INTESTINAL ANASTOMOSIS BY LATTICE-BOLTZMANN METHOD

SIMULATION OF 3D TRANSIENT FLOW PASSING THROUGH AN INTESTINAL ANASTOMOSIS BY LATTICE-BOLTZMANN METHOD

Context. Recently, the number of reconstructive operations on the digestive tract has significantly increased. Such operations have predictable negative consequences associated with disruptions of hydrodynamic processes in the anastomosis area. These negative consequences can be partially avoided by choosing anastomosis anatomical form based on mathematical modeling. Known mathematical models are cumbersome and do not allow to obtain results in real time. The proposed approach using lattice Boltzmann method allows solving this problem.

Objective. The purpose of the work is to develop a three-dimensional mathematical model of anastomosis for research of hydrodynamic parameters of fluids with complex structure in real time.

Method. The method of constructing and analyzing the mathematical model of anastomosis of the digestive tract based on lattice Boltzmann method is proposed. The method differs in that it provides simultaneous analysis of hydrodynamic parameters of the liquid and determines the nature of movement of fine-grained inclusions in the anastomosis area. The main stages of the method are the development of technology for determining the modeling area, discretization of the three-dimensional Boltzmann equation with the choice of lattice and the nature of the collision operator, taking into account the complex structure of the liquid; development of the technology of transition from the density distribution function to the distribution of pressure at the mesoscopic level, taking into account the properties of the liquid, the creation of the process of transforming the set of mesoscopic parameters into the macroscopic parameters of the liquid.

Results include determining the density of field velocity in the anastomosis area to modify its geometry. The study of the influence of gravity on the nature of motion of fine-grained inclusions has been carried out. The quantitative characteristics of the delay of particles in the area of anastomosis, depending on the dynamic viscosity of the liquid, are determined.

Conclusions. The three-dimensional mathematical model discussed in this paper is based on the application of the lattice Boltzmann method for calculating the hydrodynamic parameters of the motion of fluid in the study area. The distinctive feature of the model is that it accounts for the complex nature of the liquid having fine-grained inclusions. The model allows determining the behavior of these inclusions and the field of speed with sufficient accuracy in real time.

Keywords: mathematical model, lattice method of Boltzmann, anastomosis simulation.

NOMENCLATURE

- $x, y, z$ – continuous Cartesian coordinates of three-dimensional space;
- $t$ – time of simulation;
- $v$ – velocity of the elemental volume of liquid at the mesoscopic level;
- $v_{eq}$ – vector of velocity of the elemental fluid volume in the node $\omega$;
- $f(x, y, z, v, t)$ – density distribution function;
- $f_{eq}^{\omega}$ – density distribution function at node $\omega$;
- $f_{eq}(x, y, z, v, t)$ – equilibrium density distribution function;
- $\tau$ – relaxation factor in the direction $f_{eq}(x, y, z, v, t)$;
- $\delta$ – parameter of fine-grained inclusions;
- $c_s$ – speed of sound propagation in the studied area;
- $\lambda$ – kinematic viscosity;
- $\eta$ – dynamic viscosity;
- $\rho_f$ – liquid density;
- $p$ – pressure at the outlet;
- $n$ – number of fine-grained inclusions in the simulation area;
- $d$ – diameter of the fine-grained inclusion;
- $\rho$ – density of fine-grained inclusions;
- $u$ – vector of macroscopic velocity;
- $w_\omega$ – weight ratio in the node $\omega$;
- $\Delta t, \Delta x, \Delta y, \Delta z$ – steps in time and space.

