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Numerical Simulation of Mixing Hydrodynamics Bubble

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Abstract: A mathematical model of bubble mixing, based on the content view of the gas-liquid reactor in the form of two continuous interpenetrating and interacting media: liquid and gas bubbles pop. By numerical implementation of the model is investigated for circulating the liquid phase and found its main characteristics: the radius of the interface between the upstream and downstream, the velocity profile of the circulating fluid flow and volume flow. The analytical expressions for the calculation of the minimum duration of one cycle of mixing and power consumption for its implementation. The results of mathematical and computer modeling bubble mixing agreement with experimental data and were used in the calculation and design of biogas equipment.

Key words: Reactor, bubbling, stirring, turbulence, circulation

INTRODUCTION

Many processes in construction, chemical, biochemical and other industries conducted in bubble devices (reactors) in which the interfacial surface is formed as a result of crossing (bubbling) of gas through the liquid layer (Bogdanov *et al*., 2007).

Gas bubbles rising upwards entrain the adjacent layers of fluid that leads to the formation of its upward flow in the central zone of the reactor. This stream, reaching the free surface of the liquid, changes its direction whereby the vicinity of the reactor walls formed by the downward annular flow. Thus, the upward flow of gas bubbles bubbling liquid circulates in the meridional section of the reactor which leads to a mixing and equalizing its concentration of solutes, particulate matter and the temperature throughout the reactor volume which is an important factor for intensification occurring there in physics-chemical and biochemical processes (Koetsier and Thoenes, 1973; Sokolov and Domanski, 1976).

Currently, the main method of studying the hydrodynamics of bubbling is conducting laboratory and industrial experiments, followed by mathematical processing of the data (Sokolov and Domanski, 1976). At the same time developing methods of mathematical and computer modeling of two-phase flows (Shaptala *et al*., 2013; Kuznetsov, 2012).

THE MAIN PART

In bubbling gas-liquid reactors, liquid mixing occurs as a result of the passage (bubbling) of gas through its layer (Fig. 1) (Bogdanov *et al*., 2007).

With mass bubbling occurs turbulent fluid motion which is described by the equations for the averaged turbulent motion-Reynolds equations (Zaichik *et al*., 1994; Delnoij *et al*., 1997):

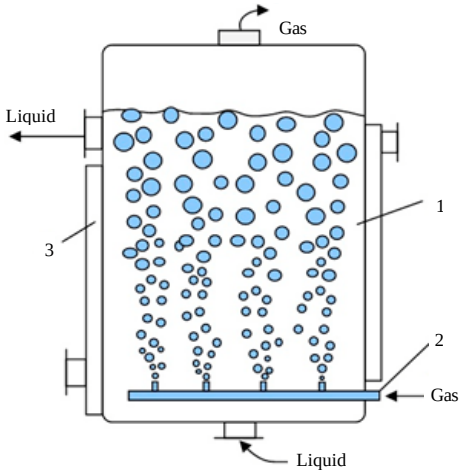

Fig. 1: Scheme hollow bubble reactor (1: reactor vessel, 2: gas distributor, 3: heat exchanger)

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$$\frac{du_j}{dx_j} = 0 \quad (1)$$

$$\rho\frac{\partial u_i}{\partial t} + \rho u_j\frac{\partial u_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \mu\frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}\pi_{ij} + F_i \quad (2)$$

Where:

i, j = 1, 2, 3; $u_1 = u_x$, $u_2 = u_y$, $u_3 = u_z$: averaged over time, the projection of the fluid velocity

ρ = Density of the fluid

P = Averaged pressure value

π_{ij} = Tensor of turbulent stresses in the fluid

$$\pi_{ij} = -\rho < u_i' u_j' > \quad (3)$$

where, u_i', u_j'; turbulent fluctuations of the projections of the fluid velocity, F_i; averaged interfacial force projection:

$$F_i = \frac{\pi d^2}{4} C_D \frac{\rho|v_i - u_i|(v_i - u_i)}{2}$$
$$C_D = \frac{24}{Re_b} + \frac{3.6}{Re_b^{0.313}},\ Re_b = \rho d|v_i - u_i|/\mu \quad (4)$$

Where:

d = Size bubbles

C_D = Drag coefficient

v_i = Bubbly medium speed

Re_b = Reynolds number of bubbles

To close the system of Eq. 1, 2 turbulent stress tensor within «k-ε» turbulence model is expressed in terms of the projection of the averaged velocity (Zaichik *et al*., 1994):

$$\pi_{ij} = -\rho\left(\frac{2}{3}k\delta_{ij} - v_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) \quad (5)$$

Where:

k = The turbulent kinetic energy of the fluid (the energy of turbulent fluctuations of its velocity)

