Three dimensional fluid dynamical analysis of convection in a diffusion sample

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Abstract

We developed the code of three-dimensional fluid dynamical analysis of convection in a liquid column of diffusion sample in a cylindrical container. Temperature reaches a steady value quickly than the velocity. Only slight convection appeared in the present simulation condition(short time). However, with the progress of diffusion, the convection may be considered to occur depending on the experimental condition. In future, its detailed comparison with experiments is to be presented in the case of laboratory experiments under 1g condition for liquid Ag+0.95Ag0.05Au.

1. Introduction

The occurrence of natural convection in melts often affects seriously the results of measurements of diffusion coefficients in melts. Recently, it has been possible to measure such diffusion coefficient under microgravity(μ g) much more precisely than under 1g condition on the ground. However, even though the measurement was performed under μ g, it is well known that the gravitational disturbance causes the convection which may inevitably spoil the measurements of diffusion coefficients in melts. In this study, we developed the code of three-dimensional fluid dynamical simulation to analyze the convection in cylindrical container, which is driven by the temperature and concentration gradients. The numerical simulation for the Ag + 0.95Ag0.05Au diffusion couple was performed and the effect of convection for these causes is evaluated. The experimental study for this diffusion couple is in progress by the present diffusion project in NASDA.

2. Analytical methods

The schematic picture of the container is shown in Fig.1(a). Thermo-couples are installed at the points, which are indicated by broken lines in this figure. They enable us to get the information on temperature profile along the container. We adopted the analytical system of sample shown in Fig.1(b). No slip condition was assumed for the boundary between the sample and the container. The temperature distribution of the system was given based on the experimental measurements. Ag + 0.95Ag0.05Au melts were non-compressible Newtonian liquid, and Boussinesq approximation was adopted for the equation of motion. That is the effect of the change of the density due to the change of the fluid temperature and Au concentration is considered only in the voyancy term in the equation of motion. Followings are the equations employed for the analysis in the cylindrical coordinate,(R,φ,Z).

(i)Melt of sample

Continuity of particle number

$$divV = 0. \tag{1}$$

Energy

$$\frac{\partial\theta}{\partial\tau} + div(\theta V) = \frac{1}{\Pr}\Delta\theta . \tag{2}$$

Transportation of mass

$$\frac{\partial C}{\partial\tau} + div(CV) = \frac{1}{Sc}\Delta C . \tag{3}$$

Motion

$$\frac{\partial U}{\partial\tau} + div(UV) = -\frac{\partial P}{\partial R} + \Delta U + \frac{V^2}{R} - \frac{2}{R^2}\frac{\partial V}{\partial\varphi} . \tag{4}$$

$$\frac{\partial V}{\partial\tau} + div(VV) = -\frac{1}{R}\frac{\partial P}{\partial\varphi} + \Delta V - \frac{UV}{R} - \frac{V}{R^2} + \frac{2}{R^2}\frac{\partial U}{\partial\varphi} . \tag{5}$$

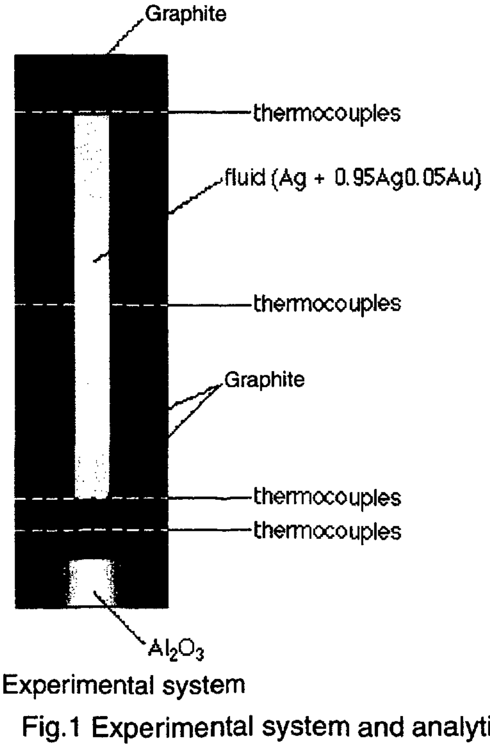
$$\frac{\partial W}{\partial\tau} + div(WV) = -\frac{\partial P}{\partial Z} + \Delta W + \frac{Ra^T}{\Pr}\theta - \frac{Ra^C}{Sc}C . \tag{6}$$