INTRODUCTION

Life science nowadays is a rapidly developing area of research. The urgent need for obtaining new results in this field of knowledge arose long ago but was constrained by the considerable complexity of research objects. Biological processes, which, as a rule, are the main objects of the study of life sciences, are characterized by variability, which is caused by the dependence on many parameters. However, the complexity of measuring these parameters is another important challenge that impedes progress in this area. In most cases, this complexity is due to the fact that there are difficulties with direct access to the object of measurement. Another negative factor is that the measuring instruments significantly affect the investigated process. Therefore, in this area, simulation has been and remains one of the most effective methods of research.
This work describes the mathematical modeling of fluid motion with fine-grained inclusions through anastomoses in the lower section of the human digestive tract. The importance of this study is based on the fact that this section of the digestive tract is characterized by high peristaltic activity and, accordingly, high sensitivity to surgical intervention. A traditional approach, in this case, is to solve a boundary value problem based on a system of equations containing the Navier-Stokes equation and the flow continuity equation. The process of solving this non-stationary nonlinear boundary-value problem is cumbersome and requires a large amount of computational resources since rapid change in parameters requires a high degree of discretization and imposes additional conditions on the convergence of computational methods. Therefore, in recent years, alternative approaches have been developing rapidly using neural networks, cellular automata and other means of description for complex processes. Among the above-mentioned methods, the method based on solving the lattice Boltzmann equation in each node of the discrete area is important and is called the lattice Boltzmann method.

1 PROBLEM STATEMENT

This work describes the development and research of a mathematical model of fluid motion with fine-grained inclusions through the anastomosis area of the lower part of the digestive tract. The objective functions of such a model are to determine the velocity field, the pressure distribution and the characteristics of sticking of fine-grained inclusions in the anastomosis area. To simplify the simulation process and achieve the possibility of mathematical modeling in real time, the lattice Boltzmann method is applied. The Boltzmann equation for 3D simulation describes the probability of the fact that the elemental volume of a liquid at a time \( t \) will be in a cube with a center at the point with the coordinates \( (x,y,z) \) and the lengths of the edges \( dx,dy,dz \), and the velocity of the motion of this elemental volume will be in the range from \( v \) to \( dv \) [1].

In general, the equation is represented by the expression:

\[
\frac{\partial f(x,y,z,v,t)}{\partial t} + v \left( \frac{\partial f(x,y,z,v,t)}{\partial x} + \frac{\partial f(x,y,z,v,t)}{\partial y} + \frac{\partial f(x,y,z,v,t)}{\partial z} \right) = \Omega \left( f(x,y,z,v,t) - f^{(eq)}(x,y,z,v,t) \right) .
\] (1)

The function of the right-hand side of the equation (1) is called the collision operator. The operator \( \Omega \left( f(x,y,z,v,t) \right) \) describes the nature of the collisions of elemental volumes during the movement of the fluid. In general, the operator of collisions is given by the following expression:

\[
\Omega \left( f(x,y,z,v,t) \right) = \frac{\delta}{\tau} \left( f(x,y,z,v,t) - f^{(eq)}(x,y,z,v,t) \right) .
\] (2)

where \( \tau \) – a constant that determines the time scale required to establish a local equilibrium, \( \delta \) – a parameter whose value depends on the presence and the compacted location of the fine-grained inclusions in the node at the moment of collision, \( f^{(eq)}(x,y,z,v,t) \) – equilibrium function of the Maxwell-Boltzmann density distribution.

Equations (1) and (2) describe the fluid behavior at each point of the investigated area at mesoscopic level. Therefore, there is a problem of transition from mesoscopic to macroscopic level, on which the fluid parameters are represented by the velocity field and the pressure distribution.

For such a transition, we will apply a Chapman-Enskog expansion [2] adapted to the conditions of this model, which forms the connection between the kinematic viscosity and the Boltzmann equation parameters:

\[
\lambda = \frac{(2\tau - \Delta \delta)c_s^2}{2\delta}.
\]

The Chapman-Enskog expansion allows replacing the solution of a boundary-value problem based on the Navier-Stokes equation by solving a set of Boltzmann equations, each of which describes the dynamics of the movement of elementary fluid volumes in the nodes of a discrete lattice covering the study area.

