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Development of Convection in Binary Mixture with Soret Effect

The future Space experiment IVIDIL is planned to study the influence of vibration stimuli on the measurements of diffusion and thermodiffusion coefficients. A binary mixture of water and isopropanol is chosen as a working liquid. The principle of the Space experiment and ground based research are outlined. In addition preparatory experiments might be performed during parabolic flights. Results of 3D numerical simulations of thermal vibrational convection in binary mixture at the conditions of the parabolic flight are presented. Heat and mass transport arising in the system with increasing of vibration actions is discussed.

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1. Introduction

Molecular diffusion processes are caused by concentration gradients in a multi-component mixture. Noticeable diffusion flux can also be induced by temperature gradients which lead to partial separation of constituent components. This cross effect between temperature and concentration is known as thermo diffusion or Soret effect. This effect can be quite important in the analysis of the distributions of components in oil reservoirs. Precise measurements of diffusion coefficients under terrestrial conditions are often perturbed by buoyancy-induced flows. The microgravity environment minimizes the effect of gravity and allows the true diffusion limit to be achieved. On the other hand the background g-jitters encountered in many space experiments may alter the benefits of the microgravity environment, e.g. see the report by Shevtsova et al.[1]. Thus a study of the effects of controlled vibrations on measurements of diffusion and Soret coefficients in liquid systems could be beneficial.

2. Principle of IVIDIL experiment

The experiment IVIDIL (influence of vibrations on diffusion in liquids) is prepared in the frame of ESA Physical Sciences program. An international group is involved in the preparation of the space experiment: ULB, Belgium (the coordinator), Canada,France and Russia.

A novel approach to measure the diffusion and the Soret coefficient simultaneously is proposed. The scientific team suggests performing the experiments in two steps. During the first step a concentration gradient is established by imposing a temperature gradient along the experimental cell that is filled with a homogeneous binary mixture. Due to Soret effect the binary mixture will separate with time. At the second step the system is reverted to an isothermal case and molecular diffusion progressively reduce the previously established concentration gradient.

There are no mechanically driven parts in contact with the liquid (no valves). Optical interferometry in combination with digital recording and processing will result in accurate determination of the optical amplitude and phase information. Such an approach allows repetition of the experiments with the same initial conditions. In this way reliability of the experimental results will be improved in an important way using statistical means. In the experimental runs with vibrational stimuli we have the possibility to study exactly the same system for several vibration parameters. Preliminary parametric analysis of the most influential frequencies and g-jitter amplitudes should be done numerically.

3. Ground based preparation

Presently the ground based preparatory experiments are running at ULB without vibrations. Fine-tuning the vibrating system is currently performed. A typical experiment is carried out as follows. The cell, shown in Fig. 1, is filled with the mixture of water and isopropanol. Then the Peltier modules establish the temperature of the top and bottom plates at the mean temperature of the upcoming experiment. A waiting period of at least two hours is allowed in order to reach a steady state. Two thermistors, inserted inside the cold and hot plates are used for temperature control. Before setting ΔT to a designated value a first image was acquired and used for the reconstruction of a reference phase. Immediately after applying the temperature gradient interferogram acquisition is quite frequent to record the developing thermal field. The time step between image acquisitions is gradually enlarged up to half an hour for tracking the much slower thermodiffusion separation. To approach solute equilibrium a typical experimental time was few days and then we turn to the measurement of the diffusion coefficient. The experimental study has multiple benefits.

