Gravity level influence on the onset and nonlinear regimes of a binary mixture convection in rectangular cavity heated from below

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Abstract. In this paper we present the results of numerical simulation of nonlinear convection regimes of a NaCl aqueous solution heated from below. The calculations are carried out for square and horizontally elongated rectangular cavities, both in the approximation of a constant thermal diffusion coefficient and in case of taking into account its temperature dependence. Other transport coefficients are considered as constant. We observe the local and integral characteristics of the realized flows at constant and variable thermal diffusion coefficients in the conditions of the Earth and reduced gravity.

1. Introduction

Convective phenomena in multicomponent liquids often accompany many technological and natural processes or cause their onset [1-5]. If there is a temperature gradient in multicomponent mixtures, it is necessary to take into account the effect of thermal diffusion. This requires knowing the values of the transfer coefficients. There are many works devoted to the determination of the transfer coefficients in specific multicomponent mixtures under various fixed external conditions (temperature, pressure) and different ratios of the mass fractions of the mixture components [6-8]. In a row of works, the dependences of the diffusion and thermal diffusion (Soret) coefficients on the temperature and concentration of the mixture components were found [6, 9-14]. The analysis of the literature shows that binary organic liquid mixtures can be divided into three groups by the nature of the Soret coefficient dependence on temperature and concentration. The first group demonstrates a nonmonotonic concentration dependence of the Soret coefficient, which persists with increasing temperature [13, 14]. The second group is characterized by diminishing of the modulus of the Soret coefficient with increasing temperature, the dependences are also nonmonotonic, and the concentration value at which the sign of the Soret coefficient changes does not depend on temperature [6]. The mixtures of the third group have a temperature invariant point, where the Soret coefficient, which is not equal to zero, does not depend on temperature [14, 15].

In this work, we study the onset and nonlinear regimes of an aqueous NaCl solution convection in square and horizontal rectangular cavities heated from below. In contrast to the work [16], the simulation
is carried out under taking into account the polynomial dependence of the thermal diffusion coefficient on temperature [9,11]. Other transport coefficients are considered constant.

2. Problem statement and solution method

We consider the thermal solutal convection of an aqueous NaCl solution in square and horizontally elongated rectangular cavities with heating from below. The density of the mixture is considered to be linearly dependent on the temperature 

\[ \rho = \rho_0 (1 - \beta_T (T - T_0) - \beta_C (C - C_0)) \, \text{kg/m}^3. \]

Here \( \beta_T \) and \( \beta_C \) are the thermal and solutal expansion coefficients, respectively, and \( \rho_0, C_0 = 0.0285 \, \text{(2.85\%)} \) and \( T_0 = 298 \, \text{K} \) are the mean values of density, solutal concentration and temperature of mixture. We assume that the effects of barodiffusion and diffusion thermal conductivity can be neglected, the thermal diffusion coefficient \( D_T(T) \) depends on temperature, and the coefficients of viscosity \( \nu \), molecular diffusion \( D \), and thermal diffusivity \( \chi \) are constant.

With these assumptions in mind, the dimensional unsteady equations of thermal solutal convection of a binary mixture in the framework of Boussinesq approximation are written in the form:

\[
\begin{align*}
\partial_t \mathbf{V} + (\mathbf{V} \cdot \nabla) \mathbf{V} &= -\rho \mathbf{C} \mathbf{V} \mathbf{p} + \nu \nabla^2 \mathbf{V} + \left[1 - \beta_T (T - T_0) - \beta_C (C - C_0)\right] g, \\
\partial_t T + (\mathbf{V} \cdot \nabla) T &= g \Delta T, \\
\partial_t C + (\mathbf{V} \cdot \nabla) C &= D \Delta C + D_T(T) \Delta T.
\end{align*}
\] (1)

Here \( t \) is the time, \( \mathbf{V} \) is the velocity vector, \( p \) is the pressure, \( g \) is the gravity acceleration. We consider the thermal diffusion coefficient as temperature dependent according to the following law [9,11]:

\[ D_T(T) = 10^{-10} (1.463 - 0.00885T + 0.000131T^2) \, \text{m}^2/\text{s} \, \text{K} \] (2)