2 LITERATURE REVIEW

There are two main approaches for simulating the flow of fluid, which use the macroscopic and mesoscopic level of process description. A traditional approach to obtaining fluid flow parameters is involves applying numerical methods for solving a boundary value problem on the basis of the Navier-Stokes equation [3]. Methods of finite differences [4], methods of finite elements [5] and methods of finite volumes are widely used [6]. These methods have common disadvantages related to stability and convergence, since through discretization of the corresponding equations these methods are reduced to the solution of the system of linear algebraic equations by iterative methods. Despite the possibility of achieving high accuracy of the solution, it is often difficult to achieve the convergence of the iterative process, provided the variability of the input data and in areas of complex geometry. Unfortunately, multiple physical processes, including those processes occurring in biological objects, have precisely such characteristics [7]. The disadvantages of numerical methods also include the complexity of parallelizing the process of solving the boundary value problem. To overcome these and some other disadvantages, alternative approaches were explored. The lattice Boltzmann method, which describes the movement of elemental volumes of liquid at the mesoscopic level, is one of the most popular approaches. The first publications on the lattice Boltzmann method have a nearly 30-year history [8]. During this time, the method received a significant theoretical basis and became one of the popular methods of simulating fluid motion in biological objects [9]. The reason for the high popularity of lattice Boltzmann method is the fact that the calculations of fluid flow parameters are performed locally for each discrete point, which allows the use of parallel algorithms [10]. The method can also be
effectively applied to simulate three dimensional areas with complex geometry [11] and to take into account the complex structure of the liquid [12]. These properties of the lattice Boltzmann method are the basis for choosing tools to study of anastomosis of the digestive tract [13, 14].

3 MATERIALS AND METHODS

The mathematical model of ileum anastomosis of the human digestive tract is considered in this paper. The shape of a three-dimensional area has the form of a rectangular parallelepiped with an internal cavity that corresponds to the investigated fragment of the ileum. The geometry of this anastomosis is based on the experience of practicing surgeons. The general view of the study area is shown in fig. 1.

Through the inner cavity flows a fluid that has a complex structure. Parameters of this fluid vary during the computational experiment in the following ranges: liquid density \( \rho_l \) [kg/m\(^3\)]: 100 \( \div \) 1000; dynamic viscosity of the liquid \( \eta \) [Pa s]: \( 10^{-3} \div 100 \); speed of the fluid through the inlet \( u \) [m/s]: 0 \( \div \) 0.09; outlet pressure \( p \) [Pa]: 105; number of fine-grained inclusions in the field of simulation \( \rho_c \): 1 \( \div \) 1000; diameter of the fine-grained inclusion \( d \) [m]: \( 10^{-4} \div 10^{-3} \); density of fine-grained inclusions \( \rho_p \) [kg/m\(^3\)]: 1000 \( \div \) 1500 [kg/m\(^3\)].

Parameters of the mathematical model vary in the following range: maximum number of time steps \( m_{\text{max}} \): 1 \( \div \) 100; number of nodes in the discretizing grid \( \Omega \): 2000 \( \div \) 500000; maximum step in the time layer [s]: 0.01.

The first step in the implementation of the mathematical model of fluid motion in the area, shown in fig. 1, is to discretize the area. In this case, the rectangular parallelepiped \( G \) is covered by a three-dimensional lattice \( \Omega \), the nodes \( \omega \left( x_i, y_j, z_k \right) \) of which are elements of the set:

\[
\Omega = \left\{ \omega \left( x_i, y_j, z_k \right) \mid i = 0, i_{\text{max}} - 1, j = 0, j_{\text{max}} - 1, k = 0, k_{\text{max}} - 1 \right\} .
\]

Each of the nodes belongs to one or three types: “wet” nodes or nodes in the fluid area, “dry” nodes or nodes of the environment and boundary nodes constituting the limiting surface.

We describe the evolution of elementary fluid volumes in the nodes of the area by a system of equations:

\[
\frac{\partial f_{\omega}}{\partial t} + v_{\omega} \nabla f_{\omega} = \frac{1}{\tau} \left( f_o - f_{\omega}^{(\text{eq})} \right), \quad \omega = 0,1,2,...\left| \Omega \right| - 1, \quad (3)
\]

where \( f_o \) – density distribution function in the direction of the mesoscopic velocity vector \( v_{\omega} \); \( f_{\omega}^{(\text{eq})} \) – an equilibrium density distribution function corresponding to the vector \( v_{\omega} \).

We discretize the system of equations (3) over time and spatial variables for numerical solutions. Let us represent the vector of the mesoscopic velocity of the elementary volume of a liquid at the point \( \omega \) by the tuple

\[
v_{\omega} = \left( v_{\omega x}, v_{\omega y}, v_{\omega z} \right) \]

of its projections on the axis \( x, y, z \).

