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COMPUTER SIMULATION OF TRANSPORT PHENOMENA IN POROUS STRUCTURES USING CELLULAR AUTOMATA METHOD

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В статті описані підстави для використання методу кліткових автоматів при моделюванні явищ переносу в текстильних структурах. Представлена модель ґратового газу, принцип роботи якої заснований на методі кліткового автомату. Також розглянуті приклади використання моделі ґратового газу при моделюванні масопереносних явищ в текстильних матеріалах

From physical point of view the textile in general is object, which can be described by the theories of classical physics and experimented with physical instruments. During few last years, the principles of modelling and simulation became to be popular in the textile industry also. For example, there is a tendency:

- to use image analysis for textile quality assessment;
- to do modelling and simulations of textile structures (to study different textile structures using computer simulation, to characterize the yarn unevenness by means of computer technologies);
- to aid the garment design with a computer;
- to study physical properties of textiles as a moisture and heat transfer using computational simulations [1].

The development of computing of textile structures and their physical properties is linked to the advances in computer hardware and software on the one side, and necessity to solve more and more complicated phenomena associated either with production or exploitation of textiles on the other side.

The most part of traditional numerical simulations are represented by the Navier-Stokes equations and relied on the continuum approach. But the approach would break down, when the length scale of the physical system decreases, concretely, when the Knudsen number became greater that about 0,2. Knudsen number (Kn) is dimensionless parameter that determines the degree of appropriateness of the continuum model – the degree of rarefaction of gases encountered in a small flows through narrow channels and for an ideal gas it is:

$$Kn = \frac{\lambda}{L} = \frac{k_B T}{\sqrt{2}\pi d^2 P L}, \qquad (1)$$

where λ is a mean free path of molecules, m;

$L = \frac{\rho}{d\rho/dx}$ – representative physical length scale, m,

ρ – fluid density;

$k_B = 1{,}38 \cdot 10^{-23} J/K$ – Boltzmann's constant

T – temperature, K;

d – particle diameter, m;

P – total pressure, Pa.

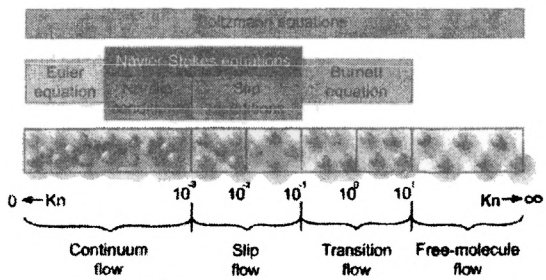


Figure 1. **Different regimes of fluid flow and methods for their description depending on Knudsen number**

As is shown at Figure 1 only Boltzmann equation, which is based on the discrete kinetic theory, is valid for the whole range of Knudsen number. As is mentioned in [2] an alternative to continuum model is the molecular one, which recognize the fluid as a swarm of discrete particles, position, inertia and state of all individual particles are calculated here either deterministically or probabilistically at all times. During last few decades a large number of molecular models/methods, which consider individual particle dynamics based on a Boltzmann distribution at the temperature of interest, have emerged. Those methods are mesoscopic and include:

molecular dynamic (MD), direct simulation Monte Carlo (DSMC), dissipative particle dynamics (DPD), smooth-particle hydrodynamics (SPH), Lattice gas cellular automata and Lattice Boltzmann model (LBM). Those methods are also used for the study of macroscopic hydrodynamics. They aren't based upon Nevier-Stokes equations, but closely related to kinetic theory and Boltzmann equation. Those methods are mentioned in literature as promising candidates effectively connecting microscopic and macroscopic scales and enabling to study mesoscopic phenomena as a fluid transport in nanopores structures.

During last few years, investigation of nanometric flow plays a crucial role in material science including textile engineering branch. Tendency to use lattice gas cellular automata for nanometric fluid flow modelling will be trashed out in this paper.

Lattice gas cellular automata model

Lattice gas cellular automata (LGCA) model is a one of the well known lattice models. The points of view from which a fluid can be described are: microscopic, mesoscopic, and macroscopic. The detailed behavior of a fluid in continuum macroscopic level is provided by partial differential equations, e.g., Navier-Stokes equations for flow of incompressible fluid. Some other numerical techniques, such as, finite-difference and finite-element methods, are used for transforming a continuum system into a discrete one. The lattice gas models based on cellular automata are newer compared to numerical methods mentioned above. These models make possible to describe the behavior of fluid systems at a molecular level under various microscopic or mesoscopic conditions. These models are based on detailed information about individual particles, such as their positions, masses, and velocities (see Figure 2) and they provide with output in terms of molecular dynamics. Thus, lattice gas models entered into the history as an alternative for fluid systems modeling.