The boundaries of the cavity are rigid and impermeable. The lateral borders are thermally insulated, the horizontal ones are maintained at constant different temperatures: \( T_L = 303 \, \text{K} \) at the lower border and \( T_U = 293 \, \text{K} \) at the upper one. Boundary conditions for concentration is the zero diffusion flux of the substance. At the initial moment of time, the concentration of the solute in the cavity is assumed to be homogeneous, and the temperature is assumed to be linearly dependent on the vertical coordinate. Thermal and physical properties of an aqueous NaCl solution are presented in Table 1.

### Table 1. Thermal and physical properties of the aqueous NaCl (2.85\%) solution

| \( \rho_0 \), kg/m\(^3\) | \( \nu \), m\(^2\)/s | \( \chi \), m\(^2\)/s | \( \beta_T \), K\(^{-1}\) | \( \beta_C \) | \( D \), m\(^2\)/s |
|--------------------------|----------------|----------------|----------------|--------|----------------|
| 1050.0                   | 1.03 \times 10^{-6} | 1.47 \times 10^{-7} | 1.9 \times 10^{-4} | -0.755 | 1.512 \times 10^{-9} |

Convection modeling was performed for two values of gravity acceleration \( g : g = g_0 \) that corresponds to Earth conditions and \( g = g_0 \times 10^{-4} \), that corresponds to the reduced gravity conditions.

The calculations are carried out using the ANSYS Fluent software package for a square cavity with 0.01 m side and a cell size of a square computational mesh equal to 5 \times 10^{-3} m, as well as for a rectangular cavity with a length \( l = 0.05 \) m and a height \( h = 0.01 \) m and a cell size of a square computational mesh equal to 1 \times 10^{-4} m, the time step is 1 s. The selected sizes of the computational grid are sufficient to resolve the viscous boundary layer. The equations were discretized using the second order of approximation in time and the third one in space.
3. Numerical results

In the considered temperature range between the upper and lower boundaries, the thermal diffusion coefficient, according to the work (2), is negative in the entire volume of the cavity. In the case of negative thermal diffusion coefficient value, the heavy component of the mixture accumulates in the warmer part of the cavity, while the light component diffuses into the colder part of the cavity. This means that in the case of heating from below examined in this work, thermal diffusion leads to the formation of a stable density stratification. In contrast, the dependence of the density on temperature when heated from below leads to the formation of an unstable density stratification. As it is known [17], in this case, at a certain value of the Rayleigh number, the mechanical equilibrium of the mixture becomes unstable and convection is always excited in a monotonic manner. Subsequently, we will make a comparison with the case of a constant value

\[ T_D = -1.58 \times 10^{-12} \text{ m}^2/\text{s K} \]

that corresponds to the average temperature value

\[ T_o = 298 \text{ K} \].

4. Square Cavity

4.1. Earth Gravity

First, we discuss the case of Earth gravity. In this case, the conditions considered in this work correspond to the Rayleigh number

\[ Ra = g \beta \Delta T h^3 / (\nu \gamma) \approx 1.23 \times 10^5 \]

which significantly exceeds the critical value of the Rayleigh number

\[ Ra_c = 2.98 \times 10^5 \] at a constant thermal diffusion coefficient.