Marking the time step as \( \Delta t \), and spatial steps for each coordinate as \( \Delta x_{\omega x}, \Delta y_{\omega y}, \Delta z_{\omega z} \), we can produce the discrete version of the Boltzmann equation:

\[
f_{\omega} \left( x_{\omega x} + \Delta x_{\omega x}, y_{\omega y} + \Delta y_{\omega y}, z_{\omega z} + \Delta z_{\omega z}, t + \Delta t \right) - f_{\omega} \left( x_{\omega x}, y_{\omega y}, z_{\omega z}, t \right) + \Delta t
\]

Figure 1 – General view and geometric dimensions of “side-to-side” anastomosis
Let's set $\Delta x_k = \Delta t = 1$. Then equation (4) will look like:

$$f_0\left(x_0, y_0, z_0, t + \Delta t\right) = f_0\left(x_0, y_0, z_0, t\right) - \frac{1}{\tau} \left[f_0\left(x_0, y_0, z_0, t\right) - f_0^{(eq)}\left(x_0, y_0, z_0, t\right)\right].$$

The simulation of the process of solving equation (5) is carried out in two stages.

1. Collision at the node $\omega$:

$$\tilde{f}_0\left(x_0, y_0, z_0, t + \Delta t\right) = f_0\left(x_0, y_0, z_0, t\right) - \frac{1}{\tau} \left[f_0\left(x_0, y_0, z_0, t\right) - f_0^{(eq)}\left(x_0, y_0, z_0, t\right)\right].$$

2. Distribution of the obtained value of the distribution function $\tilde{f}_0\left(x_0, y_0, z_0, t + \Delta t\right)$ for the moment of time $t + \Delta t$ to the neighboring nodes of the grid:

$$f_0\left(x_0, y_0, z_0, t + \Delta t\right) = \tilde{f}_0\left(x_0, y_0, z_0, t + \Delta t\right).$$

Neighborhood relationship identifies those nodes for which the interaction with the current node $\omega$ is given. For this model, the nature of such connections is unified and is called D3Q19 (fig. 2).

Equation (6) includes an equilibrium density distribution function for a node $\omega$.

We apply an expression for this function, which was first proposed in the work [15].

We consider the fluid pressure $p_\omega$ in each node $\omega$ is related to the distribution function through the expression $p_\omega = c_s^2 f_\omega$, we can write the expression for pressure in the equilibrium state:

$$p_\omega^{(eq)} = c_s^2 f_\omega^{(eq)} = w_\omega \left[p + p_0 \left\{ \frac{3 v_0 \cdot u}{c_s^2} + \frac{9 (v_0 \cdot u)^2}{2 c_s^4} - \frac{3 u^2}{2 c_s^2} \right\} \right],$$

where $p_0 = c_s^2 \rho$ — average pressure.

Let's modify equation (5), replacing $f_\omega$ with $p_\omega$:

$$p_\omega\left(x_0 + \Delta x_\omega, y_0 + \Delta y_\omega, z_0 + \Delta z_\omega, t + \Delta t\right) - p_\omega\left(x_0, y_0, z_0, t\right) = -\frac{1}{\tau} \left[p_\omega\left(x_0, y_0, z_0, t\right) - p_\omega^{(eq)}\left(x_0, y_0, z_0, t\right)\right].$$

Having solved the equation according to the scheme (6), (7), we can determine the macroscopic parameters of the pressure distribution and velocity fields from the equations:

$$p = \sum_\omega p_\omega, \quad u = \frac{1}{p_0} \sum_\omega v_0 p_\omega.$$
which is shown in fig. 1. During the simulation one of the important tasks was to determine the distribution of pressure and velocity fields in the study area, depending on the fluid parameters. Such research allows to determine areas with extreme values of measured parameters and, based on this information, formulate recommendations for choosing the geometric form of anastomosis, which would allow to critically reduce the risk of the so-called “blind bags” or unwanted additional cavities.

