭЭГ) головного мозга человека. Предлагаемый метод обработки ЭЭГ, в отличие от применявшегося ранее, основан на аппроксимации АЧХ уравнением, которое содержит набор коэффициентов, удобных для сравнения данных, полученных от разных испытуемых и, как установлено, обладающих диагностической значимостью. Ранее для оценок использовалось лишь отношение частота/амплитуда либо обратное ему. Полученные результаты указывают на возможность дифференциации пациентов различных нервно-психических профилей по значениям параметрических показателей, получаемых при аппроксимации АЧХ ЭЭГ.

Ключевые слова: количественная ЭЭГ, амплитудно-частотная характеристика, математический анализ ЭЭГ, шизофрения, деменция

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Introduction

The share of interdisciplinary research in biomedical applications is growing steadily. One potential direction for this approach are modern computer technologies and methods of mathematical data processing in neurophysiological research. These studies consider neurodynamic processes occurring in the brains of animals belonging to different types and classes, as well as in the human brain. Researchers aim to gain an understanding of the mechanisms governing the nervous system and the mind, working with individual neurons, cell populations, brain slices, and the brain as a whole, as well as with their computer models.

Electroencephalography (EEG) is a noninvasive method for recording brain activity, widely used in research and in clinical practice, along with magnetic resonance imaging (MRI), positron emission tomography (PET), computed tomography (CT). EEG records bioelectric signals of the brain taken from the electrodes placed on the surface of the scalp by measuring the voltage differences between the electrodes applied and the references [1]. The images obtained by EEG, characterizing the recorded voltage differences, are called electroencephalograms.

EEG readings reflect the synchronous synaptic activity of neuron populations. Electrical excitation of neurons generates an extracellular voltage that allows the opposing ends of the neuron (dendrites and axons) to have different charges. The general purpose of EEG is to interpret the changes in measured signals reflecting the changes in the activity of certain regions of the brain. Identifying these regions is a crucial problem, since the measurements in the surface of the scalp reflect the sum of the signals taken from different spatially distributed regions of the brain. Because neural activity is cyclic, the measured voltage fluctuates between positive and negative, and the rate of this cycle reflects the frequency of the signal.

EEG is a highly sensitive method with a resolution of up to tens of milliseconds, allowing to observe the evolution of various bioelectric processes over time, which cannot be achieved by other methods. In addition, EEG makes it possible to explore the response of such a highly complex biological system as the brain to various stimuli. However, a high-quality amplifier is necessary to adequately record and then interpret electroencephalograms, since the amplitude of the measured signal is small: it ranges from units to several tens of microvolts.

Several frequency ranges are observed in the bioelectric signal of the brain [2]: delta (0.5-4 Hz), theta (4-8 Hz), alpha (8-13 Hz), beta (13-30 Hz), and gamma (over 30 Hz). It can be seen from Fig. 1 that the measured signal contains all of these rhythms in a certain proportion which changes depending on the brain's activity.



Fig. 1. Total signal of local EEG and brain rhythms: delta, theta, alpha, beta, gamma [3]

In general, quantitative studies of electroencephalograms rely on various methods of analysis, including cross-correlation coefficients, coherence coefficients, the method of evoked potentials, etc. Different methods are also used to study the frequency response of the bioelectric signal of the brain. One of these methods is considered in our study.

The method of evoked potentials (EP) consists of recording the electrical activity of the brain in response to an external stimulus. This method is used to study such properties of the brain as excitability and susceptibility to stimuli [4]. The amplitude and the delay in the response of evoked potentials of EEG signals provide valuable data on the functional capabilities of the brain in different conditions and in different target groups. For example, an increase in time delay may be associated with attention deficit hyperactivity disorder (ADHD) in children [5], aging [6], mild cognitive impairment [7], and various psychotic conditions [8].

Applying energy-dispersive spectroscopy [9] for analysis of evoked potentials - is one of the most successful methods for identifying biomarkers. In addition, it can yield important data on the frequency composition of EEG oscillations. Typically, spectral estimates are calculated for discrete frequencies (for example, 8.5–10.0 Hz, that is, for the lower alpha band). The RMS amplitude or power (squared amplitude) of the given EEG signal frequency is used to quantify its contribution to the measured signal.

Unfortunately, spectral analysis does not provide data for the temporal evolution, that is, for the moments when frequency shifts occur over time. This problem can be solved by different methods of time-frequency analysis, including short-term Fourier transform, and wavelet analysis, which has gained popularity in recent years, making it possible to accurately convert EEG signal shapes into specific time and frequency components. EEG signals are regarded within this approach as shifted and scaled versions of a particular mathematical function (wavelet) rather than the composition of sinusoidal waves with different frequencies, as is the case with Fourier transforms. It has been found that the spectral power of alpha waves at rest and the peak frequency of the alpha rhythm can be reduced in patients with psychotic disorders [10]. A possible reason for this is that decreased alpha power is correlated with negative symptoms in schizophrenia.

Schizophrenia is a severe mental illness that affects approximately 1% of the population.

Because this disabling disorder may be caused by diverse genetic and neurobiological factors, many trials have been carried out to identify its biomarkers with a view to its early diagnosis. The biomarkers most commonly used for schizophrenia are associated with the neuroimmune and neuroendocrine systems, metabolism, various neurotransmitter systems, and neurotrophic factors. Quantitative electroencephalography has also been applied to identify possible biomarkers but such studies are very scarce. A notable paper [11] considers the theta-phase gamma-amplitude relationship as an evidence-based tool for the detection of schizophrenia.

Russian researchers compared various indicators of the alpha rhythm in the electroencephalograms of healthy subjects with the corresponding indicators in patients with arterial hypertension [12]. The values of the amplitude and frequency observed for patients with hypertension were lower than those in healthy subjects. An increase in the frequencyamplitude ratio in the frontal, parietal and occipital electrodes was found for diseased subjects, without any changes in the temporal electrodes.

Several cerebrovascular and cardiovascular diseases are associated with the onset of dementia. The neuropsychological profile of patients with such disorders [13] depends on the location and depth of vascular damage to the brain, as well as on the types of cerebrovascular pathologies. Quite often, such pathologies affect the frontal lobes; consequently, the patient's motivation begins to decrease and control over the actions deteriorates. In addition, such symptoms as forgetfulness and confusion are observed. Ref. [14] reported an increase in the spectral power in the delta range, proportional to the damage to the cardiovascular system, and a decrease in the power of the alpha rhythm in diseased subjects. Furthermore, it was found that the ratio of theta to the alpha power can serve as a reliable marker for assessing the individual degree of brain damage in cardiovascular diseases.

Our study describes a new mathematical model that adequately describes the amplitude-frequency response of the EEG.

We found the statistical distribution of the coefficient values determined by fitting the EEG frequency response obtained during examination of healthy subjects, comparing the obtained parameters between the groups of healthy subjects and those suffering from schizophrenia and age-related vascular dementia.



Fig. 2. International 10–20 system [15]; the human skull is shown in two projections (*a* and *b*) with characteristic points on it: bridge of the nose (Nasion), the crown (Vertex) and occipital protuberance (Inion); see also the explanations in the text

Materials and methods

Electroencephalograms of the subjects were obtained at the Department of Functional Diagnostics of the V.M. Bekhterev National Medical Research Center for Psychiatry and Neurology (St. Petersburg) from 2010 to 2018. A Telepath-104 electroencephalograph was used for the recordings. The electrodes were positioned in accordance with the international 10–20 system (Fig. 2) [15].

The following notations and abbreviations were introduced in the figure for the electrodes and the anatomical structures: Nasion for bridge of the nose, Inion for occipital protuberance, Vertex for crown, Preaurical point for external auditory meatus, F for lobus frontalis (frontal lobe), C for sulcus centralis cerebri (central sulcus), T for lobus temporalis (temporal lobe), P for lobus parietalis (parietal lobe), O for lobus occipitalis (occipital lobe), A for auricula (earlobe); the electrodes in the left hemisphere are denoted by odd indices, and the electrodes in the right hemisphere by even indices.

The sampling rate of the electroencephalograph was 250 Hz. A cap consisting of silicone tubes and silver chloride non-polarizing bridge electrodes were used.

