

## Numerical Simulation of Slug Flow Mass Transfer in the Pipe with Granular Layer

Dmitry P. Khramtsov, Andrey V. Vyazmin\*, Boris G. Pokusaev, Sergey P. Karlov, Dmitry A. Nekrasov,

Moscow State University of Mechanical Engineering, ul. Staraya Basmannaya 21/4, 105066, Moscow, Russia  
 av1958@list.ru

A numerical study of the process of interphase mass transfer during the motion of a gas bubble at different inclination angles in case of movement in the channel between the layers of gel is presented. The dependence of the effective dimensionless mass transfer coefficient depending on the angle of inclination of the channel was obtained. The relation between effective dimensionless mass transfer coefficient and the speed of the freely rising gas bubble was found. A new exact method for solving 3D systems of hydrodynamic equations is described based on decomposing these systems into simpler equations. It is obtained that the exact solution to a 3D nonstationary system of the Navier–Stokes equations can be expressed in terms of two stream functions.

### 1. Introduction

One of the most common flow regimes in the pipes for energy systems, oil and gas production, as well as in microchannels is the slug flow regime of two-phase flow (Hessel et al., 2005). In such flow a large gas bubble is rising in a pipe or moving under the pressure in the capillary channels, separated by a fluid layer. Mixing of gas and liquid phases, combined with diffusion and low thermal resistance through the thin film between bubble and wall, leads to a substantial intensification of the processes of heat and mass transfer. A satisfactory theory of such flows has not yet been developed. This is due, primarily, to the complexity of such flows. Problems with the theoretical description arise even for the case of motion of a single slug in an inclined pipe (Pokusaev et al., 1999).

Dynamics of gas liquid flow inside gels are not studied enough, both experimentally and numerically. Gel is a specific two-phase system. One phase represents a relatively sparse spatial network of polymer molecules which are bonded at the intersections of intermolecular bonds. The second phase is a liquid (in some cases - the water), which occupies the space between the polymer molecules. This fluid does not have any chemical bond with the polymer molecules, i.e. does not form chemical compounds with them. The transfer processes in gels have such features as unsteady and anisotropy: they are determined the nature, structure, and behavior of transfer medium (see, for example, research of Pokusaev et al., 2015). In the study of additive processes of application of gels in relation to problems of bioprinting, we found the effect of microchannels formation between the layers of gel, filled with gas and fluid (photo is shown in Figure 1).

In the case of the presence of microorganisms within the gel, a carbon dioxide is produced within the gel due to activity of microorganisms. For the normal functioning of microorganisms in the gel it is required a withdrawal of produced products. In this case, the rate of drainage is influenced by the intensity of absorption and the speed of ascent of gas bubbles, which leads to the necessity of conducting experimental and theoretical studies of the process of mass transfer of gas bubbles in the gel. The relevance of such studies is also due to the active development of technologies of three-dimensional printing of living tissues (Mironov et al., 2003) and bodies (Jakab et al., 2010).