The second group of experiments aimed to determine the trajectories and the behavior of fine-grained inclusions in the fluid under study. The main parameters of the variation during these experiments were the size and number of particles, which can simultaneously be in the area we are investigating. To simplify the calculations, it is assumed that all the fine-grained inclusions have the same shape, size and density. The tasks of this group of studies were to determine the areas of accumulation of particles, which indicate the possibility of occurrence of stagnant phenomena in the application of a particular form of anastomosis.

The study used self-created software written in the algorithmic programming language Python in the environment PyCharm. Third-party software in the form of additional modules pyLBM-0.2.1, numpy-1.12.1, Cython-0.25.2, mpi4py-2.0.0, matplotlib-2.0.2 and others was also used. To prepare geometric forms of anastomosis, the package for creating 3D computer graphics Blender-2.78 was used.

5 RESULTS

The main results are obtained through the creation and study of a mathematical model of fluid motion with fine-grained inclusions in a three-dimensional complex domain. To determine the fluid parameters, a technology based on the application of the Boltzmann lattice method was used. The created model allows to get parameters of speed of a liquid with accuracy $c < 10^{-5}$ m/s. However, the great variability of biological processes makes absolute values of field velocities less informative when evaluating biological phenomena. The simulation results presented in a graphical form allow us to qualitatively evaluate the field of fluid velocities and draw conclusions about the correction of the form of anastomosis. For example, the velocity field shown in fig. 3, displays areas that require shape correction.

The trajectory of the motion of fine-grained inclusions at each time of the modeling time was determined as the result of the action on the particle of three forces: the interaction force of the particle with the liquid, the force that is the result of collision of this particle with the adjacent particles and the force of gravity. Studies have shown a significant dependence of the location of anastomosis in space on the trajectory of fine-grained inclusions. We can observe on fig. 4 difference of arrangement of particles at different positions of anastomosis in relation to gravity. Parameters of this experiment: total simulation time – $t_{\text{max}} = 600\,\text{s}$; moment of time, shown in figure 4 – $t_{\text{cur}} = 325\,\text{s}$. Number of particles in the research area
The practical value of this work is that by applying these research results it was possible to reduce 10–15% negative consequences of reconstructive operations on the digestive tract. The further direction of research includes increasing area of modeling and accounting for peristaltic oscillations, as the main source of fluid flow through the area of anastomosis. A separate aspect of the study is the consideration of possible peristaltic oscillations of the actual anastomosis area, which has not yet been used in practice and has not been considered in mathematical modeling. In the research plan, there is also the construction and research of models of reconstructive operations on different parts of the digestive tract.

CONCLUSIONS

The work involves the development and research of a mathematical model that describes the parameters of the functioning of anastomosis in the lower parts of the human digestive tract. The importance of these studies is due to a significant increase in such operations and the presence of negative consequences of surgical intervention. The proposed approach to the description of the motion of the fluid in the anastomosis area is based on the use of lattice Boltzmann method. Due to the use of this method and the application of modern software development technologies, the adequacy of the mathematical model in comparison with the traditional mathematical models based on the solution of the boundary value problem based on the Navier-Stokes equation and the flow continuity equation is significantly increased. Experiments have shown that this method allows us to calculate the volume velocity in anastomosis zone with an accuracy of $\varepsilon < 10^{-5}$ m/s for the geometric parameters of the area and physical parameters of the fluid given in the work for 2–3 minutes.

A feature of the proposed mathematical model is the fact that it takes into account the complex nature of the liquid, which includes fine-grained impurities. The behavior of these impurities in the field of anastomosis, depending on the dynamic viscosity of the fluid, is investigated. The second advantage of the proposed approach is the possibility to reduce the simulation time by applying parallel algorithms for calculating local mesoscopic fluid parameters for each node in the investigated area. Thus, for the first time it became possible to obtain the results of model experiments using three-dimensional mathematical modeling in real time.

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\[ n = 100 \text{ Pcs}; \ \text{fluid density} \ \rho_f = 1000 \text{ kg/m}^3; \ \text{particle density} \ \rho_p = 1500 \text{ kg/m}^3; \ \text{particle size} \ d = 10^{-3} \text{ m.} \]
Математичне моделювання тривимірного нестаціонарного потоку через анестазмоз травно-го тракту решітчастим методом Болтмана

Актуальність. Останніми часом істотно зросла кількість реконструктивних операцій на травному тракті людини. Результати таких операцій мають прогнозовані негативні наслідки, що пов’язані з порушенням гідродинамічних процесів у зоні анестазму. Ці негативні наслідки можливо частиною усунути шляхом вибору форми анестазму на основі математичного моделювання. Відповідні математичні моделі є громіздкими і не дозволяють отримувати результати в реальному масштабі часу. Запропонований в роботі підхід з використанням решітчастого методу Болтмана дозволяє вирішити цю проблему.