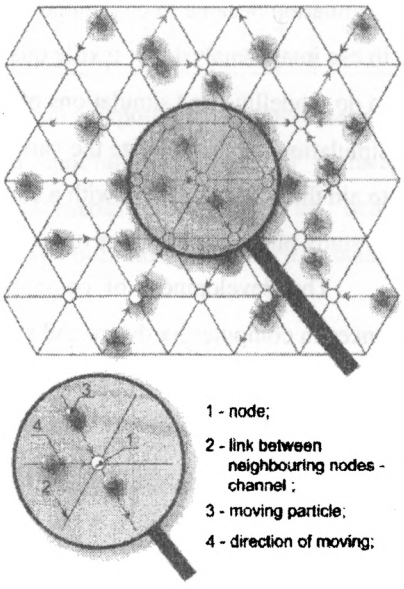


Figure 2. **Representation of LGCA model underlaid by the hexagonal Bravais lattice with triangular tilling**

Detailed description of lattice gas cellular automata method is done for example in [3-5].

The main characteristic of the LGCA model is a fully discreetness because the main parameters are discrete. Particles have the same mass m and velocity v and are moving on an underlying Bravais lattice, generally on a hexagonal one with the triangular tilling, which has the unitary distance Δl between neighbouring nodes. The maximal number of particles in a node is six, equalling the number of neighbours, i.e. to the connectivity of the lattice $B = 6$. Particles are moving from one node to other along the links called channels, connecting neighbour nodes. The moving takes place in discrete time with discrete velocity. The dynamics of LGCA model is ensured by means of collision and propagation, which come true during one time step, also known as a time unit $(t.u.)$.

Collision phase. The collision phase proceeds in accordance with collision rule, which chosen such that mass (particle number in fact) and momentum are conserved at each site on the lattice. The conservation of the local particle number n and mass m in a node $\vec{x}$ could be described as following:

$$\sum_{i=1}^{B} {}^{n}n_i(\vec{x}) = \sum_{i=1}^{B} n_i(\vec{x}) \tag{2}$$

$$\sum_{i=1}^{B} {}^{n}m_i(\vec{x})\,{}^{n}n_i(\vec{x}) = \sum_{i=1}^{B} m_i(\vec{x})\,n_i(\vec{x}) \tag{3}$$

The initial distribution of the colliding particles in the node $\vec{x}$ at individual channels i's is represented by $n_i(\vec{x})$, while their post-collision state in the same node and channel is given by "new" ${}^{n}n_i(\vec{x})$ values. The local momentum conservation during the collision phase may be expressed using its components ${}^{n}p_a(\vec{x})$ and $p_a(\vec{x})$ as:

$$\sum_{i=1}^{B} {}^{n}m_i(\vec{x})\,{}^{n}n_i(\vec{x})\,v_{ia}(\vec{x}) = \sum_{i=1}^{B} m_i(\vec{x})\,n_i(\vec{x})\,v_{ia}(\vec{x}) \tag{4}$$

The redistribution of particles in an individual node obeys the rule of keeping the total momentum in this node constant. The different types of collisions in two-dimensional LGCA model are shown on Figure 3.

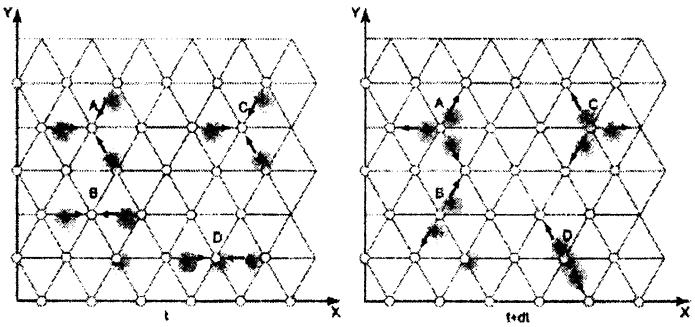


Figure 3. **Typical two- and three-particles collisions in a basic LGCA model**

Propagation phase. During the propagation phase, a particle is shifted from the node $\vec{x}$ to the node $\vec{x} + \vec{v_i}\Delta t$, i.e. is a particle is present at any moment t in a node $\vec{x}$, it is shifted to the neighbouring node in time $t + \Delta t$. It is notable here that the neighbourhood is pre-described by all practicable velocity vectors $\vec{v_i}$, according to a node-independent collision rule that covers the whole lattice.

Implementation of the lattice gas cellular automata algorithm

A large variety of computers from personal computers to powerful parallel supercomputer and a wide range of programming languages explain the existence of a quantum of lattice gas algorithms, which have been implemented since 1985. The algorithm presented in this paper makes possible the simulation of dynamical particle system – its evaluation in time. It based on a FHP-1 model and is designed for general-purpose computer using C++ programming language. The detailed description of the basic LGCA algorithm is presented in [6].