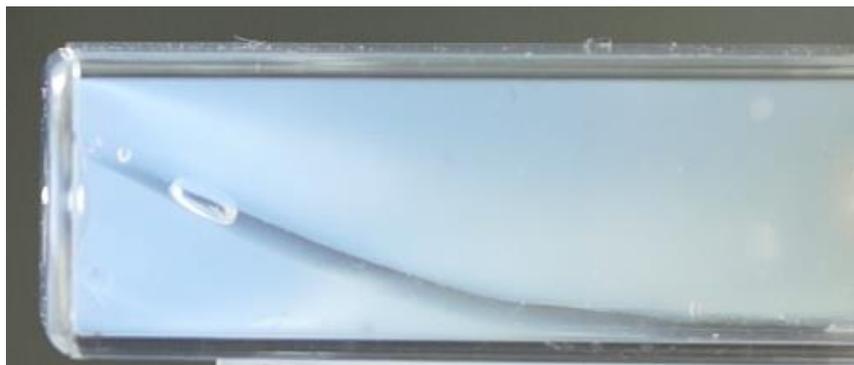


Figure 1: Gas bubble in inclined channel inside gel

Using of modern numerical techniques such as smoothed particle hydrodynamics method, allows to simplify the mathematical description, which makes possible the numerical simulation of three-phase systems with solid phases of different geometry. Method of smoothed particle hydrodynamics was used in the simulation of multicomponent mixtures (Hu and Adams, 2006), the processes of expiration of gas-liquid flows (Das and Das, 2009) and heat-mass exchange processes (Jeong et al., 2003). Method of smoothed particle hydrodynamics is also used for solving problems of fluid flow dynamics in the channels of complex shape (Monaghan, 2012), including movement in porous and gel-like structures (Zhu and Patrick, 2001). Direct numerical simulation of 3D hydrodynamic problems by solving the Navier-Stokes equations requires significant computing resources. Using the decomposition method allows to reduce the solution of the original problem to a system of simpler equations. Previously a new exact method for solving 3D linear systems of hydrodynamic equations was described based on decomposing these systems into three simpler equations. It is shown that the general solution to 3D Stokes equations can be expressed by means of solutions to two independent equations: the heat conduction equation and the Laplace equation (see, for example, Polyanin and Vyazmin, 2013a). Later this approach was extended for description of the motion of viscoplastic media (Polyanin and Vyazmin, 2013b).

The aim of this work is obtaining of new data on the intensity of interfacial mass transfer of gas bubbles depending on the angle of tilt in the motion of multiphase flow in the channel inside gel. It will also be shown that the solution to a 3D nonstationary system of the Navier–Stokes equations can be expressed in terms of two stream functions.

## 2. Mathematical model

Model movement of a gas bubble in the tube based on the process of mass transfer is developed based on the smoothed particle hydrodynamics method. The method is based on representing the fluid as a set of particles, which are located at some distance from each other, the distance called smoothing (Liu and Liu, 2003). The influence of each particle on the properties of nearby particles is calculated on the basis of its density and the distance from the particle for which parameters. For the calculation we introduce the notion of kernel functions. As a kernel function, typically uses a Gaussian function (Amada et al., 2004).

In the case of motion of a gas bubble of carbon dioxide in the channel between the layers of gel, filled with ethanol, the computational domain is a rectangular parallelepiped with a straight channel of rectangular cross section. The channel length is 40 mm, width 8 mm and thickness 1 mm (see Figure 2). The gas bubble affects lift force, which is compensated by the force of gravity. Also on the ascent rate is influenced by the hydraulic resistance of the medium, which is caused by the curvature of the bubble head. The gas bubble is defined as a collection of particles forming area in the form of a rectangular parallelepiped having a density of carbon dioxide. Within a few tens of iterations after the beginning of process of modelling the source region with carbon dioxide is converted to form a gas bubble, observed in the experiment (Figure 1).

## 3. Numerical simulation results

For verification of the developed model was used for calculation of test problem on simulation of freely rising gas bubble in a pure liquid at various angles of inclination of the tube for the purpose of comparison with previously obtained experimental data (Pokusaev et al., 2011). The results of the calculation showed that the dependence of the velocity of ascent of a gas bubble from the angle of the tube shows extreme character, and the maximum ascent rate falls at an angle of 40°, which is consistent with the experimental results.

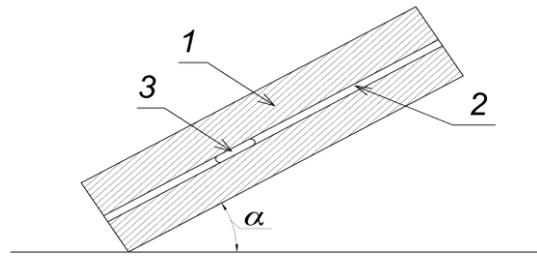


Figure 2: The computational domain of the channel in the gel: 1 – gel; 2 – channel filled with fluid; 3 – gas bubble

To determine the intensification of mass transfer of a gas bubble at various angles of tilt was introduced dimensionless effective coefficient of mass transfer, calculated as the ratio of the volume of the gas bubble at the end of the working section at a given angle of inclination  $V_\alpha$  to the volume of the gas bubble at the end of the work area when the vertical position of the tube  $V_{90}$

$$\delta = \frac{V_\alpha}{V_{90}}$$

Thus, it is possible to estimate the influence of the tilt angle of the tube at the intensity of the process of mass transfer.