• On the preparatory side: the thermal design of the diffusion cell was improved, the problem of maintaining constant ΔT

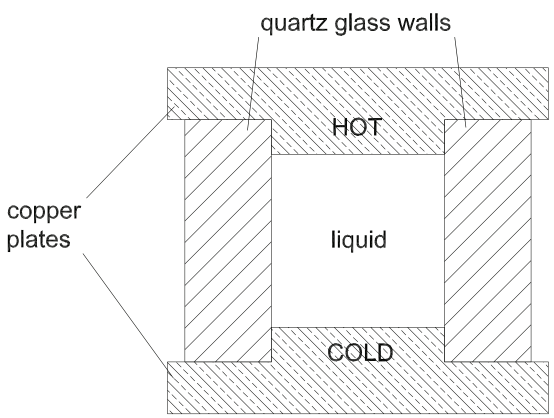

Fig. 1: Sketch of the experimental cell.

under vibrations (for few hours) was solved and the characteristic times of the system (viscous τ_v, thermal τ_{th} and diffusive τ_D) were measured. In addition ground measurements of the diffusion and Soret coefficients will be compared with future microgravity results.

• On the fundamental side: we are able to experimentally study different types of convection. It also resulted in a complementary theoretical analysis of convective flows in a cubic cell: double diffusive convection and thermal vibrational convection. The latter one is briefly discussed below.

4. Preparations on numerical side.

4.1.Thermal vibration convection; formulation of the problem

At reduced gravity the influence of vibration on Soret separation occurs due to thermo vibrational convection (TVC) in the system. So, the primarily goal is to examine the behavior of TVC as a function of vibration stimuli. The results below correspond exactly to the geometry of the set-up and to the physical properties of the liquid used in the experiments. Heat and mass transfer in a cubic cell filled with a homogeneous binary mixture with initial mass fraction of the heavier component (i.e. water) C_0, is considered. The two opposite side walls are kept at constant temperatures T_{hot} and T_{cold} with $\Delta T = T_{hot} - T_{cold}$. All other walls are assumed thermally insulated. The geometry of the problem is shown in Fig. 2. The mass flux of the heavier component in the mixture is given by

$$\mathbf{j}_c = \mathbf{V}C - D\nabla C - D\,S_T C\,(1 - C)\,D\nabla T. \quad (1)$$

D is the molecular diffusion coefficient and $S_T = D_T / D$ is the Soret coefficient. Mass conservation requires $\partial C/t = -\nabla \mathbf{j}_C$. Then the governing equations will take form:

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V}\nabla\mathbf{V} = -\frac{\nabla P}{\rho} + \upsilon\nabla^2\mathbf{V} + \mathbf{g}, \quad (2)$$

$$\frac{\partial T}{\partial t} + \mathbf{V}\nabla T = \alpha\nabla^2 T, \quad (3)$$

$$\frac{\partial C}{\partial t} + \mathbf{V}\nabla C = D\nabla^2 C + DS_T\nabla\left[C\left(1-C\right)\nabla T\right], \quad (4)$$

$$\mathbf{V}\cdot V = 0. \quad (5)$$

The boundary conditions on the rigid walls are $\mathbf{V}=0$; $\partial_n(C-T)=0$. Here $\mathbf{V}$ is the velocity vector, T, P are the temperature and the pressure; α is the thermal diffusivity and ν is the kinematic viscosity;

$$\mathbf{g} = \mathbf{e_z}\,[g_{st} + g_{os}\cos(\omega t)],\ \omega = 2\pi\, f\, L^2/\nu$$

is the gravity vector, consisting of stationary and oscillatory components. The problem (2)-(5) is solved numerically in the Boussinesq approximation when $\rho =\ (T, C)$. Nondimensional formulation of the problem includes Prandtl, Schmidt, Grashof numbers:

$$Pr = \frac{\nu}{\alpha},\ Sc = \frac{\nu}{D},\ Gr = \frac{g\beta_T \Delta T L^3}{\nu^2},$$

