

Vibrational convection of ternary mixtures in rectangular cavities in zero gravity conditions

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Abstract. The present paper is devoted to the investigation of the onset and nonlinear regimes of the vibrational convection of ternary mixtures in rectangular cavities with rigid boundaries in zero gravity conditions. We consider translational linearly polarized vibrations of finite amplitude and frequency. The axis of vibrations is perpendicular to the temperature gradient. The problem is solved by finite difference method in the framework of 2D unsteady approach. Numerical data on the time evolution of instantaneous and average fields and characteristics of convective flows and concentration fields are obtained for different vibration intensities and aspect ratios.

1. Introduction

In [1] the Soret induced convection of the binary mixtures in a horizontal layer subjected to the vertical temperature gradient and longitudinal high-frequency vibration was investigated. It was found that the vibrations exert destabilizing effect at positive values of the separation ratio and stabilizing effect at negative separation ratios. The influence of high-frequency vibrations of different orientations on the Soret-induced convection of the methane-butane mixture in square cavity in low gravity conditions was studied in [2]. As in [1], the study was performed in the framework of the averaged approach. In [3] the effect of vibrations along the axis perpendicular to the temperature gradient on three-dimensional regimes of the Soret-induced convection of water-isopropanol mixture in cubic cavity in low gravity conditions was investigated. The onset and nonlinear regimes of the Soret-induced convection of ternary mixtures in square cavity at different levels of gravity was studied in [4, 5]. The effect of longitudinal high-frequency vibrations on the onset of Soret-induced convection of ternary mixtures in horizontal layers subjected to the vertical temperature gradient was investigated in [6].

The effect of vibrations is used to control the flows in the melt, which in general is a multicomponent system, during crystal growth [7, 8]. The present work is devoted to the investigation of the onset and nonlinear regimes of the vibrational convection of ternary mixtures in rectangular cavities with rigid boundaries subjected to vertical temperature gradient in zero gravity conditions. The interest to this problem is associated with the experiments on transport phenomena in ternary mixtures conducted on board of the International Space Station.



2. Formulation of the problem

Let us consider vibrational convection of multicomponent mixture, consisting of n components, in a rectangular cavity with rigid impermeable boundaries in zero gravity conditions. We introduce Cartesian coordinate system as follows: x -axis is parallel to the long sides of the rectangle, y -axis is parallel to the short sides, the origin of coordinate system is located in lower left corner. The cavity performs longitudinal (parallel to x -axis) harmonic vibrations with amplitude a and angular frequency ω . The short sides of the rectangle are thermally insulated, at the long sides the constant different temperatures are maintained.

Unsteady equations of thermosolutal convection of ternary mixture subjected to the translational vibrations of finite frequency and amplitude in zero gravity conditions, in the Boussinesq approximation in the reference system of oscillating cavity are [9]:

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \nabla \vec{u} = -\nabla p + \nabla^2 \vec{u} + \frac{\text{Ra}_v}{\text{Pr}} \cos(\Omega t) (T + \mathbf{I} \cdot \mathbf{C}) \vec{j}, \quad (1)$$

$$\frac{\partial \mathbf{C}}{\partial t} + \vec{u} \nabla \mathbf{C} = \frac{1}{\text{SC}} (\nabla^2 \mathbf{C} - \boldsymbol{\epsilon} \nabla^2 T), \quad (2)$$

$$\frac{\partial T}{\partial t} + \vec{u} \nabla T = \frac{1}{\text{Pr}} \nabla^2 T, \quad (3)$$

$$\nabla \cdot \vec{u} = 0. \quad (4)$$

Here $\vec{u}$ is the velocity vector, p is the pressure, $\mathbf{C} = (C_1, \dots, C_{n-1})^T$ is the transpose vector of concentrations, $\mathbf{I} = (1, \dots, 1)$ is the unit vector and $\vec{j}$ is the unit vector in the direction of vibrations.

