NUMERICAL SIMULATION OF FLUID FLOW AND MASS TRANSPORT USING LATTICE-BOLTZMANN METHOD

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Introduction

The development of novel numerical methods for applications in computational fluid dynamics (CFD) has made rapid progress in recent years. The traditional approaches of CFD are based on solve the Navier-Stokes equations by some direct discretisation. In contrast to that, the lattice-Boltzmann method (LBM) uses a more rigorous description of the transport phenomena, the Boltzmann equation. Compared to other methods, the LBM makes use of several significant physically motivated simplifications that allow to construct more efficient computational codes as compared to the classical approaches. Thus, the LBM have attracted a lot of attention in the fluid dynamics community and emerged as an attractive alternative in many application areas.

Lattice-Boltzmann hydrodynamics

Historically, the lattice Boltzmann approach developed from lattice gases [1], In lattice gases, particles live on the nodes of a discrete lattice. The particles jump from one lattice node to the next, according to their (discrete) velocity. Then, the particles collide and get a new velocity. Hence the simulation proceeds in an alternation between particle propagations and collisions [3].It can be shown that lattice gases solve the Navier-Stokes equations of fluid flow [4].

The general form of the lattice Boltzmann equation is

$$f_i\left(\boldsymbol{r}+\boldsymbol{u_i}\Delta t, t+\Delta t\right)= f_i\left(\boldsymbol{r},t\right)+\Omega_i \tag{1}$$

where the f_i is the concentration of particles that travels with velocity $\boldsymbol{u_i}$. With the discrete velocity $\boldsymbol{u_i}$ the particle distributions travel to the next lattice node in one time step Δt. The collision operator Ω_i differs for the many lattice Boltzmann methods, in the Bhatnagher-Gross-Krook form can be written as [4]:

$$\Omega_i=\frac{1}{\tau}\left(f_i\left(\boldsymbol{r},t\right)-f_i^{eq}\left(\boldsymbol{r},t\right)\right) \tag{2}$$

Where $f_i^{eq}\left(\boldsymbol{r},t\right)$ is the equillibrium distribution, and τ is the relaxation parameter

The equilibrium distribution $f_i^{eq}\left(\boldsymbol{r},t\right)$ is a function of the local density ρ and the local velocity $\boldsymbol{u}$. These are the first and second order moments of the particle distribution as,

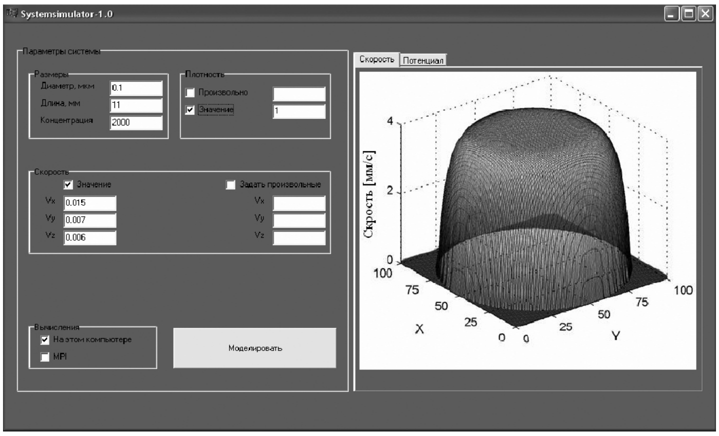
$$\rho(\boldsymbol{r},t)=\sum_i f_i(\boldsymbol{r},t) \tag{3}$$

$$\boldsymbol{v}(\boldsymbol{r},t)=\frac{1}{\rho(\boldsymbol{r},t)}\sum_i \boldsymbol{u}_i f_i(\boldsymbol{r},t) \tag{4}$$

The equillibrium density $f_i^{eq}\left(\boldsymbol{v},\rho\right)$ is calculated as

$$f_i^{eq}\left(\boldsymbol{v},\rho\right)=w_p\rho\left[1+\frac{\left(\boldsymbol{u_i}\cdot\boldsymbol{v}\right)}{c_s^2}+\frac{\left(\boldsymbol{u_i}\cdot\boldsymbol{v}\right)^2}{2c_s^4}-\frac{\boldsymbol{v}^2}{2c_s^2}\right] \tag{5}$$

in which c_s is the speed of sound, the index $p=\boldsymbol{u_i}\cdot\boldsymbol{u_i}$ and w_p is the corresponding equillibrium density for $\boldsymbol{v}=\boldsymbol{0}$. For the three-dimensional, nineteen velocity lattice (D_3Q_{19}) that we have used in our simulations, $w_0=1/3$ (rest particle), $w_1=1/18$ (particles streaming to the face-connected neighbours) and $w_2=1/36$ (particles streaming to the edge-connected neighbours) [2].



Numerical simulation

For LBE-study purposes in C++ Builder 6 modeling program was developed and electroosmotic flow (EOF) in an open-straight, cylindrical capillary with homogeneous and smoothsurface was simulated.

Figure 1. Modeling program work window

Results

Because there is no general analytical solution available for the EOF problem in a cylindrical capillary, the simulated velocity field was compared with another one obtained by numerical solution of the one-dimensional momentum balance equation.

$$\frac{d^2 v_x}{dr^2} + \frac{1}{r}\frac{dv_x}{dr} = \frac{2E_{ext} q_e n_\infty}{\eta_f} \sinh\left(\frac{q_e \Psi}{k_B T}\right) \qquad (6)$$

The solution of this equation provides the radial distribution of the axial velocity component of EOF in the cylindrical capillary. Equation (6) was solved with a very fine resolution (2×10^5 points per channel diameter). Further, the use of different capillary radii allowed to realize aspect ratios r_c / λ_D from 10 to 100. Fig. 2. compares the velocity profiles obtained via both procedures.

