Numerical investigation of heat and mass transfer processes in a spherical layer of viscous incompressible liquid with free boundaries

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Abstract. The results of mathematical modelling of the dynamics of a mixture of the viscous incompressible liquid and gas, which fills a spherical layer with free boundaries and contains a gas bubble within itself, are presented in this paper. Spherical symmetry is assumed, and it is considered that the dynamics of the layer is determined by thermal, diffusive and inertial factors. On the basis of constructed numerical algorithm the studies of the formation of the liquid glass layers, which contain the carbon dioxide gas within themselves, have been conducted. The impact of the external thermal regime, external pressure and the density of gas in the bubble at the initial time on the dynamics of the layer, diffusion and heat-and-mass processes inside it is investigated. The results of numerical investigation of the full and simplified thermal problem statement, without consideration of gas diffusion, are compared.

1 Introduction

The study of spherical liquid layers is a task of current interest in connection with the investigation of properties of some new materials, such as spheroplast or sensitizers for emulsion explosives [1, 2]. The mathematical and numerical modeling of the formation of spherical microballoons is held in [3-7].

The dynamics of a spherical layer with free boundaries, consisting of the viscous incompressible liquid and gas and containing a gas bubble within itself [3-5], is investigated numerically in this paper. It is assumed that the gas is insoluble in the liquid and all transfer coefficients depend on the temperature. The problem is considered in a short-term weightlessness, that involves a spherical symmetry of processes, i.e. only radial component of the velocity of the fluid is nonzero. All physical quantities depend on the distance from the origin and vary with time. The Navier-Stokes equations, as well as the equations of the heat transfer and diffusion of the gas form the basis of mathematical model, describing the processes within the liquid layer. Inside the gas bubble the pressure, density and absolute temperature of the gas satisfy the ideal gas law.

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2 Statement of the problem

Let the domain $R_1(t) < r < R_2(t)$ define a spherical layer, where $r = R_1(t)$ and $r = R_2(t)$ are its internal and external boundaries. The consequence of the original mathematical model is the following system of equations in the dimensionless form [4]:

$$\frac{dV}{dt} = \frac{1}{2} V^2 \frac{(R_2^2 + R_1^2)(R_2 + R_1)}{R_2^3 R_1^3} + \frac{1}{\text{Re}} \left[P_g S - P_{ex} S - 2\bar{Si}\sigma(T) \frac{R_2 + R_1}{R_2 R_1} \right] \frac{R_2 R_1}{R_2 - R_1} - \quad (1)$$

$$- \frac{4}{\text{Re}} \nu(T) V \frac{R_2^2 + R_2 R_1 + R_1^2}{R_2^2 R_1^2}, \quad t > 0, \quad V(0) = V_0;$$

$$\frac{dR_1}{dt} = \frac{V}{R_1^2}, \quad t > 0, \quad R_1(0) = R_{10}; \quad (2)$$

$$\frac{d\rho_g}{dt} = -\frac{3V}{R_1^3} \rho_g + \frac{3}{Pe_d R_1} D(T) \frac{\partial C}{\partial r}, \quad t > 0, \quad \rho_g(0) = \rho_{g0}; \quad (3)$$

$$\frac{\partial T}{\partial t} + \frac{V}{r^2} \frac{\partial T}{\partial r} = \frac{1}{Pe} r^{-2} \frac{\partial}{\partial r} (r^2 \chi(T) \frac{\partial T}{\partial r}), \quad t > 0, \quad T(0, r) = T_0(r); \quad (4)$$

$$\frac{\partial C}{\partial t} + \frac{V}{r^2} \frac{\partial C}{\partial r} = \frac{1}{Pe_d} r^{-2} \frac{\partial}{\partial r} (r^2 D(T) \frac{\partial C}{\partial r}) \quad t > 0, \quad C(0, r) = C_0(r). \quad (5)$$

Here V is the rate of change of the spherical layer's volume, $V = r^2 v$, where v is the radial velocity of the fluid, ρ_g is the density of the gas in the bubble, T is the temperature, C is the gas concentration in the fluid layer, P_g , P_{ex} are the pressure in gas bubble and external pressure, $\nu(T)$, $\sigma(T)$ are the kinematic viscosity and surface tension coefficients, $\chi(T)$, $D(T)$ are the thermal diffusivity and diffusion coefficients. The following dimensionless parameters arose as a result of bringing the system of equations to dimensionless form: the Reynolds number $\text{Re} = (v_* r_*) / \nu_*$, the Peclet number $Pe = (v_* r_*) / \chi_*$, the diffusive Peclet number $Pe_d = (v_* r_*) / D_*$ and also parameters $S = (r_* P_*) / (\rho_* v_* v_*)$, $Si = \sigma_* / (r_* P_*)$, $\bar{Si} = Si \cdot S$. Characteristic values are designated by index *. They are selected so that $r_* = t_* v_*$, $\chi_* = \kappa_* / (\rho c_1)$, ρ is the density of fluid (chosen as the characteristic value), $\kappa(T)$ is the thermal conductivity coefficient, c_1 is the heat capacity of the fluid.