Based on a fact, mentioned already in the first part of the paper that lattice gas cellular automata can describe complex hydrodynamic phenomena and that they can substitute Navier-Stokes equations, it is quite natural to check up if the simulation model fulfils basic fluid flow laws, for instance the Darcy's law.

Fluid flow in a free two-dimensional channel. The algorithm described in a previous session completed with a periodic boundary conditions and an algorithm for a pressure gradient generation was used. The following channel parameters were used: the length L of the channel was 550 lattice units ($l.u.$). Thanks to the periodic boundary conditions applied on the left and the right sides the channel is infinitely long in principle. The width d of the channel was $160\sqrt{3/2}\ l.u.$ Overhead and bottom channel sides are composed of solid walls that restrict the flow. The bounce back reflections were pre-set for the fluid particle collisions with solid wall particles. Fluid particles were generated into the free space between walls. The mass of each particle was one mass unit ($1\ m.u.$). The average microscopic mass density $m(\vec{x})$ was chosen as 3.5 particles per a node.

The pressure gradient was subsequently varied to study the flow rate – pressure gradient relationship. The pressure gradient in this works was created in terms of reversing particle momentum vectors with the chosen probability f_x at all nodes of one vertical line of nodes, the length of which was equal to the channel width d, located on the left side of the horizontal channel. To be more concrete the parameter f_x expresses the average change in the x-component of the particle momentum at a particular node during one time unit ($1\ t.u.$). This flipping mechanism acts merely on particles with negative x -components of velocity.

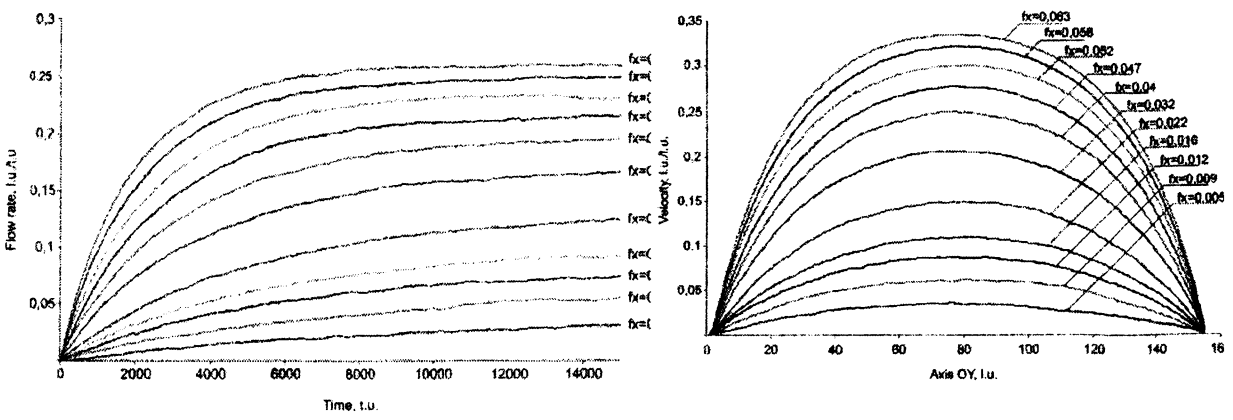
This velocity component points leftward. The "total force" applied on the line of nods is than nf_x, where n represents the number of nodes in the line that spans across the channel width. So the pressure P applied at the left hand channel side is expressed as $P = nf_x/d$. That is why the physical unit of f_x has to be the same as the unit for a pressure divided by a length, i.e. $m.u./t.u.^2$.

The pressure gradient value is got, when the "total force" nf_x is divided by the product of the channel length and the channel width $L \times d$.

The system was left to relax, i.e. to evolve to a steady state flow, after the start of each simulation trial (see Figure 4, *a*). The steady flow rate was achieved after about $10\ 000\ t.u.$ for the parameter f_x values about $0.05 \div 0.06\ m.u./t.u.^2$. The smaller the probability value f_x was the longer time period was needed for an achievement of a steady state flow. For example, for $f_x = 0.009 \div 0.002\ m.u./t.u.^2$ it took more than $13\ 000\ t.u.$, as is evident from

Figure 4.

The x -component of velocity was averaged over the whole channel length L for each horizontal node layer over $5\ 000\ t.u.$ in the steady state region to obtain velocity profiles for various pressure gradients. These computer simulation outputs exhibiting a parabolic velocity profiles typical for Poiseuille flows are presented in Figure 4, *b*.



a. *b.*

Figure 4.