Three groups of subjects were considered: relatively healthy (normal) subjects, patients with schizophrenia and patients with age-related vascular dementia. The 'normal' group consisted of relatively healthy subjects and included 17 people aged 20 to 64 (3 men and 14 women). The 'schizophrenia' group included 9 patients with schizophrenia aged 22 to 49 (4 men and 5 women). The 'age-related vascular dementia' group included 17 people aged from 54 to 80 (6 men and 11 women) suffering from age-related cerebrovascular disorders with pronounced cognitive decline.

EEG recordings were examined in the WinEEG 2.90.53 program using averagereference montage, with 16 electrodes, or (Fp1, Fp2, F3, F4, C3, C4, P3, P4, O1, O2, F7, F8, T3, T4, T5, T6) channels. The high-pass filter was set to 0.5 Hz, the low-pass filter - to 50 Hz, with a notch filter at 50 Hz. Epoch length was 5 s. Artifact-free epochs recorded while the subjects were at rest with their eyes closed (the so-called quiet wakefulness) were chosen for analysis. About 45 different values of amplitudes and frequencies were obtained for each subject. Analysis of the coefficients was carried out using the MagicPlot 2.7.2 software. We used Student's *t*-test for statistical analysis.

A physico-mathematical model was developed for quantitative analysis of electroencephalograms, reflecting the relationship between the amplitude and frequency of the bioelectric signal of the brain, which is described by the following formula:

$$A(f) = af + b + a_1 \exp[-(f - f_0)^2 \ln 2/\sigma^2],$$
(1)

where *A*, V, is the amplitude of the wave; *f*, Hz, is the wave frequency; *a*, *b*, a_1, f_0, σ are the numerical coefficients in different units: *a* in V/Hz; *b*, a_1 in V; f_0, σ in Hz.

Eq. (1) was derived empirically by approximating the frequency response. It provides the best description, giving the



Fig. 3. Example of approximated (dashed line) experimental frequency response (points) for T5 electrode for one of the subjects in the 'normal' group; the values of the obtained parameters are given

minimum error of deviation from the given response curve. The frequency response was calculated in earlier studies using simply the ratio of amplitude to frequency or the inverse ratio, which is certainly convenient for obtaining a simple estimate but has no physical basis. Eq. (1) complicates calculations but reflects the behavior of the measured signal curve, therefore, it best describes the curve corresponding to the amplitude versus frequency function. Based on these considerations, the amplitudes and frequencies for each electrode, obtained from the electroencephalograms for each subject, were approximated by Eq. (1). The biophysical nature of the proposed relationship is undoubtedly intriguing and may be the subject of a separate study. However, this task is beyond the scope of our analysis.

Results and discussion

Let us first consider the results for the 'normal' group. An example of the approximated frequency response obtained for one of the subjects using the T5 electrode is shown in Fig. 3. The frequency response for other channels had a similar appearance for each subject from the 'normal' group.

Because we observed no significant differences in the coefficient values between the channels in each of the three study groups, data for each parameter were analyzed simultaneously for all electrodes (without separating the data for different electrodes). As a result, statistical distributions of the coefficient values were obtained for the 'normal' group (Fig. 4). Evidently, the peak frequency f_0 lies in the alpha range, and so the obtained data are consistent with the general notion that the maximum amplitude of alpha waves occurs in a state of passive wakefulness with eyes closed (at rest).

Comparing the obtained values of the parameters between the three groups, we found the following differences (the paragraphs are lettered in accordance with the letters in Fig. 5):

a) in the coefficient a_1 between the 'normal' and 'age-related vascular dementia' groups (p < 0.05); between the 'schizophrenia' and 'agerelated vascular dementia' groups (p < 0.05);

b) in the coefficient f_0 between the the 'normal' and 'age-related vascular dementia' groups (p < 0.05); between the 'schizophrenia' and 'agerelated vascular dementia' groups (p < 0.05); between the 'normal' and 'schizophrenia' groups (p < 0.20);

c) in the coefficient σ between the 'normal' and 'schizophrenia' groups (p < 0.05); between the 'schizophrenia' and 'age-related vascular dementia' groups (p < 0.05).

These differences are shown graphically in Fig. 5. No other differences were found between the coefficients.

Thus, it was found that there are distinct characteristics in the behavior of the frequency response for each of the three groups, different from the other groups. For example, the



Fig. 4. Statistical distributions of frequency response coefficients (1) for subjects of the 'normal' group



Fig. 5. Statistical distributions of coefficients $a_1(a)$, $f_0(b)$ and $\sigma(c)$ for all electrodes for three groups of subjects: 'normal' (N), 'schizophrenia' (Sch), 'dementia' (D); the differences observed between the data are given in the text

characteristics for the 'schizophrenia' group are a slightly reduced peak frequency f_0 , compared to the 'normal' group (but still falling into the upper theta and lower alpha frequency ranges) and increased half-width at half-maximum σ , compared to similar coefficients from the other two groups. In the meantime, the 'age-related vascular dementia' group is characterized by a negative value of the coefficient a_1 (i.e., the Gaussian peak is deflected downwards rather than upwards) and a reduced value of the peak frequency f_0 .

Notably, the differences in data between the groups should be assessed by the entire set of values of the obtained parameters, and not by one single parameter value.

Analysis of the results has lead us to conclude that the proposed mathematical model (1) can be used to divide the subjects into groups in accordance with their specific diseases.

Conclusion

Electroencephalography is a popular method to diagnose various neuropsychiatric used disorders. Because of its high temporal resolution, EEG allows to almost instantly track the changes in brain activity. In contrast to several other methods, the procedure is non-invasive and absolutely harmless for the subjects.

EEG signals are electrophysiological responses reflecting basic neural activities that depend on the physiological states of the subject (for example, emotions, attention, and many others). The key parameters obtained by EEG are

model that we have developed, approximating amplitude-frequency the characteristic human electroencephalograms. We have found pronounced differences in the values of the coefficients obtained for different clinical groups of subjects. It has been established that the selected empirical parameters have actual diagnostic significance rather than serve for fitting

and

analysis, is important for clinical practice.

manifestations

purposes only. Thus, we have confirmed the practical significance of the proposed method for differentiating neuropsychic disorders in patients.

the amplitude and frequency of the measured

signal. Determining these parameters visually can produce serious errors; for this reason, they

are calculated by various software packages and methods. Furthermore, understanding different

functional states of the brain, identified, in

particular, by mathematical methods of EEG

This study presents a physico-mathematical

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THE AUTHORS

SOBOLEV Maxim E.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation m.e.sobolev@mail.ru

GORELIK Aleksandr L.

V.M. Bekhterev National Medical Research Center for Psychiatry and Neurology 3 Bekhterev St., St. Petersburg, 192019, Russian Federation gorelik_a@mail.ru

VLASOVA Olga L.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation olvlasova@yandex.ru

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СВЕДЕНИЯ ОБ АВТОРАХ

СОБОЛЕВ Максим Евгеньевич — аспирант Высшей инженерно-физической школы Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 m.e.sobolev@mail.ru

ГОРЕЛИК Александр Леонидович — кандидат медицинских наук, заведующий отделением функциональной диагностики Национального медицинского исследовательского центра психиатрии и неврологии им. В.М. Бехтерева, Санкт-Петербург, Российская Федерация.

192019, Российская Федерация, г. Санкт-Петербург, ул. Бехтерева 3 gorelik_a@mail.ru

ВЛАСОВА Ольга Леонардовна — доктор физико-математических наук, профессор, директор НОЦ «Фундаментальные основы медицинских и биомедицинских технологий» Высшей школы биомедицинских систем и технологии Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 olvlasova@yandex.ru

THEORETICAL PHYSICS

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SYMMETRY TRANSFORMATION PARAMETERS AS CLASSICAL DYNAMIC VARIABLES IN THE GAUGE THEORY

N.N. Gorobey¹, A.S. Lukyanenko¹, A.V. Goltsev²

¹ Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation;

² Ioffe Physical-Technical Institute, St. Petersburg, Russian Federation

A modification of the gauge theory is proposed, in which the set of generalized coordinates is supplemented with symmetry transformation parameters, and the condition is additionally imposed on the latter, which ensures the classical character of their dynamics in the quantum theory. As a result, additional dynamic variables and transverse physical degrees of freedom in the Hamiltonian become separated. The classical theory of the Yang–Mills field is considered.