The equations are written in the dimensionless form using the following quantities as the scales: the height of the cavity H for the length, ν/H for the velocity, H^2/ν for the time, $\rho_0 \nu/H$ for the pressure, temperature difference between the lower and upper boundaries ΔT for the temperature, and $\beta_T \Delta T \mathbf{B}^{-1}$ for the vector of concentrations. Here ν is the viscosity of the mixture, $\mathbf{B}$ is the diagonal matrix of the coefficients of concentration dependence on the density and β_T is the thermal expansion coefficient. Equations (1)-(4) contain the following dimensionless parameters: $\text{Pr} = \nu/\chi$ is the Prandtl number, χ is the thermal diffusivity, $\boldsymbol{\epsilon} = -\beta_T^{-1} \mathbf{B} \mathbf{D}^{-1} \mathbf{D}_T$ is the vector, consisting of $(n-1)$ separation ratios, characterizing the thermal diffusion separation in mixture for each solutes. $\text{SC} = \nu^{-1} \mathbf{B} \mathbf{D} \mathbf{B}^{-1}$ is the matrix of parameters of the dimension $(n-1) \times (n-1)$, where $\mathbf{D}$ – is the matrix of the molecular diffusion coefficients, $\mathbf{D}_T$ is the vector of thermal diffusion coefficients, $\text{Ra}_v = a \omega^2 \beta_T \Delta T H^3 / (\nu \chi)$ is the vibrational analogue of the Rayleigh number, $\Omega = \omega H^2 / \nu$ is the dimensionless frequency.

The boundary conditions are:

$$x=0, L: \vec{u}=0, \frac{\partial T}{\partial x} = \frac{\partial \mathbf{C}}{\partial x} = 0, \quad (5)$$

$$y=0, H: \vec{u}=0, T = \pm 1/2, \frac{\partial}{\partial y} (C - \boldsymbol{\epsilon} T) = 0. \quad (6)$$

3. Numerical method

In the case of binary mixture the matrix of molecular diffusion coefficients is reduced to a single number. For ternary mixtures the matrix $\mathbf{D}$ has a dimension (2×2) , that leads to the appearance of additional terms in the equation for component concentration responsible for cross-diffusion, and

complicates the calculations. Reduction of the molecular diffusion coefficient matrix to the diagonal form allows to eliminate the cross diffusion terms in the equations, decreasing the number of governing parameters of the problem, and the equations for the concentrations of the components become independent of each other. Such transformation applied to the problem (1)-(6) in dimensionless form can be written as [4, 10]:

$$\mathbf{C} = \mathbf{BV}(\mathbf{BQ})^{-1}\hat{\mathbf{C}}, \quad \boldsymbol{\varepsilon} = \mathbf{BV}(\mathbf{BQ})^{-1}\hat{\boldsymbol{\varepsilon}},$$

where $\mathbf{V}$ is the matrix whose columns are the eigenvectors $\mathbf{v}_i = (v_{i1}, \dots, v_{in-1})^T$ of the matrix $\mathbf{D}$;

$$\mathbf{Q} = \text{diag}\{q_1, \dots, q_{n-1}\}, \quad q_i = \beta_i^{-1} \sum_{j=1}^{n-1} \beta_j v_{ij}.$$

The problem (1)-(6), written in terms of stream function and vorticity, was solved numerically by finite difference method. The spatial derivatives were approximated by central differences. Unsteady equations were solved using explicit finite difference scheme with a constant time step $h^2/8$, where h is constant spatial step. The Poisson equation for the stream function was solved by successive over-relaxation method. The vorticity values at the boundaries of the cavity were calculated using the Thom formula [11].