***a* – volumetric flow rate of the channel flow as a function of time, with various values of the parameter f_x; *b* – velocity profiles for various values of the parameter f_x in the free two-dimensional channel**

Eleven independent experiments were carried out for which the parameter f_x varies from 0 up to $0.06\ m.u./t.u.^2$. The corresponding pressure gradients to these f_x values were between 0 and $4.6 \times 10^{-4}\ m.u./(t.u.^2 \times l.u.)$. This span of pressure gradients provides us with flow rates within the interval $0 \div 0.25\ l.u./t.u.$ The flow rate q is considered as volumetric flow rate and can be easily detected as $q = \overrightarrow{v_x}$, where $\overrightarrow{v_x}$ is the average x-component of velocity per particle space averaged over the entire lattice. The area,

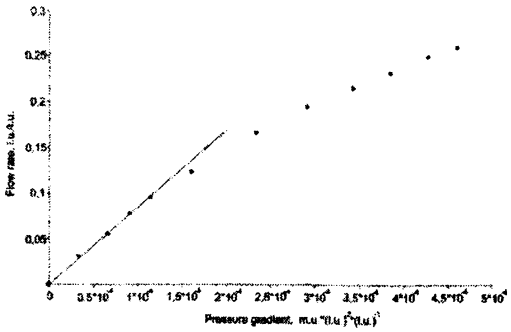


Figure 5. **The extent of linearity of the flow rate's dependency on the pressure gradient delimits the region of Darcy's law validity**

where the Darcy's law is valid for the investigated systems, is shown in Figure . It is possible to see, that the linear dependence between flow rate and pressure gradient holds for low flow rates up to $0.1\ l.u./t.u.$ For this region the Darcy's law has force. When the flow rate exceeded the value $0.015\ l.u./t.u.$, the laminar flow probably changes into the turbulent one which leads to the deviation from the linear relationship. This limit point depends, of cause, on the channel width. The wider is the channel the smaller is the pressure gradient value limit for the linear behaviour

Fluid flow through decline porous material with random structure. The series of experiments engaged in simulation of fluid flow through the decline porous structure was inspired with the Ph.D work of Jakub Hrůza. He has studied the filtration characteristics of assembled filters, produced from nonwoven materials like s spunbond or/and meltblown. This type of filters composes from fan folding textile and looks as a harmonica. An advantage of those filters is a several times biggest filtration area, that influence the pressure gradient, efficiency and durability of filter. Theoretically it is known, that good characteristics of those filters are done by a special orientation of fluid inside the filter. Filtrated dispersion tries to orient itself perpendicularly to filter area in order to minimize the distance, which has to be covered in a space filled by porous matter. Researches doing on that problem suppose only, tat fluid chooses the shortest way. As was mentioned below, it is difficult to demonstrate this type of phenomena practically. No visual proofs only theoretical assumptions were founded in literature. The aim of the study was to prove the convolution of the flow direction at the boundary with the random porous media, imitating the structure of nonwoven textile.

The algorithm described in the previous experiment was used for computer simulation again. The porous material was placed in the middle of the channel.

The size of the channel was: length $L = 450\ l.u.$, the width $d = 250\sqrt{3/2}\ l.u.$, the thickness of the porous medium was $90\ l.u.$, the density of particle per node was 3.5. The fluid flow in the channel was confined by solid walls. The type of particles reflections with each other and with the porous material, boundary conditions, the way of pressure gradient creation were pre-set as well as in previous computer experiment. In this series of computer experiments the porous material has porosity 0,85, 0,9 or 0,95 and crossed the channel axis at the angel 15°, 35° or 55°.

It is necessary to point out, that the size of the pores inside the generated porous material is small enough for approach the nanoscale flow. Several interesting features of the flow through those porous structures were exhibited during computer simulations.

The velocity fields were monitored and expressed by graphical manner for all systems for better understanding of these phenomena. Particle velocities were space averaged inside $5\ l.u. \times 5\ l.u.$ squares and simultaneously these space averaged velocities have been made time averaged over $8\ 000\ t.u.$ inside steady state regions of flows. Velocity vector arrays were obtained. If the velocity vector was located in first or second quadrants of polar coordinates, i.e. in the interval $(0, \pi]$, then it got green color, other way it got red. It is evident, that on the interface between the free channel area and the porous structure is a reorganization of fluid velocity directions – flow impacts on a solid parts of the porous medium and fluid particles try to stream to the pores inside the porous material. It is possible to see, the fluid enters into the porous material perpendicularly.

The same results were obtained when inclination α of porous material was 15°, 35° and 55°. The results of computer simulation are qualitative only, but show the nature of phenomenon. This proof was looking for.

Conclusion

In this paper the LGCA model was presented as an alternative for a mesoscopic fluid flow modelling. It was pointed out that the modern textile science uses the limited number of simulation methods for theoretical studies of transport properties of textiles. The lattice based models especially LGCA models appear as a acceptable candidates for a nanometric flows study, for example. LGCA models identified itself as a powerful approach to obtain insight into momentum transport within textile structures.

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