Contribution to the process of mass transfer makes the hydrodynamics of the bubble and the phase boundary surface. The maximum value of the effective mass transfer coefficient corresponds to the angle of inclination at which the speed of ascent of the bubble maximum. If you increase the speed of ascent of the gas bubble passes the work area in less time, respectively, the interaction time between phases decreases. The obtained dependence allows to conclude that the time of interfacial contact is the defining characteristic of the intensity of the process of mass transfer.

The data obtained by numerical simulation of the motion of a gas bubble in the channel between the layers of the gel showed that the process of ascent of a gas bubble in the gel also has an external character; however, the extremum is not so pronounced compared with the movement of the bubble in the tube. The numerical result is at angles of tilt less than  $10^\circ$  movement of the bubble with a flat channel in the form of a disk. When you increase the angle of inclination of from  $20$  to  $50^\circ$  is observed a sharp increase in speed, after which the rate decreases slightly according to the linear law (see Figure 3).

The dependence can be explained by the change in bubble shape with increasing lifting force. When the tilt angles in the range  $20 - 50^\circ$  the increase in lift leads to the growth rate of ascent. With further increase of angle of inclination of the bubble expansion is observed along the axis perpendicular to the direction of movement that causes an increase in hydraulic resistance and reduced ascent rate. The calculation of the effective dimensionless mass transfer coefficient showed that, similarly to the case with a pipe, dimensionless coefficient of mass transfer is directly dependent on the speed of ascent, the bubble (Figure 4). The nature of the dependences of the velocity of ascent of bubbles in the tube and in the channel inside the gel can be caused by changing the shape of the head bubble in the region of the critical point (Pokusaev et al., 2011).

#### 4. Reducing 3D Navier-Stokes equations to two equations for two stream functions

A closed system of the Navier–Stokes equations describes the non-steady-state flow of a viscous incompressible Newtonian fluid. In vector form, it is written as

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla \rho + \nu \Delta \mathbf{u}, \quad (1)$$

$$\text{div } \mathbf{u} = 0,$$

where the vector  $\mathbf{u}$  has components  $u$ ,  $v$  and  $w$  directed along the rectangular Cartesian coordinates  $x$ ,  $y$ , and  $z$ , respectively;  $t$  is time;  $\Delta$  is the Laplace operator;  $\nabla$  is the nabla operator;  $\rho$  is the density of the fluid; and  $\nu$  is the kinematic viscosity of the fluid.

System of four Eq(1) can be reduced to a system of two equations for two stream functions  $\varphi$  and  $\psi$ . To accomplish this, the fluid velocity vector components should be expressed in terms of stream functions by the formulas

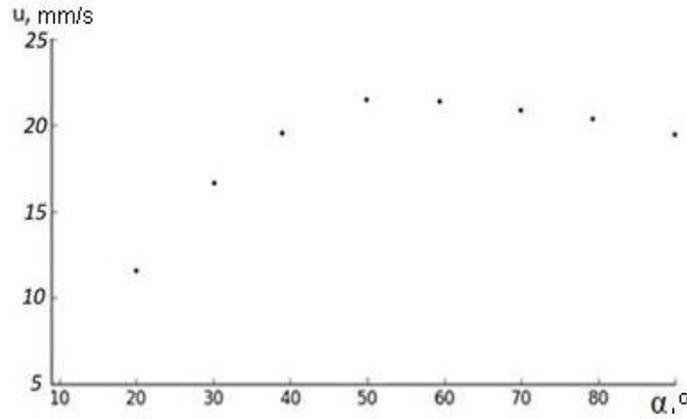


Figure 3: Ascent rate of CO<sub>2</sub> gas bubble in ethanol depending on the angle of the channel in the gel, the calculated data