Keywords: gauge theory, quantization, symmetry transformation parameters, Hamiltonian

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ПАРАМЕТРЫ ПРЕОБРАЗОВАНИЯ СИММЕТРИИ КАК КЛАССИЧЕСКИЕ ДИНАМИЧЕСКИЕ ПЕРЕМЕННЫЕ В КАЛИБРОВОЧНОЙ ТЕОРИИ

*H.H. Горобей*¹, *А.С. Лукьяненко*¹, *А.В. Гольцев*² ¹ Санкт-Петербургский политехнический университет Петра Великого, Санкт-Петербург, Российская Федерация;

> ² Физико-технический институт им. А.Ф. Иоффе, Санкт-Петербург, Российская Федерация

Предложена модификация калибровочной теории, в которой множество обобщенных координат дополняется параметрами конечных преобразований симметрии. На последние наложено дополнительно условие, обеспечивающее классический характер их динамики после квантования. Как результат, дополнительные динамические переменные и физические поперечные степени свободы в гамильтониане разделяются. Рассмотрена классическая теория поля Янга – Миллса.

Ключевые слова: калибровочная теория, квантование, параметр симметрии, гамильтониан

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Introduction

A simple and natural understanding of the dynamic structure of the gauge theory is that the initial set of dynamic variables in its mathematical apparatus is redundant and some of them should be eliminated by solving the equations of constraints and additional gauge conditions [1]. However, in the subsequent development, this reduction procedure has been replaced by the expansion of the phase space of the theory with the addition of Lagrange multipliers with the corresponding canonical momenta and ghosts, as well as the expanded BRST-symmetry [2-6]. Another option for expanding the phase space of the gauge theory was proposed in Ref. [7], where the parameters of finite symmetry transformations were added to the original dynamic variables. These finite shifts in the group space are constructed in the form of integrals of infinitesimal shifts generated by constraints. However, such an extension alone does not solve the problem of separating physical degrees of freedom and pure calibrations and a dynamic interpretation of the theory. It should be supplemented with a structure that allows connecting finite shifts in the group space with observations. In the case of the dynamics of relativistic particles with reparametrization invariance of their world lines, the intrinsic parameter of the symmetry group plays the intrinsic time of each particle. This invariant parametrization also arises naturally in the BRST-invariant representation of the propagator of covariant quantum theory for a relativistic particle [8] and reproduces the Fock [9] and Schwinger [10] formalism based on the introduction of proper time. In Ref. [11], the introduction of this parameter was proposed to be supplemented with the condition of its classical dynamics with the corresponding modification of the initial action. This addition allows us to connect the proper time with observations and get a dynamic interpretation of covariant quantum theory. It can be assumed that such a two-stage modification of the singular theory (adding finite symmetry transformations to dynamic variables and an additional condition for their classical dynamics) will be an effective way to separate physical degrees of freedom and pure gauges in the general case.

In this paper, this modification has been shown as an example of a free Yang-Mills field. The result should be a separation of the dynamics of the physical transverse components of the Yang-Mills field and the "motion" of the longitudinal components (pure calibrations) in the group space.

Modification of the Yang-Mills' action

The proposed mode caution of the gauge theory action is divided into two stages. We proceed from the canonical form of action, namely,

$$I = \int dt \Big[p_i \dot{q}_i - \lambda_a \varphi(p,q) - h(p,q) \Big], \quad (1)$$

where the constraints obey the commutation relations:

$$\{ \varphi_a, \varphi_b \} = C_{abd} \varphi_d, \{ \varphi_a, h \} = h_a \varphi_{ad},$$
 (2)

(we consider the case $h_a = 0$), and variations of the Lagrangian multipliers ensuring the invariance of the action (1) with respect to the infinitesimal symmetry transformations

$$\delta q_i = \varepsilon_a \{ q_i, \varphi_a \}, \delta p_i = \varepsilon_a \{ p_i, \varphi_a \}$$
(3)

have the form

$$\delta\lambda_a = \dot{\varepsilon}_a - C_{abd}\lambda_b\varepsilon_d. \tag{4}$$

At the first stage, according to Ref. [7], we replace the Lagrangian multipliers with explicit functions of the parameters defining the finite symmetry transformation ($\delta s_a = \varepsilon_a$):

$$\lambda_a = \dot{s}_b \Lambda_{ab} \left(s \right), \tag{5}$$

which are integrals of functional-differential Eqs. (4). At the second stage, according to Ref. [11], we add a variation generated by the infinitesimal shift of new dynamic variables to the action. We call this step a condition of classical dynamics, since it allows one to remove integration over new dynamic variables in the functional-integral representation of the propagator of covariant quantum theory. We carry out these constructions as an example of a free Yang-Mills field $A_{\mu a}$ where μ is a space-time index ($\mu = 0, 1, 2, 3$), and *a* is an internal index of the gauge theory. Here, A_{0a} are the Lagrange multipliers, so, at the first stage, the original Yang-Mills Lagrangian function takes the form

$$L = \frac{1}{2} \left[\left(\dot{A}_{ia} - \nabla_i \left(\dot{s}_b \Lambda_{ba} \right) \right)^2 - B_{ia}^2 \right], \quad (6)$$

where B_{ia} is the Yang-Mills "magnetic field" tension, and the covariant derivative is determined by the following relation [1]:

$$\nabla_i F_a = \partial_i F_a - igT_{bad} A_b F_d. \tag{7}$$

We will not have need of the explicit form of functions Λ_{ab} here. Now, following Ref. [8], we will still expand the set of new variables by adding infinitesimal shifts ε_a to them, as well to Lagrangian function (6) we add its variation generated by these infinitesimal shifts:

$$\tilde{L} = \frac{1}{2} \left[\left(\dot{A}_{ia} - \nabla_i \left(\dot{s}_b \Lambda_{ba} \right) \right)^2 - B_{ia}^2 \right] +$$

$$+ \left(\dot{A}_{ia} - \nabla_i \left(\dot{s}_b \Lambda_{ba} \right) \right) \cdot \left(\nabla_i \left(\dot{\varepsilon}_c \Lambda_{ca} + \dot{s}_c \frac{\partial \Lambda_{ca}}{\partial s_d} \varepsilon_d \right) \right).$$
(8)

The canonical form of the modified Yang-Mills' action

Now we turn to the canonical form of the modified action (8). Let us find the canonical momenta:

$$\pi_{ia} = \dot{A}_{ia} - \nabla_i \left(\dot{s}_b \Lambda_{ba} \right) + \nabla_i \left(\dot{\varepsilon}_c \Lambda_{ca} + \dot{s}_c \frac{\partial \Lambda_{ca}}{\partial s_d} \varepsilon_d \right),$$
⁽⁹⁾

conjugated to A_{ia} , and

$$p_{s_{b}} = -\Lambda_{ab} \nabla_{i} \left(\dot{A}_{ia} - \nabla_{i} \left(\dot{s}_{c} \Lambda_{ca} \right) \right) - \nabla_{i} \left(\dot{A}_{ic} - \nabla_{i} \left(\dot{s}_{q} \Lambda_{qc} \right) \right) \frac{\partial \Lambda_{bc}}{\partial s_{d}} \varepsilon_{d} - (10) - \Lambda_{ab} \Delta \left(\dot{\varepsilon}_{c} \Lambda_{ca} + \dot{s}_{c} \frac{\partial \Lambda_{ca}}{\partial s_{d}} \varepsilon_{d} \right),$$

conjugated to $s_a (\Delta = \nabla_i \nabla_i)$, and

$$P_{\varepsilon_b} = -\Lambda_{ab} \,\nabla_i \left(\dot{A}_{ia} - \nabla_i \left(\dot{s}_c \Lambda_{ca} \right) \right), \quad (11)$$

conjugated to ε_b .