The calculations were carried out for rectangular cavities with aspect ratios 1:1 and 5:1, on the grids with the numbers of nodes 41×41 and 201×41 respectively. The initial conditions corresponded to small perturbations of stream function and uniform vertical gradients of temperature and solutes concentrations:

$$\psi = 10^{-8} \sin(2\pi x) \sin(\pi y), \quad T = 1/2 - y \quad \text{and} \quad \mathbf{C} = \boldsymbol{\varepsilon}(1/2 - y).$$

The calculations were carried out for two ternary mixtures with different combinations of the separation ratios of solutes: for Mixture 1 both solutes had positive separation ratios $\varepsilon_1 = 0.3$, $\varepsilon_2 = 0.1$, and for Mixture 2 – negative separation ratios $\varepsilon_1 = -0.3$, $\varepsilon_2 = -0.1$. The molecules of solutes with positive separation ratios concentrate in the warm area of cavity, and the molecules of solutes with negative separation ratios – in cold area. The values of the Prandtl number and Schmidt numbers were taken the same for both mixtures: $\text{Pr} = 10$, $\text{Sc}_1 = 100$, $\text{Sc}_2 = 1000$. The chosen parameters are typical for the liquid mixtures. The value of the dimensionless frequency of vibrations was also fixed $\Omega = 445$. For the cavity of 1 cm height filled by ternary liquid mixture with the viscosity $\nu \sim 10^{-6} \text{ m}^2/\text{s}$ this value corresponds to the dimensional vibration frequency approximately equal to 1 Hz. Vibrational Rayleigh number was varied in the range $\text{Ra}_v = 10^3 \div 2 \cdot 10^5$.

4. Results

Figures 1-2 show the numerical data on the time evolution of the average stream function and the difference in the solute concentration values at the centers of the upper and lower cavity boundaries for Mixtures 1 and 2 for the cavity with aspect ratio 5:1. The average values were obtained by averaging of the instantaneous values over the period of vibrations.

We consider the physical situation in which the static gravity field is absent and the initial state corresponds to the established linear distribution of temperature and solute concentrations. In the case of infinite horizontal layer, in such situation at low values of the vibrational Rayleigh number the average flow is absent, convection arises in a threshold manner at a certain critical value of Ra_v . In the case of rectangular cavity with aspect ratio 1:5, as follows from our calculations (Figs. 1, 2) at low intensities of vibrations (low values of vibrational Rayleigh number) in both mixtures weak average flow is observed and the differences in the component concentrations values at the centers of upper and lower boundaries are not very different from the initial values, corresponding to the established linear distributions in the absence of convection. At large Ra_v for the Mixture 1 (Fig. 1) in the first

stage of time evolution the average flow of high intensity arises, then oscillatory decrease of flow intensity with time is observed. For the Mixture 2, significant vibration intensity is required for the development of marked average flow: the curves corresponding to $Ra_v = 5 \cdot 10^4$ and $Ra_v = 10^5$ in Figure 2a are close to the line $\bar{\psi} = 0$ and only at $Ra_v = 2 \cdot 10^5$ the value of average stream function markedly different from zero is established. The difference in the solute concentrations values for both mixtures significantly decreases with the vibration intensity growth (Figs. 1bc, 2bc) resulting in the amplification of the fluids mixing.