(ii)Container

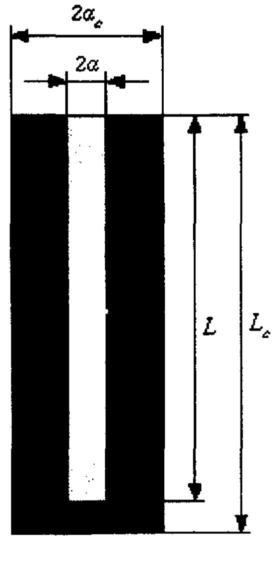
Energy

$$\frac{\partial\theta}{\partial\tau} = \frac{k}{\Pr}\Delta\theta . \tag{7}$$

In these equations U, V, W, P, θ, C, τ are respectively non-dimensional velocity of radial direction, that of angle direction, that of axis direction, pressure, temperature, concentration of Au, and time. The coordinate, velocity, time, temperature, concentration and pressure are respectively written in non-dimensional forms by the factors, a, v/a, a^2/v, ΔT, ΔC, $\rho v^2/a^2$ respectively where a, v, ρ, ΔT, ΔC are the radius of container, kinematic viscosity, density, temperature difference and concentration difference respectively.



(a) Experimental system



(b) Analytical system

Fig.1 Experimental system and analytical system of this study

Non-dimensional parameters in our analysis are Prandtl number, Schmidt number, Rayleigh number of temperature, Rayleigh number of concentration, the thermal conductivity ratio between container and sample, aspect ratio of sample and that of container and the radius ratio of container and sample. In the order described above, they are defined as below:

$$\Pr \equiv \frac{\nu}{\kappa},\quad Sc \equiv \frac{\nu}{D},\quad Ra^T \equiv \frac{\beta g \Delta T L^3}{\kappa \nu},\quad Ra^C \equiv \frac{\gamma g \Delta C L^3}{D \nu},\quad k \equiv \frac{\kappa_c}{\kappa}, \tag{8a}$$

$$asp1 \equiv \frac{L}{a},\quad asp2 \equiv \frac{L_c}{a},\quad A \equiv \frac{a_c}{a}. \tag{8b}$$

In these definitions, κ, κ_c, D, β, γ, g is the thermal conductivity of solution, that of a container, diffusion coefficient of Au in Ag, temperature coefficient of volume expansion, concentration coefficient of volume and gravitational acceleration, respectively.

The equations (1) ~ (8) were solved by a control volume method and SIMPLE algorism based method in the analysis. Though the differentiation of these equations was performed by the control volume method, we developed the algorism, Power Serious Scheme for the approximation of convection and diffusion terms. Here, the geometrical factors are taken into considerations in the control volume method in cylinder coordinate system. Conventional method was adapted for the time integral. The calculation of flow field was performed by the mixed algorism of SIMPLE algorism and conventional method.

3. Results and discussions

We observed the maximum values of velocity, temperature and concentration with the change of time at (R, φ, Z) ~ (1/2, 0, asp1/2). They are shown in Fig.2. In our calculated conditions, Prandtl number was extremely small and Schmidt number was 2000 times larger than Prandtl number. Therefore relaxation time of mass diffusion is longer than that of thermal diffusion. As is shown in Fig.2, the temperature field had achieved the stable condition quickly. On the other hand, the concentration slightly changes in the calculation time. The temperature difference between container surfaces actually caused the convection. There exists the obvious difference of the relaxation times between the velocity change and the temperature change, and it was found that the convection of fluid did not affect the temperature distributions. The Peclet number is the ratio of convection to diffusion for the transportation phenomena. If the absolute value of Peclet number is large, the transportation is governed by the convection. On the other hand if it is close to 0, the system is characterized by the diffusion.

The temperature field, concentration distribution, and flow pattern obtained by our simulation at τ = 0.5 are shown in Fig.3.