From here we immediately obtain the constraint equations,

$$p_{s_b} = -\Lambda_{ab} \nabla_i \pi_{ia} + P_{\varepsilon_a} \Lambda_{ac}^{-1} \frac{\partial \Lambda_{cb}}{\partial s_d} \varepsilon_d, \quad (12)$$

and generalized velocities in the following combination:

$$\dot{\varepsilon}_{\tilde{n}}\Lambda_{a\tilde{n}} + \dot{s}_{c} \frac{\partial \Lambda_{ca}}{\partial s_{d}} \varepsilon_{d} =$$

$$= \Delta^{-1} \Big(\nabla_{i} \pi_{ia} + \Lambda_{ab}^{-1} p_{\varepsilon_{b}} \Big).$$
(13)

Now we find the Hamilton function of the modified theory:

$$\tilde{h} = \frac{1}{2} \left[\pi_{ia}^2 + B_{ia}^2 \right] - \frac{1}{2} \left[\nabla_i \Delta^{-1} \left(\nabla_k \pi_{ka} + \Lambda_{ab}^{-1} p_{\varepsilon_b} \right) \right]^2,$$
(14)

where we used (13).

Let us see what we have got as a result. Obviously, the constraints (12) commute with the Hamiltonian (14). The Hamiltonian does not contain ε_a which means that canonical momenta P_{ε_a} (color density of a charge) are integrals of motion. We perform the orthogonal longitudinal-transverse splitting of the canonical momenta:

$$\pi_{ia} = \nabla_i \left(\chi_{0a}^L + \chi_a^L \right) + \pi_{ia}^T, \qquad (15)$$

With

$$\Lambda_{ab} \Delta \chi^L_{0b} = -P_{\varepsilon_a}.$$
 (16)

As a result, the quadratic form of the momenta in the Hamiltonian contains only the transverse components:

$$\tilde{h} = \frac{1}{2} \left[\pi_{ia}^{T^2} + B_{ia}^2 \right].$$
(17)

Thus, the longitudinal components of the Yang-Mills are completely excluded from the dynamics in time. For them, only the "dynamics" in the group space described by the constraints (12) remains. Here, the evolution parameters s_a are supplemented by dynamic variables P_{ε_a} which can be eliminated by choosing the origin of the longitudinal component of the momentum according to Eq. (16). In the gauge theory with the constraints linear in canonical momenta, these quantities do not have a dynamic meaning.

Summary

Thus, in the Yang-Mills theory, and generally in the theory with the constraints linear in canonical momenta, the introduction

of the classical parameters of symmetry transformations as additional dynamic variables allows us to separate the physical transverse and gauge longitudinal degrees of freedom. At the same time, classical external sources which are generators of classical symmetry transformations are also added as dynamic variables. These sources themselves can be set equal to zero, as long as the separation of the physical degrees of freedom is done. In theories with quadratic on the canonical momenta constraints, such as the theory of gravity, in which there is a time problem, the modification proposed here introduces the concept of proper time, which also has its own classical source – energy. In contrast to the case considered here, this energy can have a dynamic meaning. This issue will be considered separately.

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6. Ore F.R., van Nieuwenhuisen P. Local

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THE AUTHORS

GOROBEY Natalia N.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation n.gorobey@mail.ru

LUKYANENKO Alexander S.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation alex.lukyan@rambler.ru

GOLTSEV AlexanderV.

Ioffe Physical-Technical Institute 26 Politekhnicheskaya St., St. Petersburg, 195251, Russian Federation goltsev@ua.pt

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СВЕДЕНИЯ ОБ АВТОРАХ

ГОРОБЕЙ Наталья Николаевна — доктор физико-математических наук, профессор кафедры экспериментальной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 n.gorobey@mail.ru

ЛУКЬЯНЕНКО Александр Сергеевич — доктор физико-математических наук, профессор кафедры экспериментальной физики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 alex.lukyan@rambler.ru

ГОЛЬЦЕВ Александр Викторович — доктор физико-математических наук, профессор, старший научный сотрудник Физико-технического института им. А.Ф. Иоффе, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 26. golysev@ua.pt

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STUDIES IN THE AUTOREGULATION OF HUMAN CEREBRAL CIRCULATION: MODELS AND METHODS

V.I. Antonov¹, V.B. Semenyutin², V.A. Aliev³

¹ Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russian Federation;

² Almazov National Medical Research Centre, St. Petersburg, Russian Federation;

³ Elizabethian Hospital, St. Petersburg, Russian Federation

The work contains a review of modern methods and tools used to study the regulation of human cerebral circulation. The first part discusses the basic concepts of the mathematical description of regulatory processes based on the biomedical signals analysis. The Fourier transform and transfer function, signal coherence, convolution of functions, correlation analysis, fractal analysis, wavelet transform, artificial neural networks, Hilbert – Huang transform are presented. The second part is devoted to the papers where these methods were used for medical examinations. Their analysis showed that there was a discussion of specialists regarding the choice between linear and nonlinear models of functioning the cerebral blood flow autoregulation system. It was concluded that there was currently no single approach to solving the problem, and there remains a need to continue the development of new methods and models and their implementation in medical practice.

Keywords: mathematical model, cerebral blood flow autoregulation, biomedical signal

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МОДЕЛИ И МЕТОДЫ ИССЛЕДОВАНИЯ АУТОРЕГУЛЯЦИИ МОЗГОВОГО КРОВООБРАЩЕНИЯ ЧЕЛОВЕКА

В.И. Антонов¹, В.Б. Семенютин², В.А. Алиев³ ¹Санкт-Петербургский политехнический университет Петра

Великого, Санкт-Петербург, Российская Федерация;

² Национальный медицинский исследовательский центр им. В.А. Алмазова, Санкт-Петербург, Российская Федерация;

³ СПб ГБУЗ «Елизаветинская больница», Санкт-Петербург, Российская Федерация

В работе представлен обзор современных методов и средств, применяемых для исследования регуляции мозгового кровообращения человека. В первой части приведены базовые понятия математического описания процессов регуляции на основе анализа биомедицинских сигналов. Среди них можно выделить преобразование Фурье и передаточную функцию, когерентность сигналов, свертку функций, корреляционный анализ, фрактальный анализ, вейвлет-преобразование, искусственные нейронные сети, преобразование Гильберта – Хуанга. Во второй части рассмотрены результаты работ, в которых эти методы использованы для проведения медицинских обследований. Анализ показал, что сохраняется дискуссия специалистов относительно выбора между линейными и нелинейными моделями

функционирования системы ауторегуляции мозгового кровотока. Сделан вывод о том, что в настоящее время нет единого подхода к решению поставленной задачи и требуется продолжение разработки новых методов и моделей, а также их внедрение в медицинскую практику.

Ключевые слова: математическая модель, ауторегуляция мозгового кровотока, биомедицинский сигнал

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Introduction

Regulation of cerebral circulation serves as a perfect physiological mechanism maintaining the chemical and physical homeostasis of the brain. Research into this phenomenon helps establish the conceptual framework for introducing methods for controlling the system into clinical practice.

Understanding the specifics of the process is crucial for clinical practice, since pathogenic processes in various brain lesions (such as traumatic brain injuries, ischemic stroke, non-traumatic intracranial hemorrhage, brain arteriovenous malformations or anastomosis) largely depend on the state of the regulatory mechanisms.

Fig. 1 shows the main factors governing cerebral blood flow (CBF). All abbreviations of the common medical terms used in this paper are given in Appendix.

CBF is tightly regulated under normal conditions to provide an adequate response to local or systemic changes in homeostasis. The pressure gradient that regulates the level of CBF depends not only on systemic arterial pressure (SAP) and central venous pressure (CVP), but also on intracranial pressure (ICP). There are complex relationships between these values, but in practice, the value of cerebral perfusion pressure (CPP) is defined as the difference between AP and ICP or CVP (whichever is higher). The regulatory system also includes the endothelium, which is a thin semipermeable membrane separating the blood flow from the deeper structures of the vessel. The most important function of the endothelium is regulation of vascular tone.