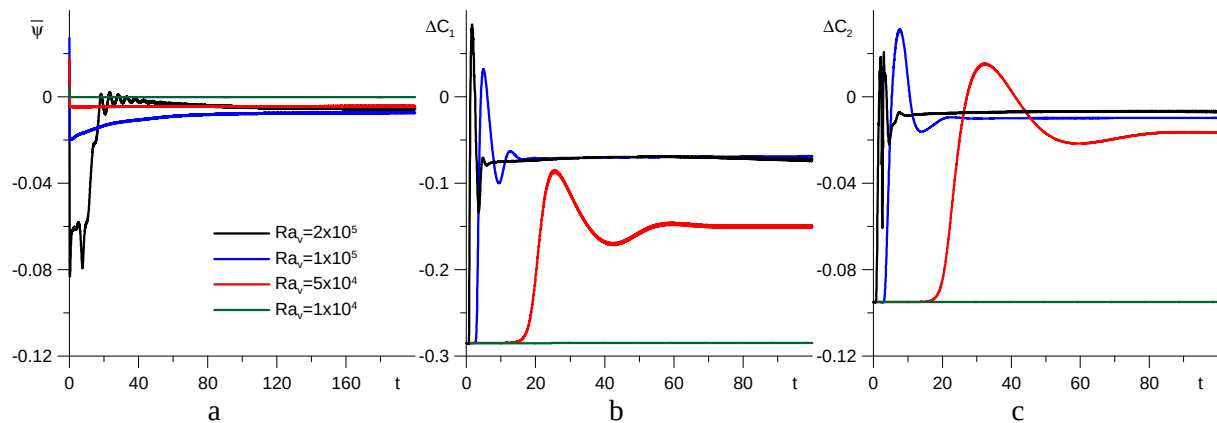


Figure 1. Time evolution of the average stream function at point (0.275;0.275) (a) and difference in the solute concentrations at the centers of lower and upper boundaries (b,c) for Mixture 1 in the cavity with aspect ratio 5:1

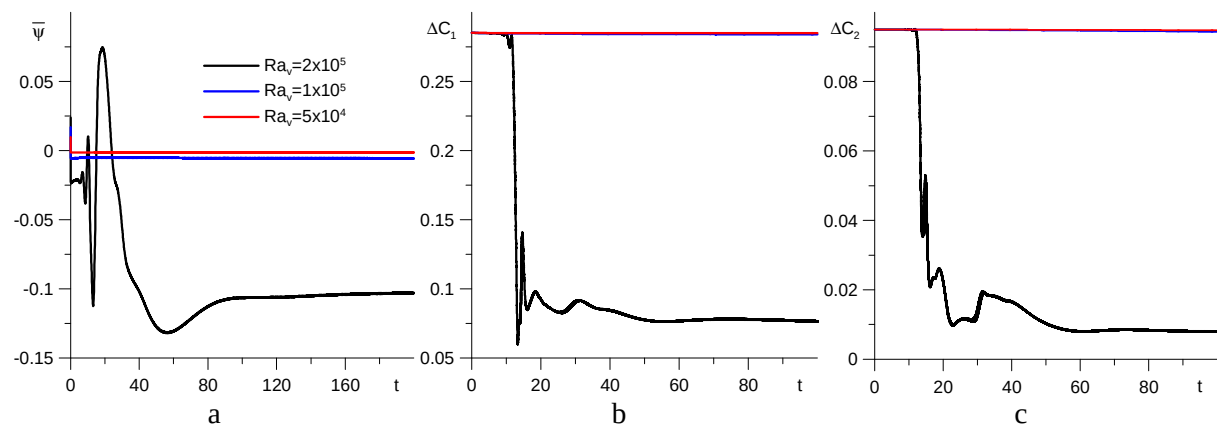


Figure 2. Time evolution of the average stream function at point (0.275;0.275) (a) and difference in the solute concentrations at the centers of lower and upper boundaries (b,c) for Mixture 2 in the cavity with aspect ratio 5:1

The transformation of the flow structure during the period of oscillations, which coincides with the period of external vibrations, for Mixture 1 at $Ra_v = 2 \cdot 10^5$ is shown in Figure 3a. Time moments for the corresponding flow structures are marked in the plot of the temporal evolution of the stream function (Fig. 3b). As one can see, during the period the change of the direction and inclination of vortices occurs.

Fig. 4 shows the fields of steady average flow and solutes concentrations for Mixtures 1 and 2 at different values of the vibrational Rayleigh number. It is seen that at low values of the vibrational Rayleigh number (Fig. 4a, b) for both mixtures the flow in the central part of the cavity is absent, there

are only four weak vortices near the side walls. The isolines of the solute concentrations are also deformed only near the side walls. At large values of Ra_v the average flow has multivortex structure, the fields of solute concentrations are strongly deformed by the flow (Fig. 4b, d). The isolines of the second solute concentration (the lower fields in Fig. 4a-d) are deformed more significantly than that of the first solute, due to the larger Schmidt number.

