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Network simulation of two-phase flows in a microfluidic chip

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Abstract. The paper presents the results of development and validation of a network mathematical model and a numerical algorithm for calculating two-phase flows of immiscible liquids in highly branched microchannel systems. The hydrodynamic model is based on the pore-network approach, which provides a significantly higher computational speed compared to the methods of computational fluid dynamics. Validation of the developed mathematical model and numerical algorithm was carried out on experimental data obtained on the problems of single-phase and two-phase flows in microfluidic chips. Satisfactory qualitative and quantitative agreement between the results of experiments and calculations was obtained.

1 Introduction

In the process of oil recovery, one of the most important roles is played by the structure of the reservoir - the size and location of pores and cracks, rock material, which determines the permeability and strength of the reservoir. Also an important indicator is the proportion of remaining oil after flooding. When studying the process of oil recovery from a rock sample, two main directions can be distinguished: 1) experimental study of core samples, and 2) study of artificially created microchannel systems from regular and two-dimensional to [1, 2], complexly structured and three-dimensional [3]. The first direction makes it possible to obtain integral information about the physical properties of the roll (determination of permeability). The second direction makes it possible to study in more detail the processes occurring in microchannels and to establish regularities expressed in mathematical form. An example of such a microfluidic chip is shown in Figure 1. Experimental oil displacement from such a chip makes it possible to visually study this process and subsequently use the result obtained to test numerical models. When modeling with computational fluid dynamics (CFD), it is necessary to build a detailed mesh for each microchannel, which ultimately leads to significant computational costs.

In recent years, the authors have been developing a universal software product for computational network fluid dynamics [4, 5]. The developed software product was previously successfully used to simulate single-phase flows in microchannels, including taking into account heat transfer [6]. At present, an original algorithm for modeling two-

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phase immiscible flows in porous media is being developed on the basis of the sNet universal network code [7, 8]. The development of an algorithm for calculating two-phase flows based on a network approach is a very attractive task in terms of a significant reduction in computational time compared to standard CFD methods. However, to close the system of equations within the framework of two-phase models, it is required to use quite a lot of different hypotheses and assumptions. Systematic testing is required to test these hypotheses. This paper presents the results of testing and approbation of the developed model of two-phase immiscible flow based on the network approach. Testing of the network approach was performed on experimental data obtained from experiments on microfluidic chips.

2 Mathematical model of network modeling of oil displacement processes

The mathematical model is described in detail in our work [8]. Here we only describe the main points of the algorithm for network simulation of two-phase flows of immiscible fluids in porous media.

1. At the first stage, the initial distribution of pressure, flow rates, and phase concentrations over the network is set.

2. Then a list of network elements is determined in which the process of phase replacement at the first time step is possible - active elements.

3. On the branches where the phase boundary is present, the capillary pressure drop is determined.

4. The hydraulic problem is solved, as a result of which a new distribution of pressure and fluid flow in the network is obtained:

4.1. The pressure field for nodes is calculated.

4.2. According to the given pressure distribution, the flow rate of the liquid on the branches is determined.

5. Based on the found distribution of flow rates in the network, a characteristic local time scale is determined for each active element of the network. From the resulting distribution, the minimum value is selected, which is the time step for a given time.

6. According to the found value of the flow rates, according to the previous distribution of the volume fraction of the phases and taking into account the set value of the time step, the current value of the volume fraction of the phases or the concentration of the components in the active elements is recalculated.

7. The list of active network elements is updated.

8. The whole algorithm from the third step will be repeated.

Separately, a technique for transferring a passive component over a network was implemented. When modeling the flow of local characteristics of the medium, such as enthalpy, concentrations of components, etc., methods of the theory of hydraulic circuits usually take into account only the convective transfer of these characteristics along the branches downstream and their sources (sinks) in the node. In this setting, the flows entering the node are mixed, and the resulting average value of the medium characteristic is carried downstream to the underlying branches and nodes.