Autoregulation of cerebral blood flow (AR) is the ability of the cerebral circulation system to maintain a relatively adequate level of CBF, with AP/CPP fluctuating within a certain range, by changing vascular resistance. CBF is regulated through interaction of different factors. These include:

myogenic response of smooth muscle cells in arteriolar walls to stretching due to the differences in transmural pressure, which is the difference between intra- (blood pressure) and extravascular pressures applied to the vessel wall;



Fig. 1. Main factors governing cerebral blood flow (CBF): CPP is the cerebral perfusion pressure; pO_2 , pCO_2 are the partial pressures of oxygen and carbon dioxide; ICP is the intracranial pressure; EM is the endothelial metabolites; SNS is the sympathetic nervous system; MA is the mental activity



Fig. 2. Curves for monitoring blood flow velocity (BFV) in the middle cerebral artery (*a*) and spectral density (SD) of spontaneous fluctuations in the Slow-Wave Activity, Respiratory-Wave Activity and Pulse-Wave Activity ranges, calculated by fast Fourier transforms (*b*)

hemodynamic shock associated with the changes in vascular tone (an increase in CBF velocity can lead to narrowing of the lumen in blood vessels);

metabolic factors, such as oxygen supply to tissues, neuronal metabolism, and the autonomic nervous system, which is involved in regulating vascular reactions [1].

Study of AR mechanisms is an important and urgent problemc currently tackled by numerous research groups. As new methods of mathematical analysis and signal processing are developed and widely introduced in practice, this greatly expands the opportunities for comprehensive study of cerebral blood flow regulation.

This paper is dedicated to comparative analysis of modern methods for studying the regulation of cerebral circulation, which can be regarded as the interaction of the input signal (AP) and the resulting response (CBF) via a regulation system with feedback.

Methods for signal processing

Data processing is used to analyze, modify and synthesize the signals received, for example, sound, images and the results of biological monitoring. Signal processing methods are used to improve transmission and storage efficiency, as well as to isolate or locate the components for further analysis in a measured signal. For example, the Fourier transform allows to extract the fundamental harmonics from a signal that at first glance appears to be noise (Fig. 2).

Types of signal conversion. Because the signals have a different nature, different methods are used for processing them.

Continuous-time processing. This group of methods is applied to signals for which the time interval can be regarded as a continuum, including both time and frequency domains. The Fourier transform of the time series allows to obtain the frequency response of the process.

Discrete-time processing. It is used to analyze signals such as samples whose elements are defined only at a finite number of points in time.

Digital processing. It consists in processing of digitized sampled signals with discrete time. Examples of algorithms for this type of processing are Fast Fourier Transform, finite impulse response filter, infinite impulse response filter, and adaptive filters such as Wiener and Kalman filters. *Nonlinear processing.* Nonlinear analysis is applied to the signals generated by nonlinear systems and can be performed in time, frequency, or space-time domains. Nonlinear systems can be used to simulate complex behaviors, including bifurcations, chaos, harmonics, and subharmonics that cannot be analyzed by linear methods. The modern approach is based on the concept of multifractals that are objects with different self-similarity characteristics in different scale ranges.

Statistical processing. Statistical processing is used for signals that can be regarded as stochastic processes with statistical properties that make it possible to apply the given methods [2]. For example, these methods can be used to reduce the effect of noise from receiving signals during medical monitoring of a patient's condition.

Mathematical methods. Mathematics possesses a powerful array of methods applicable in diverse fields of science and technology. They are also applicable in medicine. The following methods are the most important:

differential equations, recurrent procedures; Fourier and Hilbert transforms, wavelet transform, methods of nonlinear dynamics;

time-frequency analysis (producing estimate of the spectral components in analysis of time series);

stochastic analysis;

methods of computational mathematics;

data mining (used for statistical analysis of the relationship between a large number of variables representing multiple physical signals in order to extract previously unknown important properties).

Different types of relationships can exist between the processed attributes characterizing any phenomenon:

Functional relationship is the most rigid type (mainly found in inanimate nature); changing one characteristic in this relationship always leads to a change in another, for example, the dependence of the distance on time and speed. This relationship is not typical for living nature, governed by the principle of deterministic chaos.

Correlation relationship, when the value of one attribute corresponds to several values of another attribute (for example, the dependence of pulse rate on body temperature, the dependence of frequency of exacerbations of chronic diseases on age, etc.); in general, correlation is an interconnected change in indicators; it is characterized by direction, type and degree of closeness. *Pearson's correlation criterion* is a method of parametric statistics that allows to determine the presence or absence of a linear relationship between two quantitative indicators, as well as to assess its closeness and statistical significance [3]. The correlation coefficient r(X, Y) for discrete random variables can be calculated by the following formula:

$$r(X,Y) = \frac{G_{1}(x_{i}, y_{j})}{G_{2}(x_{i}, y_{j})},$$

$$G_{1}(x_{i}, y_{j} = \sum x_{i}y_{j}p_{ij} - \sum x_{i}p_{i}\sum y_{j}q_{j},$$

$$G_{2}(x_{i}, y_{jj}) = \sqrt{\sum x_{i}^{2}p_{i} - (\sum x_{i}p_{i})^{2}} \times \sqrt{\sum y_{j}^{2}q_{j} - (\sum y_{j}q_{j})^{2}},$$

where $x_{i, j}$ y_{j} are the elements of the samples; $p_{i}q_{j}$ are the probabilities with which these elements are included in the samples; p_{ij} are the their joint probabilities.

If r = 0, there is no correlation, if $r = \pm 1$, the correlation is complete and functional (the plus and minus signs express a positive or negative (inverse) relationship). Pearson's correlation values are ranked by closeness: less than 0.3 corresponds to a weak correlation; the correlation is moderate in the range of 0.3-0.7, and strong in the range of 0.7-1.0. In addition, relationships are distinguished by the nature of the changes, which can be either straight or curvilinear.

Notably, the correlation coefficients can only establish statistical associations and do not indicate the presence of causal relationships between pairs of attributes.

Spearman's rank correlation coefficient is a nonparametric measure describing the relationship between variables measured on a rank scale. It can be calculated without making any assumptions about the nature of the distributions of attributes in the statistical population. The ranking procedure begins by arranging the variables in ascending order of their values. Different values are assigned ranks that are natural numbers. The calculations are then carried out by the formula:

$$r=1-\frac{6\sum_{i=1}^{n}d_{i}}{n^{3}-n},$$

where d_i is the difference between the ranks in pairs, *n* is the number of pairs.

The *Fourier Transform* $F(\omega)$ yields the coefficients (amplitudes) for the initial function f(x) decomposed into harmonic oscillations with different frequencies. It has the form

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-i\omega x) dx,$$

where ω is the angular frequency.

An important property of the Fourier transp form is Parseval's equality:

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |F(\omega)|^2 d\omega.$$

The conversion formula can be represented as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega) \exp(i\omega x) d\omega.$$
(1)

The physical meaning of the Fourier transform is that the right-hand side of equality (1) is the sum of harmonic oscillations $\exp(i\omega x)$ with the frequencies ω , the amplitudes $\frac{1}{\sqrt{2\pi}}|F(\omega)|$ and the phase shifts $\arg F(\omega)$.

The Fourier transform makes it possible to characterize the frequency content of the signal but does not allow to determine at what point in time a particular oscillation with the frequency ω appears. If time localization of frequency components is required, for example, for analyzing signals of biological origin, a time-frequency transformation of the signal such as a wavelet transform should be applied.

Convolution of functions is an operation showing the 'similarity' of one function to a mirrored and shifted copy of another. A mathematical operation over two functions, *f* and *g*, generates a third function, which is generally considered to be a modified version of one of the initial functions. The convolution operation is a dependence of the integral over an infinite time interval of the product of the level of the first signal by the level of the second one, shifted in time relative to the first signal. The result of the convolution yields the positions where one signal is similar to another and where it is not. The definition of convolution is formulated as

$$(f*g)(t) = \int_{-\infty}^{\infty} f(\tau)g(t-\tau)d\tau.$$

In the discrete case, the convolution corresponds to the sum of f values with the coefficients corresponding to the shifted g values, i.e.,

$$(f * g)(x) = f(1)g(x-1) + f(2)g(x-2) + ...$$

Coherence is a statistic that can be used to describe the relationship between two signals or datasets. If the signals are ergodic and the system function is linear, coherence can be used to assess the causal relationship between input and output.