Equations (1), (2) are consequences of the Navier-Stokes equations and kinematic conditions at the inner boundary of the fluid layer, the equation (3) determines the change in the mass of the gas bubble, the equations (4) and (5) represent the heat transfer and diffusion processes.

The statement of the problem is supplemented by the kinematic, dynamic conditions and Henry law that links the gas concentration at the boundaries with the pressure outside this area. On the internal free surface the energy balance equation and the condition of temperature continuity are also determined. On the external free boundary the heat exchange with the atmosphere is fulfilled [3].

Inside the gas bubble the ideal gas law is prescribed:

$$P_g = \tilde{R} \rho_g T_g. \quad (6)$$

Here $\tilde{R} = R \rho T_* / P_*$ is a dimensionless parameter, R is the universal gas constant [4].

3 Numerical algorithm

The numerical computations have been carried out according to the following steps:

- Solving the Cauchy problem for a system of the ordinary differential equations (1)-(3) to find the rate of change of the spherical layer's volume V , the density of the gas in the bubble ρ_g and the internal radius R_1 by the fourth-order Runge–Kutta method.
- Determination of the external radius of the layer R_2 with the help of volume conservation law $R_2^3(t) - R_1^3(t) = R_{20}^3 - R_{10}^3$.
- Transition from the domain with moving boundaries (r, t) to the fixed region (x, t) with the help of the new dimensionless spatial variable $x = (r^3 - R_1^3(t)) / (R_{20}^3 - R_{10}^3)$.
- Computation of the temperature T within the fluid layer for finite-difference analogue of equation (4) by Thomas algorithm complicated by a parameter, which is the unknown value of temperature at the internal free boundary [6].
- Computation of the gas concentration C in the fluid layer for finite-difference analogue of equation (5) by means of the ordinary Thomas algorithm [7].
- Determination of the pressure inside the gas bubble P_g through the ideal gas law (6).

4 Calculation results

Numerical studies on the formation of the liquid glass layers, which contain the carbon dioxide gas within themselves, have been conducted. The initial state of the "gas-liquid" system is characterized by the following values: $R_{10} = 0.02$ cm, $R_{20} = 0.05$ cm. A parabolic distribution of the gas concentration $C_0(x)$ at the initial moment is assumed to be given. Initial distribution of the temperature is constant: $T_0(x) = 1171.1$ K. The external atmosphere heats up from $T_{ex1} = 1171.1$ K to $T_{ex2} = 1673$ K under the law:

$$\begin{cases} T_{ex} = T_{ex1} + \frac{(T_{ex2} - T_{ex1})}{t_2 - t_1} (t - t_1), t_1 \leq t \leq t_2; \\ T_{ex} = T_{ex2}, t > t_2. \end{cases}$$

Here $t_1 = 0$ s, $t_2 = 0.3$ s.

Figure 1. Comparison of results for internal radius change at different external pressure ($\rho_{g0} = 0.92 \cdot 10^{-3}$ g/cm³).

Figure 2. Comparison of results for internal radius change at different density of the gas in the bubble at initial time ($P_{ex} = 0.1$ atm).

The comparison of results for the full and simplified thermal problem statement, when the gas diffusion is not taken into account, at different external pressure (Fig. 1) and at different density of the gas in the bubble at initial time (Fig. 2) has been carried out. It is clear that for the full problem statement a more intense extension of the liquid layer is observed and a stationary regime is achieved

later than in the case of the thermal statement. Also Fig. 1 demonstrates that the increase of external pressure P_{ex} vastly curbs the expansion of the layer while Fig. 2 shows that the increase of density of the gas in the bubble at initial time ρ_{g0} contribute to the process.

The comparison of results for the Dirichlet and Newton conditions for the temperature at the external free boundary has been performed (see Fig. 3).

Figure 3. Comparison of results for the Dirichlet and Newton boundary conditions for the temperature at the external free boundary ($\rho_{g0} = 1.86 \cdot 10^{-3} \text{ g/cm}^3$, $P_{ex} = 0.1 \text{ atm}$): a) Variation of internal radius R_1 , b) Distribution of gas concentration C at the moment $t_0 = 0.3 \text{ s}$, c) Distribution of temperature T at the moment $t_0 = 0.3 \text{ s}$.

5 Conclusions

The problem of the dynamics of a spherical layer of viscous incompressible liquid and heat and mass transfer processes inside it is being solved. The numerical algorithm for the problem solving is constructed. Numerical studies for the "liquid glass-carbon dioxide" system for different values of the density of the gas in the bubble at initial time and external pressure are conducted. The influence of external thermal regime on the dynamics of the layer, distribution of temperature and gas concentration inside it is investigated. The comparison of results for the Dirichlet and Newton boundary conditions for the temperature at external surface of the sphere is performed. Results for the full and simplified thermal problem statement (when the gas diffusion is not taken into account) are compared. It is determined that besides the external thermal regime a significant impact on the behaviour of the spherical layer is provided by diffusion of gas.

Acknowledgments. The study was supported by the Russian Ministry of Education and Science (project identifier RFMEFI61314X0011).

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