ε = Turbulent energy dissipation rate

δ_{ij} = Kronecker delta

$v_t = C_u k^2/\varepsilon$ = Eddy viscosity fluid

C_u = Constant model

The equation of motion of a single spherical bubble shape with a diameter equal to d in a moving fluid has the form:

$$m_b\frac{dv_i}{dt} = F_i + F_{Ai} \quad (6)$$

Where:

m_b = $\pi d^3\rho_g/6$-weight bubbles

F_i = interfacial force equal to the drag force

F_{ai} = Acting on the bubble buoyancy (Archimedean) force:

$$F_{Ai} = -\frac{\pi d^3}{6}(\rho - \rho_g)g_i \quad (7)$$

where, g_i is acceleration due to gravity. In the practical case of mass bubbling when at random times generates huge amount of bubbles of different sizes to trace the movement of each of them in the framework of the lagrangian becomes impossible. In this case, it is advisable to use Euler's method according to which the entire set of bubbles is considered as quasi-solid "bubbly liquid" with their fields of density and speed. Following the methods outlined by Zaichik *et al*. (1994), Delnoij *et al*. (1997), Grace (1973) and Akhtar *et al*. (2007), we construct a mathematical model of a two-fluid mixing the contents of the bubbling gas-liquid reactors.

We make the following simplifying assumptions: a liquid and can send the sparging gas bubbles form two interpenetrating continuous and interactive environment with its physical and mechanical properties; bubble phase consists of the same average size of the bubbles; the interaction of the liquid and the bubble phase isothermal; crushing phenomena and merging (coalescence) bubbles are not considered; bubble phase does not generate static pressure; viscous interaction between a bubble and solid walls is ignored. Conditional density "bubbly liquid" can be represented as the product of the volume concentration of bubbles at the gas density:

$$\rho_b = g\rho_g \quad (8)$$

Unlike liquid density bubble medium is variable, so the continuity equation for it takes the form:

$$\frac{\partial\beta}{\partial t} + \frac{\partial(\beta v_i)}{\partial x_i} = 0 \quad (9)$$

To obtain the equation for momentum transfer bubble phase as a continuum need both parts of the equation of motion of a single bubble (Eq. 6) multiplied by the number concentration of bubbles, i.e., the number of bubbles contained in a unit volume sparged mixture: $\beta/(\pi d^3/6)$; replaced in Eq. 6 full Lagrangian derivative dv_i/dt Euler on the substantial derivative $\partial v_i/\partial t + v_j\partial v_i/dx_j$ and add to the right-hand side of Eq. 6 the turbulent stress tensor of the dispersed phase.

As a result of these transformations, we obtain the equation for momentum transfer bubble quasisolid environment:

$$\rho_g\frac{\partial(\beta v_i)}{\partial t} + \rho_g v_j\frac{\partial(\beta v_i)}{\partial x_j} = -\rho_g\beta f_D$$
$$(Re_b)\frac{v_i - u_i}{\tau} - \beta(\rho - \rho_g)g_i + \frac{\partial}{\partial x_j}(\beta\pi_{ij}^b) \quad (10)$$

Where:
$\tau = d^2\rho_g/18\mu$; dynamic relaxation time bubble
f_D = Resistance function:

$$f_D(Re_b) = \frac{Re_b}{24} C_D = 1 + 0.15 rE_B^{0.687} \quad (11)$$

π_{ij}^{π} turbulent stress tensor "bubbly liquid":

$$\pi_{ij}^{b} = -\rho_b \left(\frac{2}{3} k_b \delta_{ik} - v_{tb} \left(\frac{\partial_{vi}}{\partial_{xj}} + \frac{\partial_{vj}}{\partial_{xi}} \right) \right) \quad (12)$$

Turbulent kinetic energy per unit volume of the two phases of the same rely $k_b = k$ and eddy viscosity bubble phase is expressed through the turbulent viscosity: $v_{tb} = v_{tb} = C^2_t v_t$ where, C_t is constant model. Turbulent fluid characteristics kИε are defined by the equations k-ε turbulence model:

$$\frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{v_t}{\sigma k} \frac{\partial k}{\partial x_j} \right) + \frac{1}{\rho} \pi_{ij} \frac{\partial u_i}{\partial x_j} - \varepsilon \quad (13)$$

$$\frac{\partial \varepsilon}{\partial t} + u_j \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{v_t}{\sigma k} \frac{\partial \varepsilon}{\partial x_j} \right) + C_{\varepsilon 1} \frac{\varepsilon}{\rho k} \pi_{ij} \frac{\partial u_i}{\partial x_j} - C_{\varepsilon 2} \frac{\varepsilon^2}{k} \quad (14)$$

Included options v_t, v_{tb} and equation 13 and 14 constants have the following values: $C\mu = 0.09$; $C_t = 1.1$; $\sigma_k = 1$; $\sigma_c = 1.3$; $C_{c1} = 1.44$; $C_{c2} = 1.92$.