Coherence (sometimes called the squared amplitude) between two signals x(t) and y(t) is a real function, which is defined as

$$C_{xy}(f) = \frac{|G_{xy}(f)|^2}{G_{xx}(f) G_{yy}(f)},$$

where $G_{xy}(f)$ is the cross-spectral density between x and y; $G_{xx}(f)$, $G_{yy}(f)$ are the autospectral densities of x and y, respectively. The magnitude of the spectral density is denoted as |G|.

In view of the above limitations (ergodicity, linearity), the coherence function allows to assess the degree of confidence with which the form of the function y(t) can be predicted by the form of x(t) by choosing the optimal linear function by the least-squares method.

The power spectrum $S_{xx}(f)$ of a time series x(t) describes the power distribution over the frequency components of this signal.

The *transfer function* can be used to describe a dynamic system. It represents the differential operator expressing the relationship between the input and output of a linear stationary system. If the signal input to the system and the transfer function are known, the output signal can be reconstructed. Let us prove this.

Let u(t) be the input signal of the linear stationary system, and y(t) its output signal. Then the transfer function W(s) of such a system is written in the following form:

$$W(s) = \frac{Y(s)}{U(s)},$$

where s, rad/s, is the operator of the transfer function, $s = j\omega$; U(s), Y(s) are the Laplace transforms for the signals u(t) and y(t), respectively:

$$U(s) = \int_{0}^{\infty} u(t) \exp(-st) dt,$$
$$Y(s) = L y(t) = \int_{0}^{\infty} y(t) \exp(-st) dt.$$

Let us consider the case of discrete systems. Let u(k) be the discrete input signal of such a system, and y(k) its discrete output signal (k = 0, 1, 2,...). Then the transfer function W(z) of such a system has the form

$$W(z) = \frac{Y(z)}{U(z)},$$

where U(z), Y(z) are z transforms for signals u(k) and y(k), respectively:

$$U(z) = Z u(k) = \sum_{0}^{\infty} u(k) z^{-k},$$
$$Y(z) = Z y(k) = \sum_{0}^{\infty} y(k) z^{-k}.$$

Methods of nonlinear dynamics. The main methods are fractal analysis and fractional differentiation, as well as artificial neural networks. Let us consider these methods.

Fractal analysis is used for assessing the fractal characteristics of the data. It includes methods for determining the fractal dimension and other fractal characteristics of an object. An important limitation of fractal analysis is that an empirically determined fractal dimension does not necessarily prove that a model is fractal.

The concept of fractal is associated with objects that meet two criteria: self-similarity and fractional dimension. The first criterion means that the object consists of several levels of units resembling the structure of the entire object. The second criterion for a fractal object is the presence of fractional dimension. This requirement distinguishes fractals from Euclidean objects, which are characterized by integer dimensions.

To process signals of medical origin, the time-series approach is substituted by introducing a new object formed in a phase space of finite dimension, called a reconstructed attractor. It can be characterized by different measures, the most fundamental being the fractal dimension [6, 7].

The Rényi dimension seems to be the most convenient for studying the autoregulation of cerebral circulation.

Rényi entropy is a family of functionals used as a measure of uncertainty or randomness of a system. If some system has a discrete set of available states $X = \{x_1, ..., x_n\}$, which corresponds to the probability distribution p_i for i = 1, n (i.e., p_i are the probabilities of the system being in the states x_i), then the Rényi entropy with the parameter q (for $q \ge 0$) of the system is defined as

$$H_q(p) = \frac{1}{1-q} \log \sum_{i=1}^{N} p_i^q.$$

Since $\sum_{i=1}^{N} p_i = 1$, then, provided that $q \to 1$

it converges to the Shannon entropy, which has the form

$$H(p) = -\sum_{i=1}^{N} p_i \ln p_i.$$

However, analysis of signals from medical monitoring more often involves phenomena that require expanding the concept of fractals to complex structures with several dimensions. Complex fractals, called multifractals, are found in medicine (and in nature in general) more frequently than others. The multifractal approach actually means that the object under study can be divided into parts, each with its own properties of self-similarity. A large number of characteristics are required to describe these parts quantitatively. In particular, the spectrum of such processes cannot be described by a power law with a single exponent β .

The Wavelet Transform Modulus Maximum (WTMM) is a method for detecting the fractal dimension of a signal. It involves constructing the line of the local maximum of the wavelet transform, allowing to partition the time and scale domains into regions of fractal dimension. The continuous wavelet transform of the function f(x) is found by the following formula:

$$W_{\psi}(a,b) = \frac{1}{\sqrt{|a|}} \int_{-\infty}^{\infty} f(x) \psi^*\left(\frac{x-b}{a}\right) dx,$$

where a is the scale parameter, b is the coordinate or time.

The initial signal f(x) is divided using the function $\psi(x)$, generated from soliton-like functions, with the singularities obtained during its scale measurements and shifts. In the simplest version (using the Hulder exponent h), the scaling of one of the lines (for example, the maximum) is considered:

$$|W_{\psi}(t_i,s)| \sim s^{h(t_i)}$$

Most of the information transmitted by the signal is carried by its singularities in the form of irregular structures and transient phenomena. The wavelet transform is an effective method for detecting and characterizing these singularities because the transform can decompose the signal into blocks that are localized in both time and frequency. This makes it possible to determine the local regularity of the signal [8].



Fig. 3. Simple neural network. Black circles represent the input and output nodes, gray circles represent hidden nodes (https://ru.wikipedia.org/wiki/Нейронная_сеть)

The local regularity of a function is often measured using Lipschitz exponents [8], also called the Hulder exponents. We can explain this as follows.

Let *n* be a positive integer, and $n \le \alpha \le n + 1$. The function f(x) is called an α -Lipschitz function at the point x_0 if and only if there are two positive constants *A* and h_0 , as well as the polynomial $P_n(x)$ (of the order *n*), such that the following inequality holds true for $h \le h_0$ [9]:

$$|f(x_0 + h) - P_n(h)| \le A |h|.$$

We believe that a function has a singularity at x_0 if it is not a 1-Lipschitz function at x_0 . As a matter of fact, if a function is continuously differentiable at some point, its Lipschitz exponent is equal to unity at this point and therefore there is no singularity at this location. In practice, it is too difficult to verify the above conditions, so simpler and less stringent criteria are used for the singularity of functions.

Artificial neural networks (ANN). Modern medical expert systems make it possible to track substantial changes in the human body; they also support decision-making about medical interventions. Artificial neural networks are capable of self-learning based on medical monitoring data. They are a system of interconnected simple processors (artificial neurons). Each processor interacts with the signals it receives and the signals it sends to other processors. An important advantage of neural networks is their training capacity. Technically, training consists in finding the coefficients of connections between neurons.

An artificial neuron is usually represented as a nonlinear function (activation or firing) of a linear combination of input signals (Fig. 3). The result obtained is sent to a single output. The outputs of some neurons are then connected to the inputs of other neurons, forming a network. In practice, the network is based on perceptrons. A perceptron consists of sensors, associative and responsive elements [9].

A radial basis function network is an artificial neural network using radial basis functions (RBF) as activation functions. These functions have the form

$$f(x) = \varphi\left(\frac{x^2}{\sigma^2}\right),$$

for example,

$$f(x) = \exp\left(-\frac{x^2}{\sigma^2}\right),$$

where x is the vector of the neuron's input signals, σ is the window width, ϕ is a decreasing function.

The *error backpropagation* method is an iterative gradient algorithm used to minimize the error of the multilayer perceptron (MLP) and obtain the desired output. The gist of the method is in transmitting the error signals from the outputs of the network to its inputs, in the direction opposite to forward propagation of signals in normal operation.

Orthogonal complement of the signal. Hilbert–Huang transform. Natural physical processes are nonlinear and nonstationary. The widespread approach superimposing a linear structure on a nonlinear system does not always provide reliable results. Analysis should cover the detailed evolution of the data over time, since an important characteristic of nonlinear processes is their variation in the time-frequency domain.

