Numerical investigation of double-diffusive convection at vibrations

Nikolai Kozlov

1 Perm National Research Polytechnic University, Prof. Pozdeev St. 11, 614990, Perm, Russia
2 Institute of Continuous Media Mechanics UB RAS (Perm Federal Research Center UB RAS), Ac. Korolev St. 1, 614013, Perm, Russia
E-mail: kozlov.n@icmm.ru

Abstract. The problem of convection in a rectangular vertical cell, located in the gravity field and under the action of high-frequency vertical vibrations, is solved using the direct numerical simulation. At the initial moment of time, the system is formed by two horizontal layers of miscible liquids: the lower (heavy) layer is an aqueous solution of sodium chloride, while the upper one is a sugar solution. A two-dimensional formulation is considered; ANSYS Fluent software package is used as a solver. The impermeability and no-slip conditions are satisfied at the cell boundaries. As a result of the difference in the diffusion coefficients of dissolved species, layers with unstable stratification are formed over time near the contact zone. This leads to the onset of convection in the form of thin ascending and descending fingers. The vibrations, on average, lead to a decrease in the growth rate of fingers and the velocity of convection. In the case of relatively high vibrational overloads, a more regular convective structure forms in the diffusion layer leading to a more pronounced mixing of fluids.

1. Introduction
The systems of miscible liquids, between which a diffusion of solutes or a chemical reaction take place, are prone to the development of convection. One among numerous types of instability, creating the motion, is the double diffusion. As a consequence of difference between the diffusion coefficients of the two species, the unstably stratified domains emerge near the zone of contact of the two liquids. The less dense (denser) parts of fluid rise (sink) in the surrounding liquid in the form of “fingers” [1–4].

The vibration fields allow altering the behavior of hydrodynamic systems inhomogeneous in density [5]. A bright example to this is the stabilization of an unsteady (turned over) interface between two immiscible liquids [6]. In a similar experiment with miscible liquids the dynamics is more complicated: partial stabilization is observed [7, 8]. In the case of non-isothermal systems, vertical vibrations (oriented along the temperature gradient) make the convection regime change and are even able to suppress the convection entirely [9, 10]. Another well-known effect is the excitation of parametric resonance, observed on free surface [11] or liquid–liquid interface [12] and in stratified systems [13, 14].
In the present work, double-diffusive convection is studied numerically in a two-dimensional two-layered system formed by aqueous solutions of sodium chloride and glucose and subject to vertical high-frequency vibrations.

2. Problem formulation

The working volume is a rectangular cell with the following inner dimensions: height \( H = 0.1 \) m, width \( L = 0.05 \) m (Fig. 1a). Its orientation is vertical in the gravity field; the coordinates \( x \) and \( y \) are directed as shown in Fig. 1a. The cell is filled in equal proportion with two miscible liquids of different density. The upper layer is formed by an aqueous solution of glucose with the initial concentration \( C_{1_{\infty}} = 0.0318 \), while the bottom layer is an aqueous solution of sodium chloride whose initial concentration is \( C_{2_{\infty}} = 0.0344 \). Glucose diffusivity is \( D_{1} = 4.878 \times 10^{-10} \) m\(^2\)/s, its volumetric expansion coefficient is \( \beta_{1} = -0.3719 \), while for the sodium chloride these parameters are, respectively, \( D_{2} = 1.477 \times 10^{-9} \) m\(^2\)/s and \( \beta_{2} = -0.6892 \) [4]. At the initial moment of time, this system is characterized by a stable step-like density profile. The initial contact line is at the middle-height of the cell, \( y = 0.05 \) m. The considered system has a stability ratio \( R_{0} = \beta_{2} C_{2} / (\beta_{1} C_{1})|_{\infty} = 2.00 \) and a diffusivity ratio \( D_{2} / D_{1} = 3.03 \). These parameters correspond to the region of delayed double-diffusive convection [15].

![Figure 1. Problem formulation. (a) Hele-Shaw cell in the vibration field; (b) mesh used in calculations](image)

3. Numerical model

The numerical simulation was done with ANSYS Fluent software. A two-dimensional (2D) pressure-based transient solver was used. For viscosity, Laminar model was applied. For mass transport, Species Transport model was applied, a mixture material was defined containing 3 volumetric species: liquid water, sodium chloride, NaCl, and glucose, \( C_{6}H_{12}O_{6} \). Mixture density was computed according to the volume-weighted mixing law. For mass diffusivity, the dilute approximation (Fick's law) was applied, which means that diffusion coefficients were defined as constant for each species. The mixture viscosity was set equal to \( \eta = 0.001 \) kg/(m\( \cdot \)s); according to [16], in the considered range of concentrations the variation of \( \eta \) is small. To model vertical vibrations, frame motion was applied via a user-defined
function (UDF), which set the velocity of every fluid element as \((0, b\Omega \cos(\Omega t), 0)\). The above-mentioned parameters give the following system of equations:

\[
\frac{\partial v}{\partial t} + (v \nabla) v = -\nabla p + \nu \Delta v - e_g + e_b \Omega^2 \cos(\Omega t),
\]

\[
\frac{\partial}{\partial t} (\rho C_i) + \nabla (\rho v C_i) = -\nabla J_i,
\]

\[
J_i = -\rho D_i \nabla C_i.
\]