Figure 1 shows the comparison of the temporal evolution of the maximum value of the stream function in the cavity and the difference in NaCl concentrations between the centers of the upper and lower boundaries cavity, obtained at a constant value of the thermal diffusion coefficient (dashed lines) and under taking into account dependence (2) (solid lines). As can be seen, in the considered temperature range, taking into account the dependence \( T_D(T) \) does not qualitatively affect the onset of instability, the formation of the flow, and its intensity. At the initial stage, which lasts about 20 s, the intensity of the convective motion is very low (the maximum value of the stream function in the cavity is close to zero, Fig. 1a); this motion practically does not influence on the separation of the mixture, which is close to that observed in a purely diffusion regime. At \( t \approx 20 \text{ s} \), a sharp increase in the movement intensity occurs, which is also reflected in the nature of the separation of the mixture (a change in the nature of the increase \( \Delta C(t) \) with time is observed, it becomes much sharper). After this, dependences \( \Psi(t) \) and \( \Delta C(t) \) take on an oscillatory form. These oscillations become stationary over time. When we take into account the dependence \( D_T(T) \), the concentration gradient inside the cavity caused by the effect of thermal diffusion is less than at a constant \( D_T \), therefore the separation of the mixture is less (Fig. 1b). The structure of the flow and the distribution of the NaCl concentration in the cavity (the instantaneous fields at time \( t = 100 \text{ s} \) are shown in Fig. 1a, b) do not change when the dependence of the thermal diffusion coefficient on temperature is taken into account in comparison with the case of a constant \( D_T \). A four-vortex flow with reconnection of vortices is established in the cavity. Due to the high flow intensity the distribution of the NaCl concentration is almost homogeneous in the central part of the cavity, and varies greatly near the horizontal boundaries (Fig. 1c).
Figure 1. Temporal evolution of the maximum value of the stream function in a square cavity (a), the temporal evolution of the concentration difference between the centers of the upper and lower boundaries (b), the concentration profiles at time moment $t=100$ s (c) at Earth gravity $g = g_0 \cdot 10^{-1}$

At $g = g_0 \cdot 10^{-1}$ a non-convective period, during which the maximum value of the stream function in a square cavity is practically equal to zero, and the separation of the mixture occurs in a diffusion manner, is approximately 200 s (Fig. 2a). After the onset of instability, a stationary regime is observed. With a decrease in gravity, the flow intensity diminishes, and the maximum separation of the mixture components rises (Figures 1-2). It can be seen from Figure 2a, that the flow intensity changes little when the dependence $D_T(T)$ is taken into account, however, the maximum separation of the mixture in this case decreases in comparison with the case of a constant thermal diffusion coefficient due to the smaller value of the concentration gradient (Fig. 2b, c).

The steady flow under the conditions $g = g_0 \cdot 10^{-1}$ has the form of a diagonally elongated vortex (Fig. 2a). The NaCl concentration is homogeneous in the central part of the cavity and changes significantly near the boundaries due to the high flow intensity (Fig. 2b, c). Taking into account the temperature dependence of the thermal diffusion coefficient has little effect on the flow structure or the NaCl concentration distribution.

Figure 2. Temporal evolution of the maximum value of the stream function in a square cavity (a), the temporal evolution of the concentration difference between the centers of the upper and lower boundaries (b), the concentration profiles at time moment $t=1000$ s (c) at $g = g_0 \cdot 10^{-1}$
5. Rectangular Cavity

5.1. Earth Gravity

We study the case when the gravity acceleration is equal to that of the Earth \( g = g_0 \). In the case of a rectangular cavity, as in the case of a square cavity, with the Earth gravity, the value of the Rayleigh number exceeds the threshold value, which is obtained in the case of a constant thermal diffusion coefficient. In the entire volume of the cavity, the coefficient of thermal diffusion \( D_T(T) \), expressed by formula (2), takes negative values when the temperature difference between the horizontal boundaries is equal to 10 degrees. Figure 3a,b demonstrates the temporal evolution of the maximum value of the stream function in the cavity and the difference in concentration between the centers of the upper and lower boundaries. During the initial stage, when convection is practically absent, purely diffusional separation of the mixture occurs, the flow intensity begins to increase noticeably at \( t \) approximately equal to 10 s for a given gravity acceleration (Fig.3a), the separation of the mixture also sharply intensifies. We observed the irregular oscillations after the convection onset. If we compare the plots for the cases of constant and variable thermal diffusion coefficients, we can see that the qualitative effect of taking into account \( D_T(T) \) on the flow structure and the distribution of NaCl concentration is rather small, however, since with a polynomial dependence of the thermal diffusion coefficient on temperature, the flow intensity is somewhat higher, then at reaching the regime of irregular oscillations in this case, the mixture is separated weaker.