$$\begin{aligned}
 u &= a_1 \frac{\partial \varphi}{\partial y} - a_3 \frac{\partial \varphi}{\partial z} + b_1 \frac{\partial \psi}{\partial y} - b_3 \frac{\partial \psi}{\partial z}, \\
 v &= a_2 \frac{\partial \varphi}{\partial z} - a_1 \frac{\partial \varphi}{\partial x} + b_2 \frac{\partial \psi}{\partial z} - b_1 \frac{\partial \psi}{\partial x}, \\
 w &= a_3 \frac{\partial \varphi}{\partial x} - a_2 \frac{\partial \varphi}{\partial y} + b_3 \frac{\partial \psi}{\partial x} - b_2 \frac{\partial \psi}{\partial y},
 \end{aligned} \tag{2}$$

where  $a_i$  and  $b_i$  are arbitrary constants (their number is redundant)

Substituting Eq(2) into the continuity equation (the last equation in Eq(1)) reduces it to an identity. Pressure  $p$  is eliminated from the first three equations in Eq(1) by cross differentiation, which leads to the following two equations:

$$\begin{aligned}
 \frac{\partial}{\partial y} \left[ \frac{\partial u}{\partial t} + (\mathbf{u} \cdot \nabla) u \right] - \frac{\partial}{\partial x} \left[ \frac{\partial v}{\partial t} + (\mathbf{u} \cdot \nabla) v \right] &= \nu \frac{\partial}{\partial y} (\Delta u) - \nu \frac{\partial}{\partial x} (\Delta v), \\
 \frac{\partial}{\partial z} \left[ \frac{\partial u}{\partial t} + (\mathbf{u} \cdot \nabla) u \right] - \frac{\partial}{\partial x} \left[ \frac{\partial w}{\partial t} + (\mathbf{u} \cdot \nabla) w \right] &= \nu \frac{\partial}{\partial z} (\Delta u) - \nu \frac{\partial}{\partial x} (\Delta w).
 \end{aligned} \tag{3}$$

Substituting Eqs(2) into (3) yields two equations for  $\varphi$  and  $\psi$ .

A special case where  $a_1 = a_2 = a_3 = b_2 = b_3 = 0$  and  $b_1 = 1$  in Eq(2) corresponds to the well-known representation of the fluid velocity vector components by means of a single stream function for two-dimensional flows as follows:

$$u = \frac{\partial \psi}{\partial y}, \quad v = -\frac{\partial \psi}{\partial x}, \quad (w = 0, \quad \psi = \psi(x, y, t)).$$

Setting  $a_1 = a_2 = b_1 = b_3 = 0$ ,  $a_3 = -1$ , and  $b_2 = 1$  in Eq(2), we obtain the following simple representation for the fluid velocity vector components in the case of a three dimensional flow by means of two stream functions:

$$u = \frac{\partial \varphi}{\partial z}, \quad v = \frac{\partial \psi}{\partial z}, \quad w = -\frac{\partial \varphi}{\partial x} - \frac{\partial \psi}{\partial y}.$$

Any of Eq(3) can be replaced by the equation

$$\frac{\partial}{\partial z} \left[ \frac{\partial v}{\partial t} + (\mathbf{u} \cdot \nabla) v \right] - \frac{\partial}{\partial y} \left[ \frac{\partial w}{\partial t} + (\mathbf{u} \cdot \nabla) w \right] = \nu \frac{\partial}{\partial z} (\Delta v) - \nu \frac{\partial}{\partial y} (\Delta w), \tag{4}$$

which is derived by different methods when pressure is eliminated.

Eq(4) can be used to check exact solutions derived using set of Eq(3) (since, generally speaking, exact solutions to Eq(3) can contain additional arbitrary constants and functions).