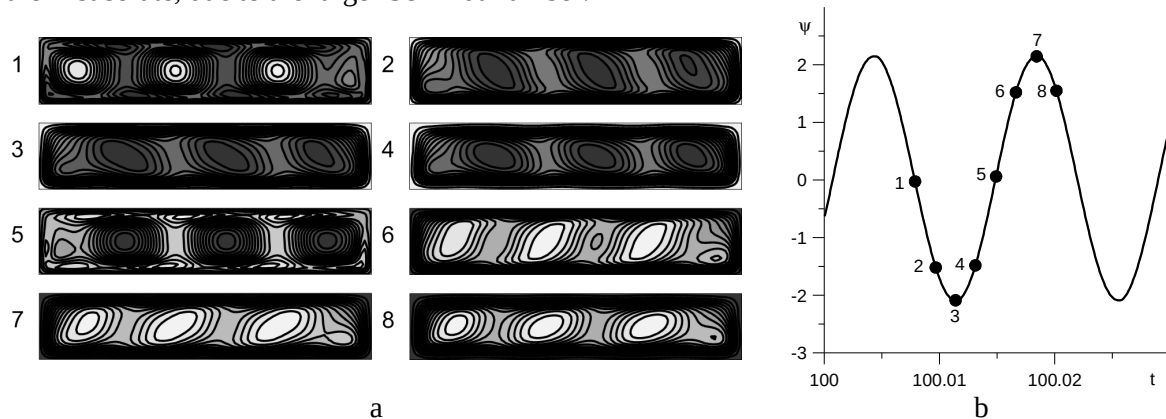


Figure 3. Transformation of instantaneous stream function fields (a) during the period of stream function at point $(0.275;0.275)$ oscillations (b) for Mixture 1 at $Ra_v = 2 \cdot 10^5$

In the case of square cavity at low values of the vibrational Rayleigh number for both mixtures the average four-vortex flow is observed (Fig. 5b). At large Ra_v for Mixture 1 the regime with large diagonal vortex and two smaller vortices in the corners of the cavity is realized (Fig. 5b). For Mixture 2 such regime was not found in the considered range of Ra_v . Four-vortex structure of average flow in square cavity is the limit case of four-vortex structure of average flow in a rectangular cavity when the distance between side walls becomes smaller. The isolines of the first solute as well as in the case of rectangular cavity with aspect ratio of 5:1, are less deformed than the isolines of the second solute. Temporal evolution of the flow characteristics in square cavity is qualitatively similar to that for the rectangular cavity with aspect ratio 5:1 (Figs. 1, 2).

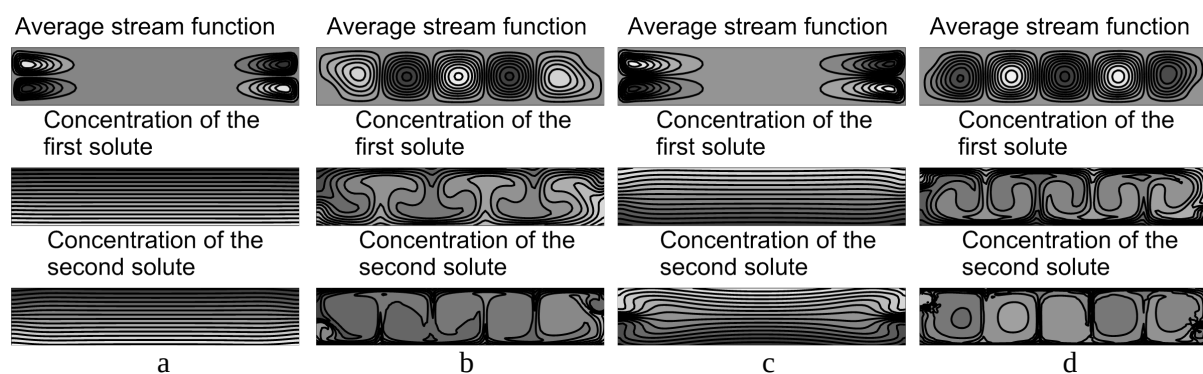


Figure 4. Streamlines of average flow and solute concentration distributions for Mixture 1 at $Ra_v = 1 \cdot 10^4$ (a) and $Ra_v = 1 \cdot 10^5$ (b) and for Mixture 2 at $Ra_v = 1 \cdot 10^5$ (c) and $Ra_v = 2 \cdot 10^5$ (d)