3 Validation of the developed algorithm for modeling two-phase flows based on the network approach

To validate the mathematical model and the calculation algorithm, the problem of oil displacement from a microchannel chip with regular porosity was considered. For this, a

microchannel chip was fabricated, the geometry of which is shown in Figure 1. The number of cells is 30×30 (the number of microchannels is 31×31), the size of the cell side is 250 μm. The width and height of the microchannels are 250 and 200 μm, respectively. The length of the inlet section is 2.36 mm. The length of the outlet section is 4.9 mm.

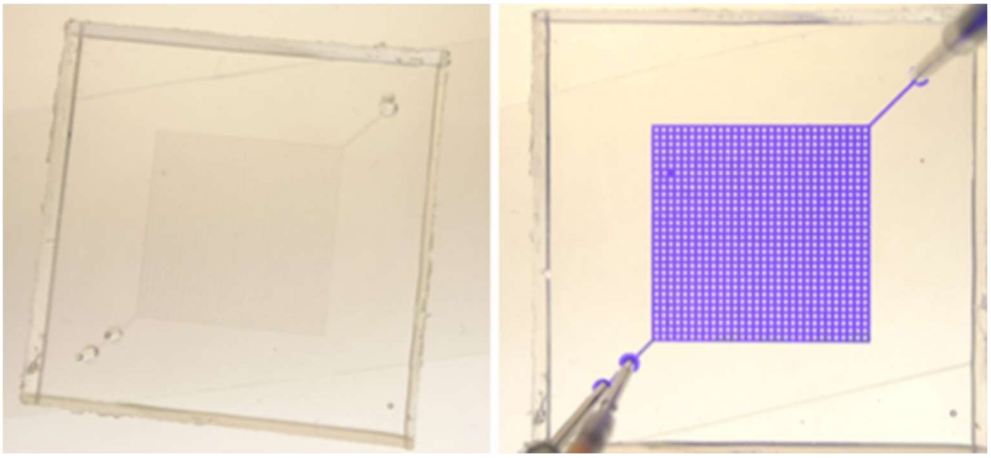

Fig. 1. Photograph of a microfluidic chip.

To verify the mathematical model, the simulation results were compared with the experiment. For this, a network model of the pore space of a microchannel chip was built, consisting of 961 microchannels of rectangular cross section interconnected (Fig. 2).

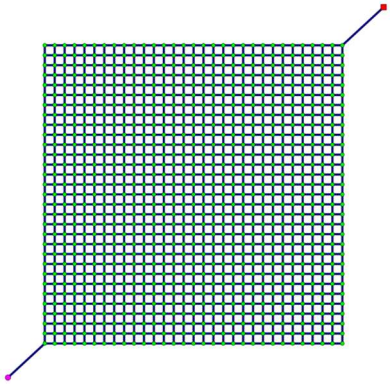

Fig. 2. Hydraulic network topology simulating the pore space of a microfluidic chip.

At the beginning, the verification of the mathematical model was carried out on a single-phase flow. For this purpose, the problem of the flow of water tinted with different dyes was considered in the experiment. The paint does not affect the properties of water, and can be considered as a passive impurity. The flow occurs diagonally from the lower left corner to the upper right. The flow rate of water at the entrance to the microchip is 1 ml/min. The density and viscosity of water were set equal to $\rho = 998.2$ kg/m^3, $\mu = 0.001$ Pa·s, diffusion coefficient $D = 2.63 \cdot 10^{-10}$ m^2/s.

Comparison with the experiment is shown in Figure 3. As can be seen, there is a fairly good agreement between the results of calculations using the network model and the microfluidic experiment on the dynamics of advancement and diffusion of the dye front in the pore space of the microchip.