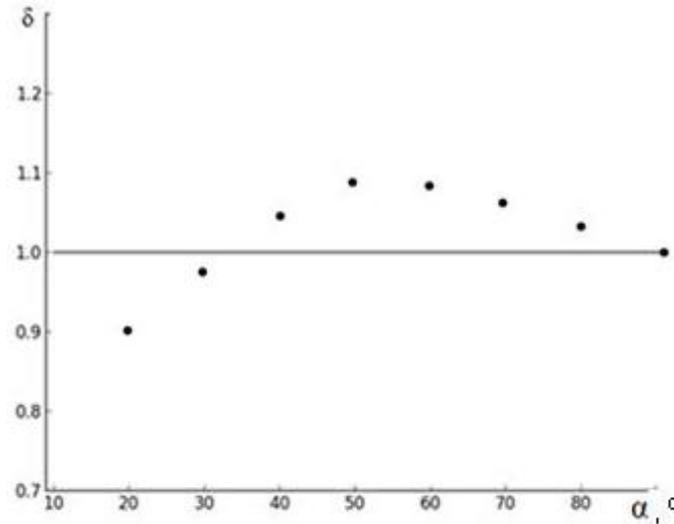


Figure 4: Dimensionless effective coefficient of mass transfer, depending on the angle of the channel in the gel, the calculated data: dots – model; line – vertical pipe

### 5. Motion of viscoelastic incompressible media

Some models of viscoelastic incompressible media (for example, gels) lead to integrodifferential equations, which, for creeping flows, appear as

$$L[u] = -\frac{\partial P}{\partial x}, \quad L[v] = -\frac{\partial P}{\partial y}, \quad L[w] = -\frac{\partial P}{\partial z}, \quad (5)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0,$$

where  $u$ ,  $v$ , and  $w$  are the fluid velocity components;  $P$  is the pressure divided by the density of the fluid; and  $L$  is the linear differential operator with respect to variables  $x$ ,  $y$ ,  $z$ , and  $t$

$$L[u] = \frac{\partial u}{\partial t} - \nu \Delta u - \int_0^t K(t, t') \Delta u(\mathbf{x}, t') dt', \quad (6)$$

The kernel  $K(t, t')$  of the integrodifferential operator in Eq(6) is usually a difference kernel, in particular for the Oldroyd model, we have  $K(t, t') = a \exp[-\lambda(t-t')]$  (Araujo et al., 2009). The kernel  $K(t, t') \equiv 0$  corresponds to the ordinary Navier–Stokes equations.

The solution to system of Eqs(5), (6) can be represented as

$$u = \frac{\partial \varphi}{\partial x} + \xi, \quad v = \frac{\partial \varphi}{\partial y} + \eta, \quad w = \frac{\partial \varphi}{\partial z} + \zeta, \quad P = -L[\varphi] + p_0,$$

where  $p_0$  is an arbitrary constant (for non-steady-state problems,  $p_0 = p_0(t)$  is an arbitrary function); functions  $\xi = \xi(x, y, z, t)$ ,  $\eta = \eta(x, y, z, t)$  and  $\zeta = \zeta(x, y, z, t)$  satisfy the three similar independent equations

$$L[\xi] = 0, \quad L[\eta] = 0, \quad L[\zeta] = 0,$$

and the pseudopotential  $\varphi$  is the arbitrary solution to Poisson equation

$$\Delta \varphi = -\frac{\partial \xi}{\partial x} - \frac{\partial \eta}{\partial y} - \frac{\partial \zeta}{\partial z}.$$

Without loss of generality, one of the functions  $\xi$ ,  $\eta$ , and  $\zeta$  can be set to be zero.

If the  $K(t, t')$  is a difference kernel, i.e., has the form  $K(t-t')$ , solutions to Eq(5) are sought using the Laplace transform with respect to time.

## 6. Conclusions

It is shown that in the case of the process of mass transfer in granular layer is the speed of the bubble depending on the angle of inclination of the tube is nonmonotonic, extreme nature and max speed when inclination angle is  $60^\circ$ . In the case of bubble movement in a flat channel inside a gel ascent rate monotonically increases up to  $50^\circ$ . Further increase of tilt angle leads to a slight monotonous decrease speed. Using the smoothed particle hydrodynamics method applied to the modelling of the gas bladder showed the effectiveness of this method in solving such problems. Smoothed particle hydrodynamics method allowed to simplify the mathematical description of the task and improve the speed of numerical calculation. To assess the intensification of interfacial mass transfer a dimensionless coefficient of mass transfer was introduced, the calculation of which showed the intensity of interfacial mass transfer is directly dependent on the average rate of ascent of the bubble. In general, the process of mass transfer is determined by the hydrodynamics of the bubble and the surface section of phases. The developed model allows simulation of multiphase flows in channels of complex geometry formed by filling spherical, and also allows to solve problems of mass transfer in gels.