The earlier equations and closure relations constitute two-fluid mathematical model of the bubbling liquid mixing. The advantage of this is the use of two-fluid model to describe the motion of the two phases of the same type of equations that allows us to apply the same computational algorithm to solve them. Equations conditions are complemented by the surfaces bounding the reactor contents. These include: solid impermeable walls of the reactor [gamma] Γ_w, bubbler hole Γ_m and the free liquid surface Γ_s. At a solid wall all the components of the fluid velocity vanish (slip and impermeability conditions):

$$u_{i|\Gamma_w} = 0 \quad (15)$$

Normal velocity component bubble phase at a solid wall also becomes zero and the tangential components are stored (for wall bubbles feel perfectly smooth):

$$u_{n|\Gamma_w} = 0,\ u_{\tau|w} = u_{\tau-1|w} \quad (16)$$

Bores bubbler bubble phase velocity is assumed to be the ascent rate averaged bubble size:

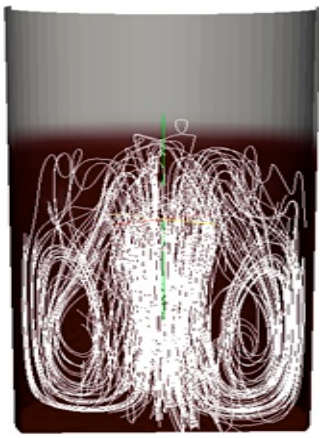

Fig. 2: Streamlines bubbled liquid

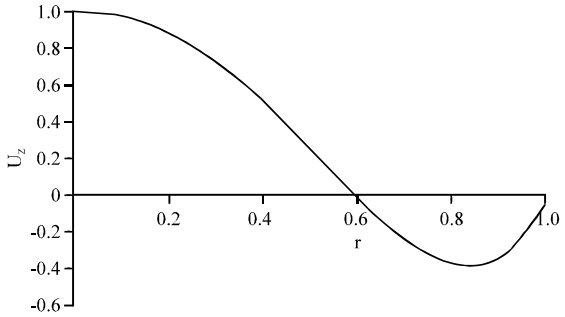

Fig. 3: Profile axial velocity component of the liquid bubbled

$$u_{n|\Gamma_{in}} v_{\pi} \quad (17)$$

Neglecting the distortion of the free liquid surface, the normal velocity components of the two phases on it will be assumed to be zero and the tangential components will assume continuing. Similarly, the boundary conditions are formulated for the other calculated values.

The foregoing mathematical model of bubble mixing numerically implemented in the package OpenCFD and OpenFOAM (2009). Finite Volume Method (FVM) were calculated velocity field and bubble liquid phase (Fig. 2).

Dignity FVM is the possibility of using unstructured grids consider spatial area of any geometrical shape as well as the opportunity to meet with a given precision the laws of conservation of mass, momentum and energy for the local and global levels (Boivin *et al*., 2000).

By polynomial approximation of the results of computational experiments found the average height of the liquid layer profile of the axial component of its velocity u_z (r) (Fig. 3):

$$\frac{u_z(x)}{U_{oc}} = Ax^4 + Bx^3 + Cx^2 + 1 \quad (18)$$

Где $u_{oc} = u_z(0)$; $x = r/R_r$; the radius of the reactor; A, B, C; coefficients depending on the $x_0 = r_0/R_r$, r_0; the radius of the interface upstream and downstream fluid flows: $u_z(r_0) = 0$.

Processing of numerical results shows that the parameters u_{ax} and r_0 in the operating range of their values can be approximately represented as a function of the Reynolds number $Re = u_m D\rho/\mu$:

$$\frac{u_{ax}}{u_m} = 1.06\lg^2 Re - 12.43Re + 37.25$$
$$x_0 = 0.66 - 0.022\lg Re \quad (19)$$

where, $u_m = Q/F_r$ is superficial velocity of the gas bubbling, Q is its consumption, F_r is reactor cross-sectional area, D is the diameter.

Volumetric flow rate of the circulating fluid flow Q_c determined by the relation:

$$Q_c 2\pi\int_0^{ro} U_z(r)rdr = \frac{\pi R_P^2 U_{oc} x_0^2\left(\begin{matrix}x_0^5 - 3x_0^4 + 2x_0^3\\ +2x_0^2 - 3x_0 + 1\end{matrix}\right)}{3x_0^2 - 5x_0 + 2} \quad (20)$$

Intensity of vertical mass transfer of the reactor can be characterized by the coefficient of the bubble mixing $k_{бп}$:

$$K = \frac{Q_c}{v} \quad (21)$$

Reciprocal of K equal to the duration of one cycle minimal bubble mixing Δt, during which mass transfer involved in circulating the entire liquid V:

$$\Delta t = \frac{1}{K} = \frac{v}{Q_c} \quad (22)$$

The results of mathematical and computer simulation of the bubbling liquid mixing agreement with experimental data and can be used for the calculation and design of industrial gas-liquid reactors.

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FINDINGS

Building mathematical model is an effective tool for studying the hydrodynamics of bubble mixing.

Numerical implementation of two-fluid model allows us to calculate the quantitative characteristics of bubbling gas-liquid mixing the contents of the reactor.

CONCLUSION

The study presents a mathematical model of two-fluid mixing the contents of gas-liquid bubble reactors. By numerical implementation of the mathematical model studied hydrodynamics recirculating flow of the liquid phase. With the help of polynomial approximation results of computational experiments an analytical expression for the profile of the axial component of the fluid velocity, based on the calculated ratio is found for the flow of recirculating flow, cycle time and energy bubbling mixing for its implementation.

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