Consider a signal S(t). The orthogonal complement of this signal is a signal $S_{or}(t)$, such that

$$\int_{-\infty}^{\infty} S(t) \cdot S_{or}(t) dt = 0.$$

The Hilbert transform calculates the orthogonal complement of the signal:

$$S_{or}(t) = \int_{-\infty}^{\infty} \frac{S(\tau)}{\pi (t-\tau)} d\tau.$$

The Hilbert transform is the result of convolution of the signal S(t) with the function $h(t) = 1/\pi t$, called the kernel of the given transformation. The frequency and phase characteristics of this transform can be obtained using the Fourier transform:

$$H(\omega) = \int_{-\infty}^{\infty} \frac{1}{\pi t} \exp(-i \omega t) dt = -i \operatorname{sign} \omega.$$

The modulus and phase shift of the Hilbert transform are found by the following formulas:

$$|H(\omega)| = 1, \omega \neq 0, \quad \Phi(\omega) = -\frac{\pi}{2} \operatorname{sign} \omega.$$

The Hilbert-Huang transform (HHT) is the decomposition of a signal into functions. which are called 'empirical modes' (EMD method), with subsequent application of the Hilbert transform to the resulting decomposition components. It consists of the following.

Let X(t) be the analyzed signal. The method of Empirical Mode Decomposition (EMD) involves sequential calculation of empirical modes c_i and residuals

$$r_j = r_{j-1} - c_j (j = 1, 2, ..., n),$$

 $r_0 = X(t).$

As a result of the calculations, we obtain a decomposition of the signal in the form

$$X(t) = \sum_{j=1}^{n} c_j + r_n,$$

where n is the number of empirical modes that is found during the calculations.

Applying methods for signal processing

to study of regulation of cerebral blood circulation

Different methods of signal processing are given in [10]; notably, the influence of these methods on the results and their reproducibility are not discussed. Another study [11] argues that the response of cerebral blood flow velocity (CBFV) can be interpreted as a kind of step response of the control system and quantified using the autoregulation index (ARI) in the range from 0 to 9.

Another approach to quantitative assessment of dynamic cerebral autoregulation (DCA) consists of analyzing the transfer function (TFA) of the hypothetical linear control system, where SAP is taken as the input signal, and CBFV is taken as the output signal [12– 14]. The gain and the phase of the transfer function are estimated by the auto- and crossspectra of SAP and CBFV, while the level of linear relationship between SAP and CBFV is expressed by the consistency of the system. Analysis of the transfer function allows to find the step response function and then estimate the ARI of the system using the least-squares method. The sum of the squared differences with the TFA response is determined for each of the 10 ARI responses. High variability observed in the calculated parameters such as gain, phase and ARI is a factor limiting the clinical use of DCA.

The transfer function was calculated as follows [12–14]:

$$H(f) = \frac{S_{xy}(f)}{S_{xx}(f)},$$

where $S_{xx}(f)$ is the auto-spectrum of SAP changes, $S_{xy}(f)$ is the cross-spectrum between SAP and CBFV signals.

The value of the transfer function H(f)| and the phase spectrum U(f) were obtained from the real $(H_R(f))$ and imaginary $(H_I(f))$ parts of the transfer function as

$$H_f \Big| = \sqrt{\left[H_R(f)\right]^2 + \left[H_i(f)\right]^2},$$
$$U(f) = \operatorname{arctg} \frac{H_i(f)}{H_R(f)}.$$

The squared coherence function $\gamma^2(f)$ was calculated as

$$\gamma^{2}(f) = \frac{|S_{xy}(f)|^{2}}{S_{xx}(f)S_{yy}(f)},$$

where $S_{yy}(f)$ is the autospectrum of the changes in CBFV.

The squared coherence function reflects the closeness of the linear relationship between SAP and CBFV for each frequency, ranging from 0 to 1.

An alternative approach to overcoming some of the difficulties of the above method involves spectral Fourier analysis of the data obtained by multimodal pressure-flow analysis (MMPF) [14, 15]. It was established that MMPF analysis can be less sensitive to nonstationary data and their variation. The data obtained using MMPF for patients with traumatic brain injuries were found to have better reproducibility compared to ARI [16]. Attempts were also made to apply nonlinear approaches to assessing DCA [17, 18] but there is as yet no clear evidence for the advantages of such approaches.

To reliably interpret the results of DCA assessment, the coherence levels must be considerably above zero. The calculations based on degrees of freedom yielded a minimum

required squared coherence level of 0.06 for 15-minute episodes of spontaneous breathing and 0.20 for 5-minute breathing periods of 6 cpm.

Some authors recommend to assess dynamic autoregulation of cerebral blood flow based on analysis of the transfer function for a coherence level of at least 0.5–0.6 [19].

The algorithm for cross-spectral analysis consists in the following:

Step 1. The amplitudes of BFV and SAP are calculated in the ranges of intracranial *B* waves and Mayer waves (*M* waves).

Step 2. The coherence between M waves of arterial pressure and BFV is calculated; the important area is where the coherence is at least 0.5.

Step 3. The phase shift between M waves of arterial pressure waves and BFV is calculated.

Figs. 4–7 show examples of calculated frequency dependences obtained by the above algorithm. The frequency of slow oscillations of systemic and cerebral hemodynamics is plotted on the horizontal scale. Evidently, the most informative part of the corresponding dependences lies in the region where the coherence exceeds 0.5.

Ref. [20] considered the effect of beat-tobeat spontaneous fluctuations in mean arterial pressure and breath-to-breath end-tidal fluctuations of carbon dioxide on beat-to-beat cerebral blood flow velocity variations using the Laguerre–Volterra network methodology for multiple-input nonlinear systems. The results obtained also indicate that cerebral autoregulation (dependence on the frequency of slow oscillations of systemic and cerebral hemodynamic frequency) is nonlinear and dynamic. Nonlinearities are typically active in the low frequency range (below 0.04 Hz). The models also confirm that beat-tobeat fluctuations of CBFV are considerably nonstationary, and the effect of carbon dioxide on the evolution of this velocity is rather variable.

Ref. [21] compared the effects of different methods for spectral estimation of signals using simulated and clinical data. It was established that data in the absence of a trend can produce an artificial peak in the low-frequency region of the estimated power spectra. This is a shortcoming of the model used, meaning that the peak cannot be taken to prove that these oscillations have a physiological basis. A quantitative method for assessing low-frequency oscillations is also described in [21]. Low-frequency oscillations in linear blood flow velocity in the main cerebral arteries, measured by transcranial Doppler sonography, were detected using the method in 10 out of 17 healthy adults (the average frequency of these oscillations was 0.021 ± 0.007 Hz), which is consistent with earlier results.

It is emphasized in [22] that traditional mathematical approaches based on theories of stationary signals cannot solve the problems related to nonstationarity, and, therefore, do not allow to reliably assess nonlinear interactions in physiological systems. The authors discuss a new MMPF method using the Hilbert-Huang transform to quantitatively assess dynamic cerebral autoregulation (DCA). The method is used to study the interaction between non-stationary CBFV and SAP. DCA is an important mechanism responsible for controlling cerebral



Fig. 4. Continuous recording (4 min) for Systemic Arterial Pressure (SAP, upper curve) and Blood Flow Velocity (BFV) in the right (R) and left (L) middle cerebral arteries (middle and lower curves, respectively).

blood flow in response to fluctuations in SAP over a period of several beats. DCA has traditionally been assessed by the relationship between pronounced systemic variations in SAP and BFV observed in clinical trials. However, reliable non-invasive assessment of DCA remains an unresolved problem in clinical and diagnostic medicine. A brief review in [22] provides the following information:

results of the transfer function analysis (TFA) traditionally used to quantitatively assess the DCA;

description of the MMPF method and its modifications;

algorithm and technical aspects of the improved MMPF method;

review of the clinical use of MMPF and its sensitivity for detecting DCA abnormalities in clinical trials.

