THE INFLUENCE OF GAS DIFFUSION ON THE
DYNAMICS OF A SPHERICAL LAYER OF
VISCOUS INCOMPRESSIBLE LIQUID AND HEAT
AND MASS TRANSFER IN IT

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Abstract. The formation of spherical microballoons in the case of short-
term weightlessness is investigated numerically. The algorithm of the
numerical solution of the problem is described and the results of numerical
studies of the formation of liquid glass microballoons, saturated with
carbon dioxide, are presented. The results of calculations for the problem
in the full statement (mathematical model includes the influence of inertial,
thermal and diffusive factors) and simplified statement, when the process of
gas diffusion is not taken into account, are compared.

1 Introduction

The results of numerical investigation of the dynamics of a spherical liquid layer containing
a gas bubble within itself are presented in this paper. Some quantity of the gas is dissolved
in the liquid, and it is assumed that liquid with dissolved in it gas is viscous and
incompressible [1-3]. The study of liquid layers, called microballoons, is connected with
the investigation of such materials as sensitizers of emulsion explosives and spheroplast
used in various constructions as a reinforcing additive and filler [4, 5].

The mathematical model that describes the processes within the liquid layer includes the
Navier-Stokes equations and equations of the heat transfer and gas diffusion [1-3]. Inside
the gas bubble the ideal gas law is carried out. The condition of short-term weightlessness,
under which the statement of the problem is studying, allows us to consider a spherically
symmetric process. Physical quantities depend on time and radial coordinate.

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2 Statement of the problem

Let \( R_1(t) < r < R_2(t) \) be a domain, filled with viscous incompressible liquid, where \( r = R_1(t) \) and \( r = R_2(t) \) are the internal and external free boundaries of the spherical layer. The following equations are obtained as a consequence of the initial mathematical model [2] (see also [6]):

\[
\frac{dV}{dt} = \frac{1}{2} r^2 \left( \frac{R_2^2 + R_1^2}{R_1^2} (R_2 + R_1) + \frac{1}{\text{Re}} \left( \frac{P_g S - P_{es} S - 2 \sigma \sigma(T)}{R_2 + R_1} \right) \right) \frac{R_2 R_1}{R_2 - R_1}, \quad t > 0, \quad V(0) = V_0; \tag{1}
\]

\[
\frac{dR_i}{dt} = \frac{V}{R_i^2}, \quad t > 0, \quad R_i(0) = R_{i0}; \tag{2}
\]

\[
\frac{d\rho_g}{dt} = -3V \frac{\rho_g}{R_i^2} + 3 \frac{D(T)}{\text{Pe}_{g,i}} \frac{\partial C}{\partial r}, \quad t > 0, \quad \rho_g(0) = \rho_{g0}; \tag{3}
\]

\[
\frac{\partial T}{\partial t} + \frac{V}{r^2} \frac{\partial T}{\partial r} = \frac{1}{\text{Pe}_d} r^{-2} \frac{\partial}{\partial r} \left( r^2 \chi(T) \frac{\partial T}{\partial r} \right), \quad t > 0, \quad T(0, r) = T_0(r); \tag{4}
\]

\[
\frac{\partial C}{\partial t} + \frac{V}{r^2} \frac{\partial C}{\partial r} = \frac{1}{\text{Pe}_{d,i}} r^{-2} \frac{\partial}{\partial r} \left( r^2 D(T) \frac{\partial C}{\partial r} \right), \quad t > 0, \quad C(0, r) = C_0(r). \tag{5}
\]

Here \( V \) is a rate of change of the microballoon’s volume, \( V = r^2 \nu \), \( \nu \) is the radial component of the velocity of the liquid, \( \rho_g \) is the density of gas in the bubble, \( T \) is the temperature, \( C \) is the concentration of gas in the liquid, \( P_g, P_{es} \) are the pressure in the bubble and external pressure. It is assumed, that coefficients of kinematic viscosity \( \nu(T) \), surface tension \( \sigma(T) \), thermal diffusivity \( \chi(T) \) and diffusion \( D(T) \) depend on the temperature. The equations are presented in dimensionless form with following parameters, emerged during the transition: the Reynolds number \( \text{Re} = (\nu, r_*) / \nu_\ast \), the Peclet number \( \text{Pe} = (\nu, r_*) / \chi_\ast \), the diffusive Peclet number \( \text{Pe}_d = (\nu, r_*) / D_\ast \) and dimensionless complexes \( S = (r_* P_\ast) / (\rho_\ast \nu_\ast) \), \( Si = \sigma_\ast / (r_* P_\ast) \), \( Si_* = Si \cdot S_\ast \). Characteristic values of physical quantities are designated by *. Herewith \( n_\ast = \nu_\ast / \nu_\ast \), \( \chi_\ast = \kappa_\ast / (\rho_\ast c_\ast) \), where \( \rho \) is the density of the liquid (characteristic density), \( \kappa(T) \) is the thermal conductivity coefficient, \( c_\ast \) is the heat capacity of the liquid.

Let us explain that equations (1), (2) arise out of the Navier-Stokes equations, dynamic and kinematic conditions at the free boundaries, the equation (3) represents the change in mass of the gas in the bubble, the equations (4) and (5) define the heat transfer and gas diffusion processes.