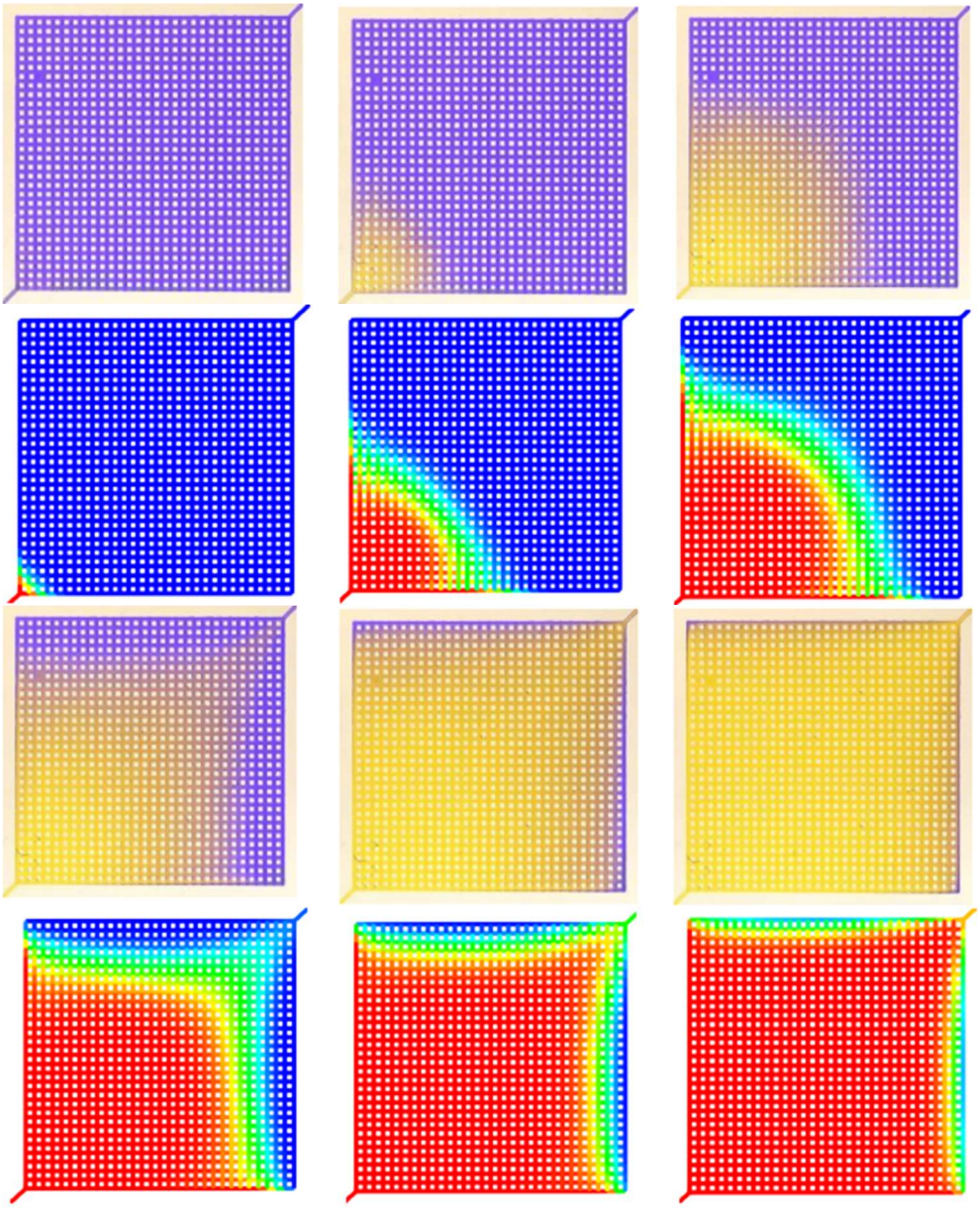

Fig. 3. Dynamics of microchip filling with colored water: experiment above, network calculation below.

Next, the pore-network model was validated on the problem of a two-phase flow when oil was displaced from a microfluidic chip. The formulation of this problem is as follows. At the initial moment of time, the pore space of the chip is completely filled with oil. Further, distilled water was supplied to the lower left input of the chip, which displaced the oil. Using a video camera and a microscope, the dynamics of oil displacement was obtained and the values of the pressure drop over time were measured at a fixed flow rate of 3 ml/min. In the experiment, the oil had the following physical properties: density 851 kg/m^3, dynamic viscosity 0.0246 Pa·s. Physical properties of water: ρ =998.2 kg/m^3 and μ = 0.001 Pa·s. The surface tension coefficient is σ = 0.027 N/m.