The MMPF method makes it possible to adaptively decompose complex nonstationary SAP and CBFV signals into several empirical modes, so that the fluctuations caused by a certain physiological process can be represented



Fig. 5. Normalized frequency response for SAP (upper curve) and BFV in the right (R) and left (L) middle cerebral arteries (middle and lower curves, respectively) in the range of B and M waves. Example of calculated result



Fig. 6. Example of calculated coherence between M waves for SAP and BFV in the right (R) and left (L) middle cerebral arteries in the range of B and M waves (the area where the coherence is at least 0.5 is important)



Fig. 7. Calculated frequency characteristics of phase shift between M waves for SAP and BFV in the right (R) and left (L) middle cerebral arteries in the range of B and M waves

by the corresponding empirical mode. This technique was used to establish, for example, that DCA is characterized by specific phase delays between SAP and CBFV fluctuations and that phase shifts are significantly reduced in hypertensive, diabetic and stroke patients with impaired DCA. Furthermore, the new method allows to reliably assess the DCA by using not only the data collected in clinical trials but also spontaneous fluctuations in SAP/CBPV under resting conditions.

Dynamic autoregulation of cerebral hemodynamics in healthy volunteers was studied in [23, 24] using the Laguerre–Volterra network for systems with fast and slow dynamics. Since autoregulation of the brain depends on diverse physiological mechanisms with significantly different time factors, this approach is used to demonstrate the effectiveness of the new method. The results are given in time and in frequency domains. They prove that cerebral autoregulation is a nonlinear and dynamic frequency-dependent system with significant nonstationarity. Quantitative estimates of the latter point to great variability in certain frequency bands for each subject in the low and medium frequency ranges below 0.1 Hz. Nonlinear dynamics is also clearly observed in the lower and middle parts of the range, where the frequency response of the system is less pronounced.

The goal of the study in [25] was to analyze low-frequency variations in MAP and ICP using an alternative algorithm developed based on the pressure reactivity index (PRx); the latter uses minute-by-minute MAP and ICP values to correlate them with patient follow-up at 6 months. The L-PRx value was calculated as the moving linear (Pearson's) correlation coefficient using a minute value in a time window of 20 min from 20 consecutive MAP and ICP values. Episodes without MAP and ICP artefacts and the resulting CPP, L-PRx, and MD values were averaged over time, so each patient was characterized by one dataset. Nonparametric statistical methods were used because most of our variables did not fit the normal distribution, in particular Spearman's rank correlation coefficient. Statistical analysis was performed using the SPSS v18.0 statistical package (SPSS, Chicago, IL, USA).

It is pointed out in [26] that the deciding which method to use to for quantitative assessment of cerebral autoregulation remains a matter of personal choice. However, TFA continues to be a popular approach adopted in studies considering spontaneous fluctuations in blood pressure.

Ref. [26] aimed to improve the standardization of parameters and settings adopted for TFA in studies of dynamic cerebral autoregulation. The dynamic relationship between blood pressure and cerebral blood flow (CBF) has the characteristics of a high-pass filter. It is assumed that adapting cerebral arterioles in response to pressure changes is not fast enough to withstand highfrequency oscillations (over 0.20 Hz) in CPP. Consequently, high-frequency oscillations are easily converted to CBF fluctuations. In contrast, slower-frequency oscillations (below 0.20 Hz but most effectively below 0.05 Hz) can counteract the cerebral arterioles and are therefore attenuated.

It is concluded in [26] that different methods of non-invasive assessment of DCA have been developed, based on spontaneous fluctuations of SAP and CBF at rest, i.e.,

analysis of the correlation coefficient (Mx), determination of the autoregulation index, transfer function analysis (TFA),

nonlinear analysis using Laguerre expansions of Volterra kernels, or autoregression,

Multimodal pressure-flow analysis

However, it would be a simplification to assume that all of these methods allow to measure dynamic autoregulation. The methods only provide metrics for describing the relationship between pressure and flow; in reality, these parameters are influenced by numerous other factors besides CA. The coherence function can be used to determine the conditions where gain and phase estimates may prove unreliable. The coherence can vary from zero to unity at each frequency. This is the equivalent of the squared correlation coefficient. It essentially expresses the fraction of the output variance that can be interpreted as the corresponding input power at each frequency. The coherence equals unity for linear systems with high signalto-noise ratio (SNR) and one-dimensional input/output power ratio. On the other hand, coherence approaches zero if the SNR is low, the systems have significant non-linearity, or if there are other variables that affect the output power.

Despite the extensive theoretical experience accumulated on using TFA, its practical implementation involves a relatively large number of parameters and settings. The literature describing TFA for DCA reports on significant differences in practical use, limiting the comparison of results from similar studies and hindering the potential clinical applications of these methods. For example, one of the consequences of this lack of standardization is the difficulty of establishing clear limits for normal and impaired autoregulation [27, 28].

Ref. [29] presents modern data on the TFA method, its place among the methods for studying cerebral autoregulation, as well as on its benefits and drawbacks. It was found that autoregulation of cerebral blood flow largely determines the relationship between cerebral blood flow and cerebral perfusion pressure; for this reason, data on autoregulation are important for diagnosing and forecasting cerebrovascular Dynamic autoregulation disorders. of cerebral blood flow is a frequency-dependent phenomenon, functioning as a high-pass filter. Transfer function analysis is one of the three most commonly used methods for studying dynamic cerebral autoregulation, which has considerably evolved over the past two decades, finding diverse applications.

Conclusion

Analyzing modern studies on the regulation of human cerebral circulation, we have found that the most common methods used are for processing signals from measuring complexes and converting them into digital form. Whether the regulation processes should be considered linear or nonlinear is a question that remains open for debate. In the first case, a set of wellknown analysis methods has been developed, aimed at simplifying the study. However, real processes are strictly nonlinear. Analysis of nonlinear systems is a rapidly developing area of modern science but no consensus has been reached on the best methods for describing the real interactions in the body. Clearly, processing of signals received from medical equipment is a task that can be solved by applying the wide range of tools available in mathematical science. Thus, much work remains to be done on developing and improving systems for monitoring and analysis of the system regulating cerebral circulation.

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Appendix

Abbreviation	Term
CVP	Central venous pressure
ICP	Intracranial pressure
CPP	Cerebral perfusion pressure
SAP	Systemic arterial pressure
AR	Cerebral autoregulation
BFV	Blood flow velocity
MCA	Middle cerbral artery
ARI	Autoregulation index
DCA	Dynamic cerebral autoregulation
CBFV	Cerebral blood flow velocity
MMPF	Multimodal pressure-flow analysis
MD	Microdialysis
CBF	Cerebral blood flow
FFT	Fast Fourier transform
WTMM	Wavelet transform modulus maxima
ANN	Artificial neural networks
RBF	Radial basis functions
HHT	Hilbert–Huang transform
EMD	Empirical mode decomposition
TFA	Transfer function analysis
SNR	Signal/Noise ratio

Common abbreviations of medical terms used in the study

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THE AUTHORS

ANTONOV Valerii I.

Peter the Great St. Petersburg Polytechnic University 29 Politechnicheskaya St., St. Petersburg, 195251, Russian Federation antonovvi@mail.ru

SEMENYUTIN Vladimir B.

Almazov National Medical Research Centre 2 Akkuratov St., St. Petersburg, 197341, Russian Federation lbcp@mail.ru

ALIEV Vulgar A.

Elizabethian Hospital 14 Vavilovs St., St. Petersburg, 195257, Russian Federation neurosurrgery2@eliz.ru

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СВЕДЕНИЯ ОБ АВТОРАХ

АНТОНОВ Валерий Иванович — доктор технических наук, заведующий кафедрой высшей математики Санкт-Петербургского политехнического университета Петра Великого, Санкт-Петербург, Российская Федерация.

195251, Российская Федерация, г. Санкт-Петербург, Политехническая ул., 29 antonovvi@mail.ru

СЕМЕНЮТИН Владимир Борисович — доктор биологических наук, заведующий лабораторией церебральной патологии Национального медицинского исследовательского центра им. В.А. Алмазова, Санкт-Петербург, Российская Федерация.

197341, Российская Федерация, г. Санкт-Петербург, ул. Аккуратова, 2. lbcp@mail.ru

АЛИЕВ Вугар Али оглы — доктор медицинских наук, заведующий нейрохирургическим отделением СПб ГБУЗ «Елизаветинская больница», Санкт-Петербург, Российская Федерация. 195257, Российская Федерация, г. Санкт-Петербург, ул. Вавиловых, 14. neurosurrgery2@eliz.ru