Here, (1) is the Navier–Stokes equation, (2) is the mass conservation equation, and (3) is Fick's law, which determines the mass flux due to concentration gradient. Velocity \(v\), kinematic viscosity \(\nu\) and pressure \(p\) are defined for the mixture; mass fraction \(C_i\), diffusion coefficient \(D_i\) and mass flux \(J_i\) are defined for each species. Equations (2) and (3) are solved for each species independently, \(i\) stands for either glucose, or sodium chloride. On all boundaries the impermeability and no-slip boundary conditions are applied.

It is worth mentioning that in some particular cases one should take into account the dependence of diffusivity on concentration \([17]\). The impact of concentration manifests itself when there are strong concentration gradients near the contact zone between the solutions, which is particularly noticeable in reacting systems. In the present case, concentrations are weak. Therefore, the use of Fick's law is justified.

The following solution methods were used. Pressure and velocity were computed according to a coupled scheme. Spatial discretization of gradients was done using Least Squares Cell Based method. Spatial discretization of pressure was performed using PRESTO! model, and for the discretization of momentum and transport equations Third-Order MUSCL model was applied. Temporal discretization was done with the second order implicit formulation. Flow Courant number was set equal to 200.

In the absence of vibrations, the time step was equal \(t_m = 0.025\) s, which was equivalent in terms of diffusion time to \(t_m D_2 / H^2 = 3.693 \times 10^{-9}\).

The simulation was performed for the frequency \(f = 40.0\) Hz (\(\Omega = 2\pi f = 251.3\) rad/s) and the amplitude \(b = (0–10)\) mm. The corresponding dimensionless acceleration was \(\Gamma = b\Omega^2 / g = 0–65\). Time step was set equal to \(t_m = 0.01 f^{-1} = 0.00025\) s, which corresponds to \(t_m D_2 / H^2 = 3.693 \times 10^{-11}\).

In the vicinity of the contact line, an adaptive mesh with rectangular cells was used (Fig. 1b). It had 500 cells of the equal size, \(L_x = 10^{-3} H\), along the horizontal direction, and 200 cells increasing with the distance from the contact line (\(y / H = 0.5\)). In the first rows on both sides of the contact line, the cells had the thickness \(h_{(1)} = 10^{-4} H\), while in each next row the cell thickness increased as \(h_{(n)} = 1.02 h_{(n-1)}\). Triangular cells were used above and below the adaptive mesh (Fig. 1b).

In order to test the horizontal mesh resolution, mapped rectangular meshes were used. In the case of natural convection, the mesh convergence was tested versus the mesh step size with the following values: 0.25, 0.2, 0.125, 0.1 mm (which make, respectively, \(1/200\), \(1/250\), \(1/400\), \(1/500\) of cavity transverse size \(L\)). The concentration of sodium chloride in the top half of the cell (initial value was zero) was compared at the moment \(t = 30.0\) s (\(\tau = (tD_2 / H^2) 10^6 = 4.43\)), before the initiation of convection. The difference in mass transfer was the following: 4.6 % – for 0.25 and 0.2, 4.2 % – for 0.2 and 0.125, 0.84 % – for 0.125 and 0.1. Therefore, the step 0.1 mm (\(10^{-3} H\)) was considered sufficient to provide an adequate precision.
4. Results
At the initial time moment, the system possesses a density drop at the contact line between the solutions of salt and sugar. On the initial stage ($\tau < 4$), a diffusive mass transfer is observed, and near the line of initial contact, a diffusion zone with an unsteady density profile is formed. When $\tau = 4$, inside the diffusion zone the formation of “fingers” begins (Fig. 2a, d): in the figure, near the left vertical boundary, density inhomogeneities in the form of spots on the horizontal isolines may be noticed. Gradually, the fingers become more pronounced (Fig. 2b, e), and finally the convection spreads to the entire width of the layer (Fig. 2c, f). A comparison of the density fields obtained with and without vibrations reveals that the vibrations reduce the speed of finger growth (compare figures 2c and 2f). At the same time, with the increase in $\Gamma$ the density structures become more extended in the horizontal direction. Besides, alongside with the reduction in height of the fastest fingers, those fingers that are in the process of formation are more distinct (Fig. 3). As a consequence, the mixing of the diffusion zone becomes more homogeneous with respect to the $x$ coordinate (Fig. 3d).

