Bio-Particles Flow Model for Computer-Aided Design of Lab-Chip Devices

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Abstract - **Paper describes the multiscale flow model and its numerical solution for bioparticles motion in microchannels, which is important for the designing and operation of microfluidic Lab-Chip devices.**

Keywords - **microfluidics, flow, model, multiscale, Lab-Chip.**

I. Introduction

Last two decades microfluidic Lab-Chips are widely used in biotechnology research, life sciences diagnostic and point-of-care test devices. Such devices manipulates with biofluidic mixtures in micro-/nano- liter amounts. Biofluid mixtures may contain various inorganic solid contaminants, organic biocomponents or biocells, which should be transported and separated at definite points. Particle's motion in biofluidic mixtures has a crucial importance for the designing and operation of microfluidic Lab-Chip devices. Here, fluid composition, flow parameters, particles and channel sizes/geometries, applied forces and others are tightly connected in such microsystems. All such effects should be integrated and solved in one joint model to receive adequate results of particles movement and sorting possibilities.

A number of software tools, which implements different numerical methods, are available and may be used for Lab-chip analysis. Although, bioparticles strictly influences the behavior of fluid flow and changes the velocity profile. Small bioparticles may interact and form bigger clusters, big particles may break the flow, all particles interact with each other, walls, etc. Besides, different forces may influence particle movement and change the flow profile as well [1].

Motion of micro- and nano- sized bioparticles or living cells usually subordinated by the drag force in a fluid flow. To simplify the model, we will consider continuous fluid phase with immersed particles, so the flow system become randomly dispersed. In this case, the volume fraction of the bio-impurities may be relatively high - up to 20%, which cause problems for several commercial CAD/CAE tools. For example, in the COMSOL particles tracing module, the volume fraction of the discrete phase should be much smaller than the volume fraction of the continuous phase, generally less than 1%. When the volume fraction of the particles is not small, the fluid system is categorized as a dense flow and this require different modeling approach.

II. Problem Statement

The main aim of this study is to create a model for the advection of bioparticles in fluidic microchannels. This allows Lab-chip engineers to design various microfluidic species separators. The basic separation technique in a continuous flow mode was described in [1]. A biofluidic mixture of test sample, buffer solution and carrier fluid continuously flows through a microfluidics chamber and can be separated into several sub-flows by using various force fields. Different mixture components have different response in case of different types of fields (electric, magnetic, optic, etc). As result, mixture components may be located at different microchannel outlets for further processing, as it is shown on Fig.1.

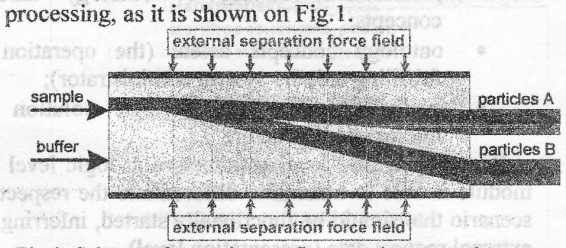

Fig.1. Scheme of a continuous flow species separation system.

To describe particles trajectories, one have to consider: channel geometry, fluids content, particles size and type, various external forces. In general, the presence of bio-particles and cells in microfluidic flow requires to formalize following effects:

1. particles - fluid interactions (particles solubility, bulk biochemical reactions);
2. particles - microchannel interactions (materials, hydrophobicity, adsorption, roughness, surface reactions);
3. particles self transformations (deformations, clustering, multiphase coalescent transformations);
4. particles sensitivity and respond on internal-external forces (electric, magnetic, optic, acoustic fields, and various biological forces).

Thus, in actual research we have to:

- formulate multiscale flow model, including bioparticle motion in microchannels under the influence of various internal and external forces;
- choose or develop appropriate numerical method for the solution of model equations;
- implement model equations in custom software tool and compare its solution results with commercial CAD/CAE tools.

III. Model Equations

In each fluid system, the type of flow plays a key role in fluid flow simulation. To determine the flow type in a arbitrary system, the most important parameters, which should be considered are: type of fluid mixture, type and amount of impurities, dimensions of the fluid channels, and fluid's velocity. For microfluidic devices we accept assumption of is laminar and parabolic flow.