Метою роботи є розробка тривимірної математичної моделі області анестазму для дослідження з достатньою точністю гідродинамічних параметрів рідин зі складною структурою в реальному масштабі часу.

Метод. Запропоновано метод побудови та аналізу математичної моделі анестазму травного тракту на основі решітчастого методу Болтмана. Метод відрізняється тим, що забезпечує одночасний аналіз гідродинамічних параметрів рідин та визначає характер руху дрібнозернистих включення у зоні анестазму. Основні етапи методу: розробка технології задавання області моделювання, дискретизація тривимірного рівняня Болтмана з вибором реальнісі та характеру оператора колій, який враховує складну структуру рідини; розробка технології переходу від функції розподілу густини до розподілу тиску на мезоскопічному рівні з урахуванням особливостей властивостей рідини; перехід від мезоскопічних до макроскопічних параметрів рідини.

Результати моделювання включають визначення розподілу поля швидкостей в зоні анестазму з метою модифікації його геометрії. Проведено дослідження впливу сил тяжіння на характер руху дрібнозернистих включень. Визначено кількісну характеристику затримки частинок в області анестазму в залежності від динамічної в’язкості рідини.

Висновки. Розглянута в даній роботі тривимірна математична модель базується на застосуванні решітчастого методу Болтмана при обчисленні гідродинамічних параметрів рідини в зоні анестазму. Особливість моделі полягає в використанні складного характеру рідини, яка включає дрібнозернисті включення. Модель дозволяє визначити характер поведінки цих включень та поля швидкостей з достатньою точністю в реальному масштабі часу.

Ключові слова: математична модель, решітчастий метод Болтмана, моделювання анестазму.
Математическое моделирование трехмерного нестационарного потока через анастомоз пищеварительного тракта. Метод Больцмана

Актуальность. В последние годы существенно возросло количество реконструктивных операций на пищеварительном тракте человека. Результаты таких операций имеют прогностические негативные последствия, связанные с нарушениями гидродинамических процессов в зоне анастомоза. Эти негативные последствия возможно частично устранить путем выбора формы анастомоза на основе математического моделирования. Известные математические модели являются громоздкими и не позволяют получать результаты в реальном масштабе времени.

Цель работы. Работа является разработкой трехмерной математической модели области анастомоза для исследования с достаточной точностью гидродинамических параметров жидкости со сложной структурой в реальном масштабе времени.

Метод. Предложен метод построения и анализа математической модели анастомоза пищеварительного тракта на основе решетчатого метода Больцмана. Метод основан на анализе гидродинамических параметров жидкости и одновременно определяет характер движения мелкозернистых частиц в зоне анастомоза. Основные этапы метода: разработка технологии задания области моделирования, дискретизация трехмерного упрощения Бульмана с выбором решетки и характеристики определения зависимости давления на мезоскопическом уровне с учетом особенностей свойств жидкости, переход от мезоскопических к макроскопическим параметрам жидкости.

Результаты моделирования включают в себя определение распределения поля скоростей в зоне анастомоза с целью модификации его геометрии. Проведено исследование влияния силы тяжести на характер движения мелкозернистых частиц. Определены количественные характеристики исследуемой области анастомоза в зависимости от динамической вязкости жидкости.

Выводы. Рассмотренная в данной работе трехмерная математическая модель базируется на применении решетчатого метода Бульмана при вычислении гидродинамических параметров движения жидкости в области анастомоза. Особенность модели заключается в учете сложного характера жидкости, содержащей мелкозернистые включения. Модель позволяет определять характер поведения этих включений и поле скоростей с достаточной точностью в реальном масштабе времени.

Ключевые слова: математическая модель, решетчатый метод Бульмана, моделирование анастомоза.

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