Figure 4 shows a comparison of the results of numerical simulation with experiment. The figure shows the dynamics of oil displacement by water at three different points in time. The comparison results show that the network model reproduces well the shape and position of the oil displacement front in the experiment at similar time points. Nevertheless, it is clear that in the calculation after the passage of the displacement front, the residual oil saturation remains close to zero. While in the experiment, oil remains in the form of thin bridges and films that wet the grains of the porous medium. This is a weak point of all pore-network models of two-phase flows. At this stage of development, network models do not take this into account. This requires appropriate refinement, which will need to be done in the future.

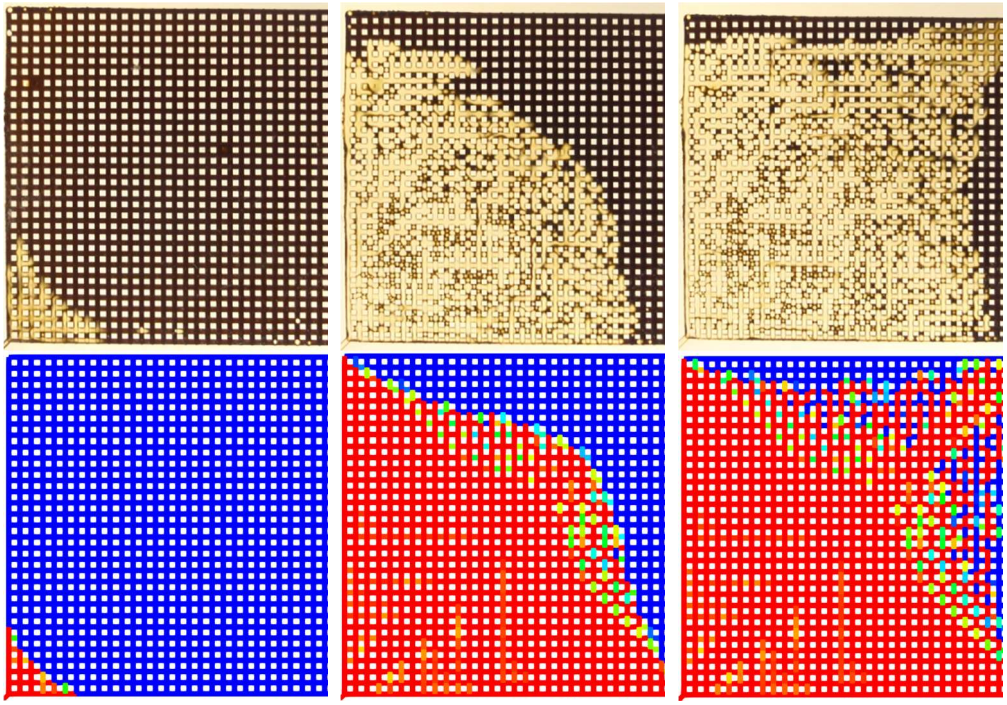

Fig. 4. Dynamics of oil displacement by water. Above - experimental photographs, below - the result of simulation.

4 Conclusions

A network mathematical model of two-phase (immiscible) fluid flow in a highly branched microchannel system has been developed. The model is divided into two parts, the hydraulic model and the phase boundary transfer model. The hydrodynamic model is based on the well-proven theory of hydrodynamic chains, which provides a significantly higher calculation speed compared to the methods of computational fluid dynamics. The physical properties of the fluid in each element of the network depend on the component composition according to the mixture rule. The phase boundary is taken into account by the contribution of the capillary force to the momentum conservation equations on the branch. Phase transfer modeling is carried out by an explicit method with an adaptive time step. This mathematical model was verified on various tests of single-phase flow and oil displacement flows in microfluidic chips. Satisfactory qualitative and quantitative agreement between the results of experiments and calculations was obtained.

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