Besides kinematic condition (2) on the internal free boundary \( r = R_1(t) \) the following boundary conditions are fulfilled [1-3] (see also [7] about the formulation of boundary conditions at the interface): the condition of temperature continuity \( T = T_g \), the energy balance equation \( \frac{1}{3} \alpha_1 P_g \frac{dR_2^3}{dt} + \alpha_2 \frac{dT}{dt} = R_2^2 \frac{\partial T}{\partial r} + \alpha_3 \left( \frac{d}{dt} \left[ R_2^2 T^2 \frac{d}{dT} \left( \sigma_\ast \right) \right] + \sigma \frac{dR_2^2}{dt} \right) \), the Henry law \( C = HA(T_g) P_g^n \). On the external free boundary \( r = R_2(t) \) the kinematic
condition $\frac{dR_i}{dt} = \frac{V}{R_i^2}$, $t > 0$, $R_i(0) = R_{i0}$, the heat exchange with the atmosphere of the first type (Dirichlet boundary condition) $T = T_{ex}$ and the Henry law $C = HA(T_{ex})P_{ex}^n$ take place. Here $\alpha_1 = P_r\nu_s/(\kappa T_s)$, $\alpha_2 = c_p\nu_s/(4\pi^2\kappa_s)$, $\alpha_3 = \nu_s\sigma_s/(\kappa T_s)$, $H = AP_s^m/\rho$ are dimensionless parameters, the Biot number $Bi = \beta r_s/\kappa_s$, $T_g$, $T_{ex}$ are the temperature of the gas in the bubble and external temperature, $m$ is the mass of gas in the bubble, $c_p$ is the heat capacity of the gas at constant volume, $A$ is the coefficient in Henry law, $n$ is the index in Henry law, $\beta$ is the heat transfer coefficient.

Inside the gas bubble the ideal gas law is determined: $P_g = \bar{R}\rho g T_g$, where $\bar{R} = R\rho T_g/P_s$ is a dimensionless complex, $R$ is the universal gas constant [2].

3 Algorithm of numerical solution

The problem is solved with the help of numerical algorithm, which is described in detail in [6, 8] and includes the solution of the Cauchy problem for a system of ordinary differential equations (1)-(3) by means of the fourth-order Runge-Kutta method [9] (determination of the rate of change of the microballoon's volume $V$, the density of gas in the bubble $\rho_g$ and the internal radius $R_i$), the transition from a region with moving boundaries to the fixed area, the construction of finite-difference schemes for the equations (4) and (5), the calculation of the temperature distribution $T$ within the liquid layer by Thomas algorithm with a parameter [10] and the computation of the gas concentration $C$ in the liquid layer by an ordinary Thomas algorithm [11].

4 Results of investigation

Numerical studies on the formation of spherical microballoons of liquid glass containing carbon dioxide gas are conducted. At the initial time the internal radius of the liquid layer $R_{i0} = 0.02$ cm, the external radius $R_{e0} = 0.05$ cm, the temperature is set as a constant $T_0(x) = 1171.1$ K, the concentration of gas in the liquid $C_0(x)$ is distributed by parabolic law. The temperature of the external atmosphere is increasing from $T_{e0} = 1171.1$ K to $T_{e2} = 1673$ K under the law:

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

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

The calculation results for the system “liquid glass – carbon dioxide gas” in the case when the density of gas in the bubble at the initial time $\rho_g(0) = 0.92 \cdot 10^{-3}$ g/cm³ and the external pressure $P_{ex} = 0.3$ atm are presented onwards. When the gas diffusion is taken into account (i.e. when the problem is considered in the full statement) the liquid layer expands more intensively, and the steady state is reached much later than in the case of the problem consideration in the simplified statement (the so-called thermal approximation) (fig. 1a). Furthermore, in the case of thermal approximation at the time $t_0 = 0.45$ s the temperature
inside the entire layer is already a constant $T=1673$ K (fig. 1b), while when the problem is solving in the full statement the constant distribution of the temperature is not achieved even when $t_0=1.2$ s (fig. 2b). fig. 2a shows that the distribution of gas concentration within the liquid layer also continues to change after the heating has stopped.

Fig. 1. a) Comparison of the internal radius $R_1$ variation within time for the problem in the full statement (solid line) and the problem in the thermal approximation, without the consideration of gas diffusion (dashed line), b) Temperature distribution $T$ inside the liquid layer at the moment $t_0=0.45$ s for the thermal statement of the problem.

Fig. 2. The distribution of gas diffusion $C$ (a) and the distribution of temperature $T$ (b) inside the liquid layer at different moments of time for the problem in the full statement.

5 Conclusions

The formation of spherical shells in the case of short-term weightlessness is investigated numerically. The mathematical model of the problem and the numerical algorithm of its solving are presented. Numerical studies for the system “liquid glass - carbon dioxide gas” are conducted, and the comparison of results obtained for the problem in full and simplified statements is carried out. The calculation results show that the diffusion of gas has a significant influence on the dynamics of a spherical layer.
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