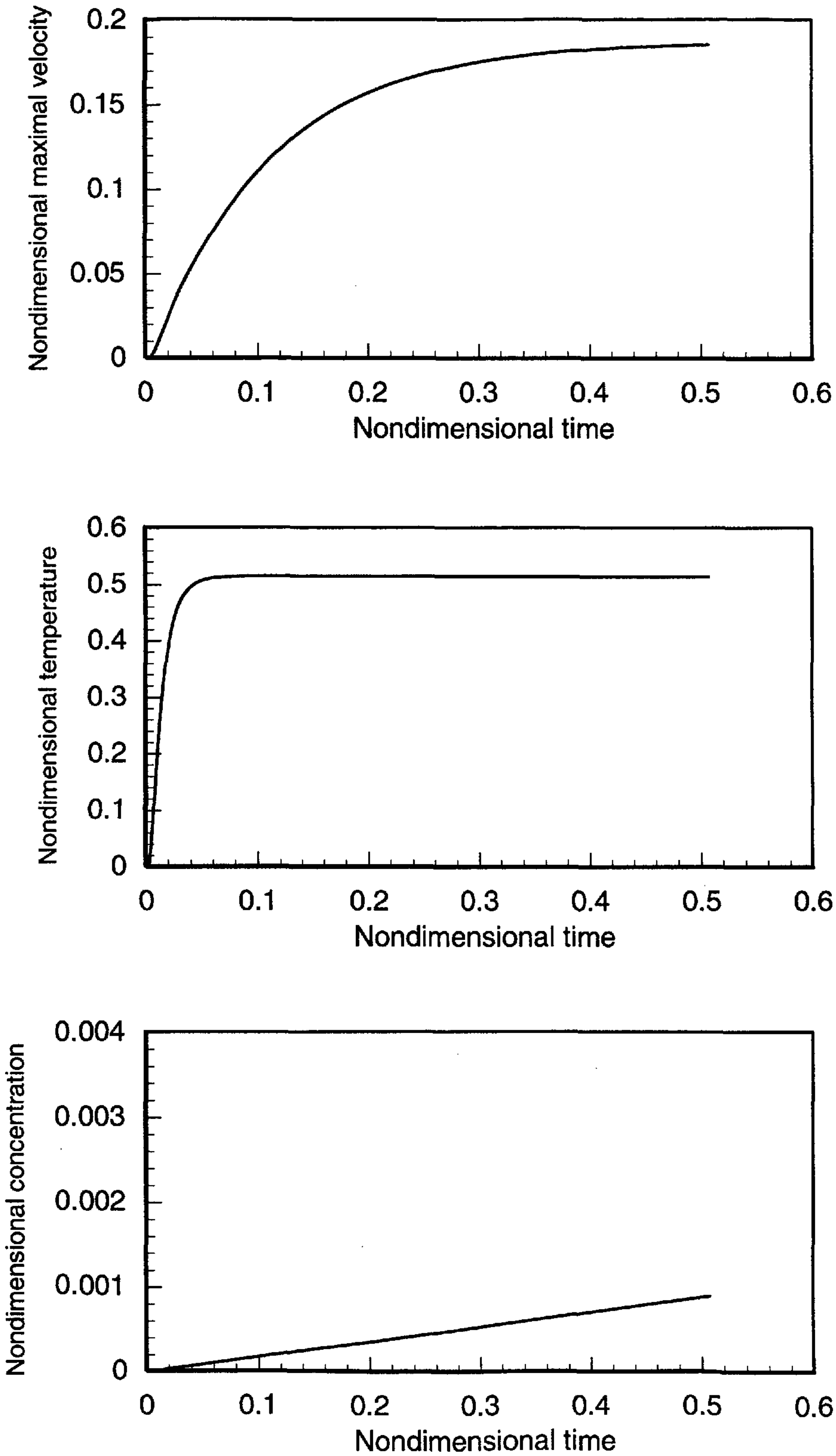


Fig.2 Nondimensional maximum velocity, temperature and concentration

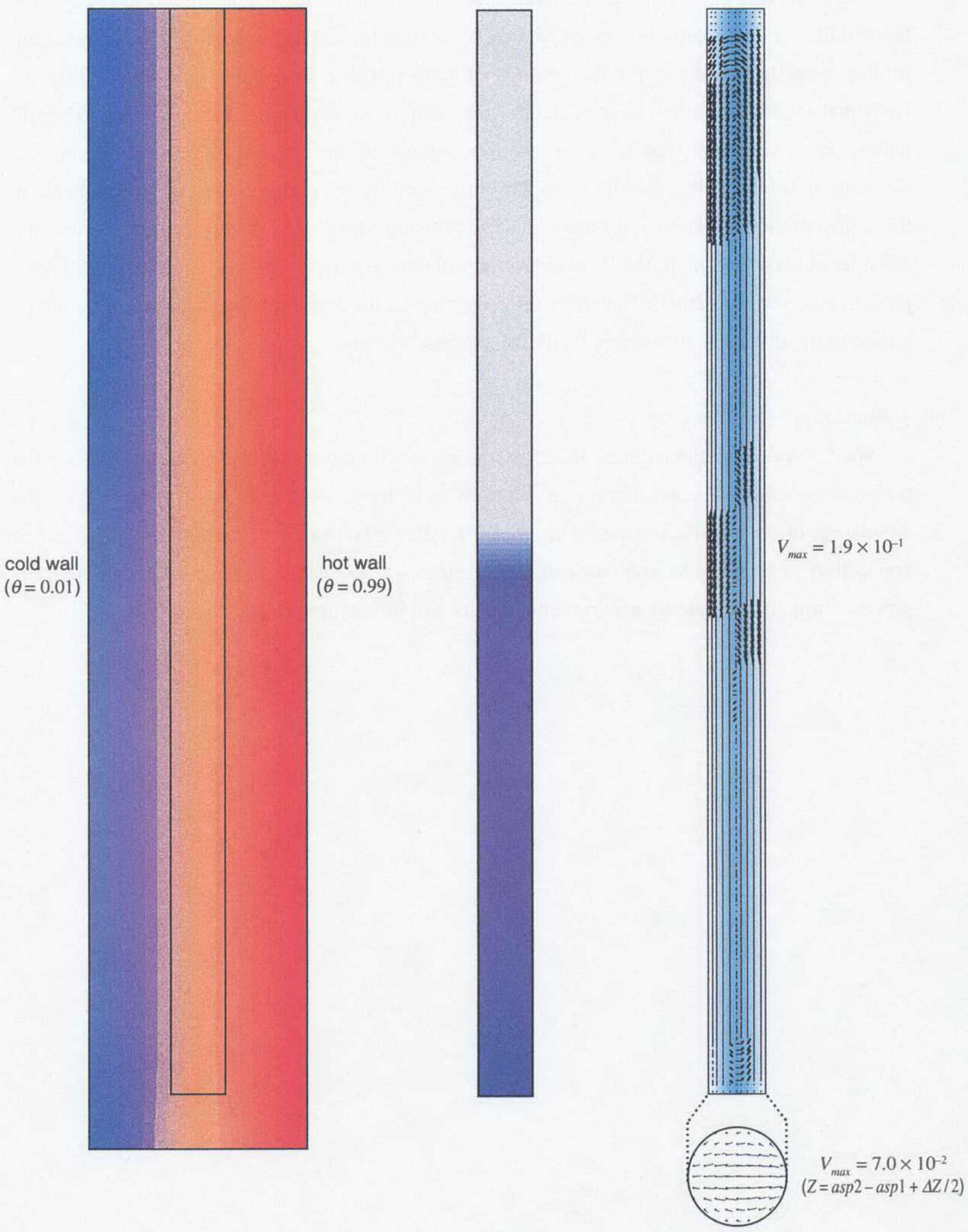


Fig. 3 Temperature distribution (right), concentration distribution (middle) and flow pattern (left) calculated in this simulation ($\varphi = \pi/2 - \Delta\varphi/2$, $\tau = 0.5$).

The temperature distribution of container is also shown in Fig.3(right). It was found that the temperature of the system was governed only by conduction not by convection. The temperature profile seemed to be linear, but the gradient of temperature in the sample was largely different from that of container. It was attributable to the difference of thermal conductivities. The roll pattern of convection was observed in the bottom of the system. To the contrary, the concentration field (Fig.3(middle)) was not influenced by the convection at $\tau = 0.5$, because the concentration gradient is limited in the extremely small area in the sample. If the area considered becomes small, the Peclet number, which relates to the convection and the diffusion phenomena, becomes small. The effect of convection on the concentration distribution should be larger, as the diffusion are enlarged with the progress of time.

4. Summary

We developed the three dimensional CFD(computer fluid dynamical) software to analyze the temperature and the concentration profiles in cylindrical container. It was applied to the simulation of the diffusion experiment of Ag + 0.95Ag0.05Au in 1g condition. The effect of convection on temperature and concentration profiles was evaluated based on this simulation. Its precise comparison with the experimental results will be performed later in this project.