Figure 6 shows the dependence of the Nusselt number per unit length on the vibrational Rayleigh number for cavities with aspect ratios 1:1 and 1:5. In both cases, the change of the regime in Mixture 1 occurs at $Ra_v = 5 \cdot 10^4$. As one can see, the transformation of flow structure is accompanied by the change of slope of the curve $Nu/L(Ra_v)$, as well as it occurs in single-component fluid [9].

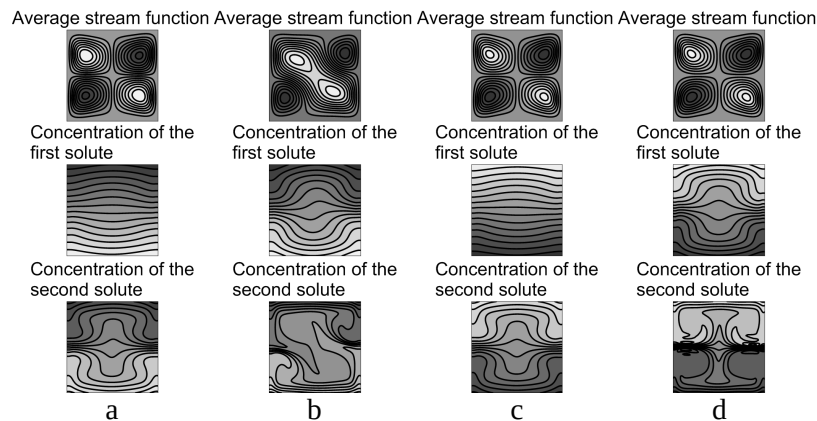


Figure 5. Streamlines of average flow and solute concentration distributions for Mixture 1 at $Ra_v = 5 \cdot 10^4$ (a) and $Ra_v = 1 \cdot 10^5$ (b) and for Mixture 2 at $Ra_v = 1 \cdot 10^5$ (c) and $Ra_v = 2 \cdot 10^5$ (d)

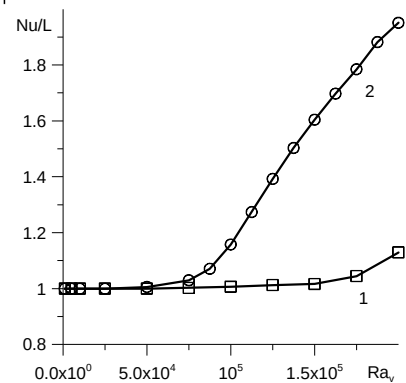


Figure 6. Dimensionless heat flux per unit length versus Ra_v for Mixture 1: 1 – aspect ratio 1:1, 2 – aspect ratio 5:1

5. Conclusions

Vibrational convection of ternary mixture in square and horizontally-elongated rectangular cavities is studied numerically on the basis of 2D unsteady approach. It is found, that in the case of square cavity, at small vibrational Rayleigh numbers four-vortex average flow of low intensity is generated. With the increase of Ra_v the transformation of average flow structure occurs – large diagonal vortex and two smaller vortices in the cavity corners are formed.

In the case of rectangular cavity elongated in the horizontal direction, at small vibrational Rayleigh numbers the average flow consists of two pairs of low intensive vortices located near the sidewalls whereas in the main part of the cavity the average flow is nearly absent. With the increase of Ra_v the transformation of average flow structure occurs – the multivortex average flow occupying the whole cavity is formed.

The transformation of average flow structure in both cases is accompanied by the change of the slope of the curve $Nu/L(Ra_v)$.

Acknowledgments

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