To give a quantitative description of the convection, let us define the following parameters.

1) The dimensionless velocity $v = v_{\text{vol}} H / D_2$ calculated from the volume-averaged velocity, $v_{\text{vol}}$. In the case of vibrations this velocity is also averaged over the oscillation period $T = 1 / f$:

$$v_{\text{vol}} = \frac{1}{V_T} \frac{1}{T} \int_{V_T} v_{\text{fluid}} dV dt.$$

2) The dimensionless height of fingers $h = 2 h_f / H$. Here, $h_f$ is the average height of the fastest fingers in the top and in the bottom layers that is measured from the images exported during the calculations (Fig. 3).

![Figure 2](image1.png)

**Figure 2.** Density fields (fragment near the contact zone) in the absence of vibrations (a–c) and at vibrations with the acceleration $\Gamma = 29$ (d–f) at the consecutive time moments: $\tau = 4.43$ (a, d), 8.86 (b, e), 13.3 (e, f)
Figure 3. Density fields (full layer width, near the contact zone) at $\tau = 13.3$ for accelerations $\Gamma = 0$ (a), 9.6 (b), 29 (c), 64 (d).

3) The volume-averaged mass fraction of NaCl in the upper half-volume:

$$C_{2\text{vol}} = \frac{1}{V_1} \int_{V_1} C_2 dV.$$

When the convection begins, the velocity $v$ gradually increases in a non-monotonous way (Fig. 4a). With the increase in the vibrational acceleration, $\Gamma$, the velocity is reduced (compare $\Gamma = 0 - 30$), but at high acceleration ($\Gamma = 64$), on the opposite, the convection is slightly intensified on the early stage ( $\tau = 6 - 8$). The evolution of convection is clearly marked by the growth of fingers. On the early stage of the convection their height slightly depends on $\Gamma$, while at $\tau > 10$ the values of $h$ split according to $\Gamma$ (Fig. 4b). The discrepancy between the series of points increases with time, and the height of fingers taken at any given moment decreases monotonously with $\Gamma$. 
The average concentration of salt in the upper half-volume, which is zero at $t = 0$, characterizes the mass transfer. The discrepancy in $C_{\text{vol1}}$ between the calculations for different values of $\Gamma$ becomes noticeable at $\tau \approx 11.5$ (Fig. 4c). $C_{\text{vol1}}$ increases non-monotonously with the vibrational acceleration: the highest mass transfer rate is observed at $\Gamma = 64$, and the lowest one at $\Gamma = 10$.

Comparison of figures 4a–4c reveals that in the range $\tau = 11–12$ a bifurcation takes place in the system, and afterwards all the processes are intensified. This is the moment when the convection becomes global, i.e. the finger structures appear along the entire layer width $L$, as may be noticed from the comparison of figures 2b, e and 2c, f. On this stage of convection, the dynamics of $v$ and $C_{\text{vol1}}$ is altered, and in the case of the highest vibrational acceleration ($\Gamma = 64$) both parameters become larger than those at lower $\Gamma$. This demonstrates that, despite the oscillations reduce the fingers length, they provide a more intensive fluid mixing in the diffusion zone that forms in the vicinity of the initial contact line, as one may also notice from Fig. 3d. Thus, when $\Gamma \sim 10$, the vibrations reduce the mass transfer rate by means of slowing down the growth of fingers. On the other hand, when $\Gamma$ reaches the next order of magnitude ($\Gamma \sim 10^2$) the vibrations seem to prevent the propagation of the convective fingers into the bulk volume due to the intensification of mass transfer in the diffusion zone. Presumably, this may be a feature of the delayed DDC, presently considered, because in this regime the fingers are formed inside the diffusion zone.
5. Conclusion
The action of vertical high-frequency vibrations on a system of miscible liquids with double-diffusive instability has been studied numerically. The performed study demonstrates that the oscillating inertial field leads to the transformation of the convective finger structures. Namely, the height of the fastest fingers is reduced and the slow fingers, situated inside the diffusion zone, become more regular. In general, the vibrations reduce the intensity of convection, this effect becoming stronger with the vibrational acceleration. However, considering the mass transfer, the effect is non-monotonous: at higher accelerations the mass transfer rate increases over the one observed in the absence of vibrations. One possible reason for this may be the fact that the finger-type convection spreads over the entire width of the fluid layer leading to the increase of the integral mass transfer. The obtained results can be useful for the investigation of vibrational convection in reacting systems and are of potential interest for the chemical industry.

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