The flow in the cavity, as well as the distribution of the NaCl concentration, are approximately the same for the cases when the thermal diffusion coefficient is constant and when it depends on temperature; therefore, the graphs for these cases have a similar form, but since when we take into account the dependence \( D_T(T) \), the flow becomes somewhat more intense, the maximum separation of the mixture becomes less than in the case of a constant thermal diffusion coefficient. The structure of the resulting flow is multi-vortex (Fig. 3a). The solute is distributed fairly homogeneously in the central part of the cavity due to the high flow intensity, but there is a sharp change in this distribution near the horizontal boundaries. (Fig. 3b, c). The time for which the contours in Figure 3 and concentration profiles in Figure 3c are given, corresponds to the moment when irregular oscillations take place in the cavity.

![Figure 3](image-url)

*Figure 3.* Temporal evolution of the maximum value of the stream function in a rectangular cavity (a), the temporal evolution of the concentration difference between the centers of the upper and lower boundaries (b), concentration profiles at time moment \( t = 200 \) s (c) at Earth gravity
Case of $g = g_o \cdot 10^{-1}$

When $g = g_o \cdot 10^{-1}$, convection emerges at a time value of approximately 100 seconds (Fig. 4a). Until this time, there is no convection, the separation occurs in a diffusion manner. The maximum value of the concentration difference for a given gravity level is slightly less than for the earthly one, and the flow itself is weaker (Fig. 3, Fig. 4). Fig. 4 shows that the behavior of the liquid at constant and polynomial temperature-dependent thermal diffusion coefficients is similar, but at $D_T(T)$ the maximum difference in solute concentrations is less (Fig. 4b).

![Figure 4](image.png)

**Figure 4.** Temporal evolution of the maximum value of the stream function in a rectangular cavity (a), the temporal evolution of the concentration difference between the centers of the upper and lower boundaries (b), concentration profiles at time moment $t = 400$ s (c) at $g = g_o \cdot 10^{-1}$

The structure of a stationary flow under the condition $g = g_o \cdot 10^{-1}$ is multi-vortex (Fig. 4a). Isolines of NaCl concentration (Fig. 4b) and the concentration profile along a line connecting the centers of the upper and lower boundaries at the same time (Fig. 4c) show its homogeneity in the central part of the cavity and the greatest change in this value near the boundaries due to the flow intensity. The effect of $D_T(T)$ on the flow intensity and the location of the NaCl in the cavity is not very large.

6. Conclusion

This paper presents the results of numerical modeling of the onset and nonlinear regimes of an aqueous NaCl solution convection in square and horizontally elongated rectangular cavities. The case of heating from below and a temperature difference of 10 K between the horizontal boundaries is considered. The calculations are performed under taking into account the dependence of the thermal diffusion coefficient on temperature according to the polynomial law; a comparison with the case of a constant thermal diffusion coefficient was performed. The onset and development of convective regimes under conditions of the Earth and reduced gravity is investigated.

It is found that a four-vortex flow with reconnection of vortices is established in a square cavity under the Earth gravity, the flow characteristics fluctuate in a regular manner. At a reduced gravity, a stationary single-vortex flow occurs.

For a rectangular cavity in both cases of the considered values of the gravity force, a multi-vortex convective flow arises in the cavity. In the case of the Earth gravity, the intensity of the arising flow is
high, irregular oscillations in the flow characteristics are observed. At a reduced gravity, a stationary multi-vortex flow is formed.

The intensity of the emerging flows is sufficient for strong mixing of the liquid in the central part of the cavity; a significant gradient of the solute concentration is observed near the boundaries. The polynomial thermal diffusion coefficient dependence on temperature decreases the maximum separation of the mixture due to the lower value of the concentration gradient compared to the case of a constant thermal diffusion coefficient.

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