It is found that the solution to a 3D nonstationary system of the Navier–Stokes equations can be expressed in terms of two stream functions. The linearized equations of motion for a viscoelastic fluid are studied. The generalization of a method for constructing solutions to arbitrary linear hydrodynamic systems is proposed. It is shown that the solution of this system of equations can be reduced to solving set equations that take into account the rheological properties of the medium and to the Poisson equation.

## Acknowledgments

The work is supported by Russian Scientific Foundation (project No. 15-19-00177).

## Reference

- Amada T., Imura M., Yasumuro Y., Manabe Y., Chihara K., 2004, Particle-based fluid simulation on GPU, Proc. ACM Workshop on General-Purpose Computing on Graphics Processors. Los Angeles, 342-343.
- Araujo G.M., Menezes S.B., Marinho, A.O., 2009, Existence of solutions for an Oldroyd model of viscoelastic fluids, *Electronic Journal of Differential Equations*, 69, 1-16.
- Das A.K., Das P.K., 2009, Bubble evolution through submerged orifice using smoothed particle hydrodynamics: Basic formulation and model validation, *Chemical Engineering Science*, 64, 2281-2290.
- Hessel V., Lowe H., Muller A., Kolb G., 2005, *Chemical Micro Process Engineering*. Wiley VCH, Weinheim, Germany.
- Hu X.Y., Adams N.A., 2006, A multi-phase SPH method for macroscopic and mesoscopic flows, *Journal of Computational Physics*, 213, 844-861.
- Jakab K., Norotte C., Marga F., Murphy K., Vunjak-Novakovic G., Forgacs G., 2010, Tissue engineering by self-assembly and bio-printing of living cells, *Biofabrication*, 2, 20-34.
- Jeong J.H., Jhona M.S., Halowb J.S., Osdol J., 2003, Smoothed particle hydrodynamics. Applications to heat conduction, *Computer Physical Communications*, 153, 71-84.
- Liu G.R., Liu M.B., 2003, *Smoothed Particle Hydrodynamics: A Meshfree Particle Method*. World Scientific, Singapore.
- Mironov V., Boland T., Trusk T., Forgacs G., Markwald R., 2003, Organ printing: computer-aided jet-based 3D tissue engineering, *Trends in Biotechnology*, 21, 157-161.
- Monaghan J.J., 2012, Smoothed particle hydrodynamics and its diverse applications, *Annual Review of Fluid Mechanics*, 44, 323–346.
- Pokusaev B.G., Zyatsev A.A., Zyatsev V.A., 1999, Transfer processes under slug flow conditions in three-phase media, *Theoretical Foundations of Chemical Engineering*, 33, 539-549.
- Pokusaev B.G., Kazenin D.A., Karlov S.P., Ermolaev V.S., 2011, Motion of a gas slug in inclined tubes, *Theoretical Foundations of Chemical Engineering*, 45, 640-645.
- Pokusaev B.G., Karlov S.P., Vyazmin A.V., Nekrasov D.A., 2015, Diffusion phenomena in gels, *Chemical Engineering Transactions*, 43, 1681-1686, DOI:10.3303/CET1543281.
- Polyanin A.D., Vyazmin A.V., 2013a, Decomposition and exact solutions of three-dimensional nonstationary linearized equations for a viscous fluid, *Theoretical Foundations of Chemical Engineering*, 47, 114-123.
- Polyanin A.D., Vyazmin A.V., 2013b, Decomposition of three-dimensional linearized equations for Maxwell and Oldroyd viscoelastic fluids and their generalizations, *Theoretical Foundations of Chemical Engineering*, 47, 321-329.
- Zhu Y., Patrick J.F., 2001, Smoothed particle hydrodynamics model for diffusion through porous media, *Transport in Porous Media*, 43, 441-447.