For the fluid flow model, the full set of Navier-Stokes equations was used:

$$\rho\frac{\partial\vec{u}}{\partial t}-\nabla\cdot\eta\left(\nabla\vec{u}+\left(\nabla\vec{u}\right)^{T}\right)+\rho\left(\vec{u}\cdot\nabla\right)\vec{u}+\nabla p=\vec{F}$$

$$\nabla\cdot\vec{u}=0, \qquad (1)$$

where ρ - fluid density, $\vec{u}$ - velocity vector, η - fluid viscosity, p - pressure, and $\vec{F}$ - volume force vector. Here the inertia terms was remain in order to check the contribution of this effect at $Re \sim 0{,}1$.

For the particles movement model, various external forces were considered to influence particle's motion in a flow. Such forces cause particles to accelerate in some direction, related to applied external/internal force.

- *Hydrodynamic chromatography* (particle diffusion is based on the Stokes-Einstein diffusivity equation) [1]

$$D=kT/6\pi r\cdot\eta, \qquad (2)$$

where D - particle diffusivity; r - particle radius, T - fluid temperature; k - Boltzmann constant.

- *Microelectrophoresis* (electrophoretic mobility according to Helmholtz-Smoluchowski equation) [2]

$$\mu_e=\xi\cdot\varepsilon\cdot\varepsilon_0/\eta, \qquad (3)$$

$$\xi=q/\varepsilon\cdot\left(1/r+1/\lambda_D\right), \qquad (4)$$

where ε - dielectric permittivity of the fluid; ε_o - the permittivity of free space; ξ - zeta potential which correlates the particle charge to the electric double layer of the fluid; q - surface charge of the particle; λ_D - Debye length, related to the electric double layer of the solvent.

- Magnetophoresis (calculated via magnetophoretic mobility μ_m, which is magnetically induced velocity divided by magnetic energy gradient) [3]

$$F_m=\mu_m\cdot\nabla B_0 \quad v_m=F_m/6\pi r\cdot\eta$$

$$\mu_m=\Delta\chi(H)\cdot V/6\pi r\cdot\eta \qquad (5)$$

where $\Delta\chi$ - difference in magnetic susceptibility between particle and suspending fluid; H, B - magnetic field strength and intensity vectors; B_0 - applied magnetic field.

- Acoustic forces (F_a) generated by vertical standing waves [4]

$$F_a=4\pi r^3kE\left(\frac{\rho_p+\frac{2}{3}(\rho_p-\rho)}{2\rho_p+\rho}-\frac{k_p}{3k}\right)\sin(2kz), \qquad (6)$$

where $k=2\pi/\lambda$; λ - wavelength acting on the particles; z - vertical coordinate; E - energy density; ρ, ρ_p - density of fluid and particle; k, k_p - compressibility of fluid and particle.

IV. Numerical Solution

The complexity and multiscale nature of bioparticles fluid mixtures directed to the hybrid numerical technique. The flow chart of sequential mode coupling of macroscopic FEM and mesoscopic LBM presented in Fig. 2.

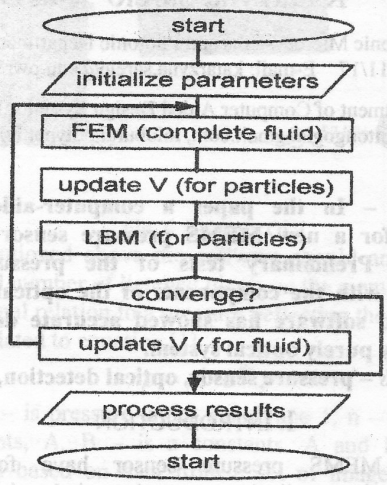

Fig.2. Scheme of a continuous flow species separation system.

Above iterations will stop when solutions for fluid and particles at the interface boundaries became compatible.

V. Conclusion

The influence of microchannel geometries, flow mechanisms and external forces on particles behavior was investigated. Bioparticles flow model, based on Stokes flow and particle dynamics, was constructed. Multiscale flow model and hybrid combination of FEM and LBM solution methods had proved their ability to simulate flow and track bioparticle's motion in Lab-Chip.

The draft simulation results were analyzed, which shown reasonable agreement with predictions published in the literature. Although, further model improvements need to be added, like particles stiffness and deformability, particles-particles interactions and others.

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