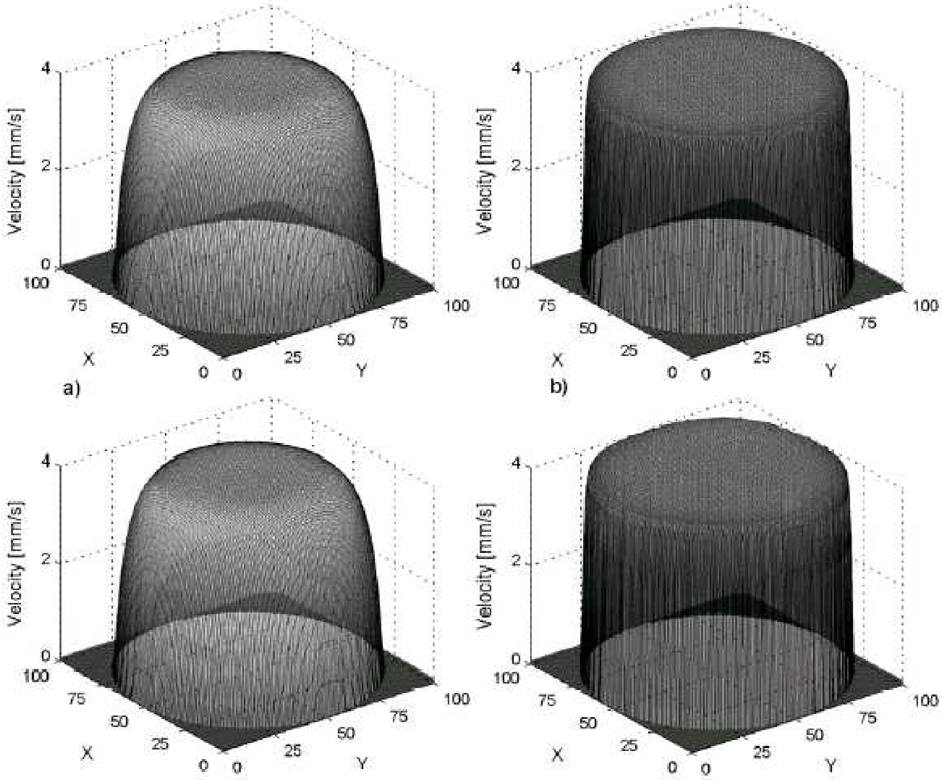


Figure 2. The EOF velocity field in an open-straight, cylindrical capillary with homogeneous and smoothsurface: Solution of the momentum balance equation (top) vs. the LB approach (bottom) for a) $r_c / \lambda_D = 10$ ***and b)*** $r_c / \lambda_D = 100$.

Accuracy of the LBE approach depends on spatial resolution with respect to the capillary radius, e.g., the use of 100 grid points over one capillary diameter results in γ_{vf} of less than 6% for all aspect ratios.

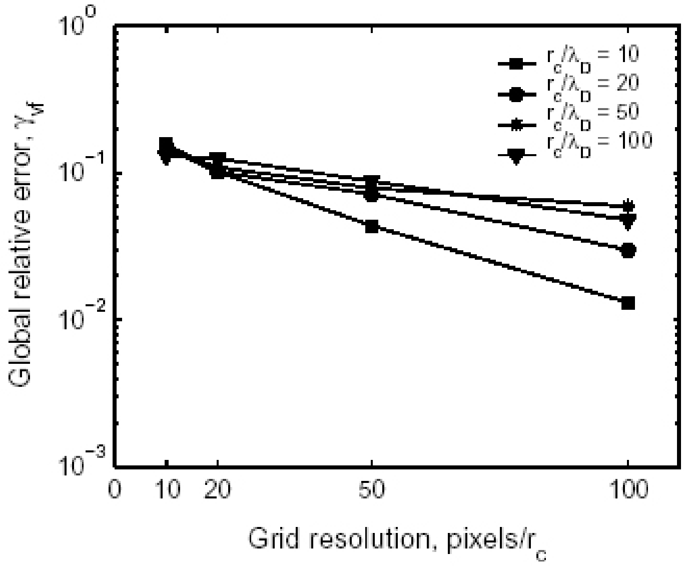


Figure 3. Global relative error of a simulated velocity field (γ_{vf}) relative to the solution of the momentum balance equation

Conclusion

As a result of work the following conclusions have been made:

1) LBE-method has been studied
2) A modeling program for EOF simulation has been developed
3) Derived results have been analysed

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УСЛОВИЯ СУЩЕСТВОВАНИЯ СТАЦИОНАРНЫХ РЕШЕНИЙ ОГРАНИЧЕННОЙ КОЛЬЦЕОБРАЗНОЙ ЗАДАЧИ ШЕСТНАДЦАТИ ТЕЛ

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Рассматривается ограниченная кольцеобразная задача с неполной симметрией [1] для шестнадцати тел P_0, P_i $(i=\overline{1,14})$, P с массами m_0, m_i $(i=\overline{1,14})$, μ соответственно. Тела взаимно притягиваются друг другом в соответствии с законом всемирного тяготения и двигаются в одной плоскости. При движении тела P_i $(i=\overline{1,14})$ образуют два правильных семиугольника, равномерно вращающехся вокруг тела P_0 с угловой скоростью ω. Угловая скорость вращения точно определяется из условия теоремы Банка-Эльмабсута [2], а также из геометрических и гравитационных параметров модели [2]. Согласно понятию «ограниченная задача трех тел» [3] и интерпретации понятия «ограниченная задача любого конечного числа