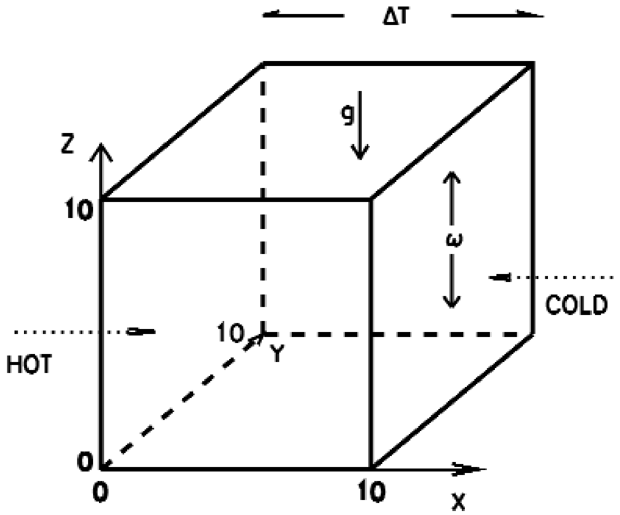

Fig. 2: Geometry of the problem.

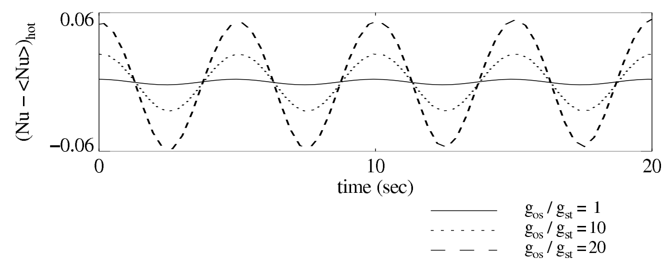

Fig. 3: Oscillatory behaviour of the hot wall Nu around its mean value at different g_{os}.

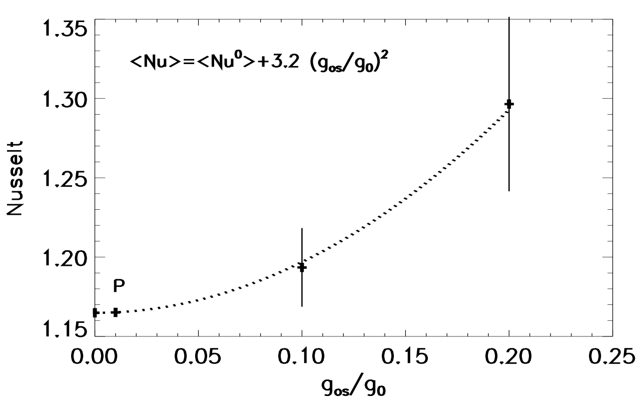

Fig. 4: Dependence of the time-averaged Nu_h on the oscillatory acceleration; at point P $g_{os} = g_{st} = 10^{-2} g_0$.

and the separation ratio

$$\Psi = C_0\left(1 - C_0\right)\frac{\beta_C}{\beta_T} S_T,$$

where β_T and β_C are the thermal and solutal expansions. For our system the fixed parameters are Pr =10.85, Sc = 1620, ψ = -0.4 and ΔT =10*K* while Gr is varied according to the gravity level. The numerical code used in this work has been tested in a benchmark study between the participants in the future experiment; details of the formulation are in Ref.[2].

4.2. Results

The results presented below are obtained for a single-frequency idealized g-jitter with the value of the residual gravity vector g_{st}=$10^{-2}g_0$. This value of the stationary component is typical for parabolic flights which will be performed in the preparatory phase for the space experiment on ISS. A parametric study of the frequency and g_{os} is conducted. The chosen ranges are representative of existing in laboratory vibrating system 0.01 *Hz* < f < 1.0 *Hz* and $0 < g_{os} / g_0 < 0.2$.

Heat transfer is characterized by the Nusselt number, which is defined as the ratio of total heat transport to conductive heat transport. Hereafter the heat transport either through the cold or hot wall is considered as other walls are thermally insulated.

$$Nu_{c,h} = q_{total} / q_{cond} = 1 - \frac{1}{\Delta T}\int_{c,h} \frac{\partial T}{\partial x} dydz$$

The control test for numerical code showed that at the absence of oscillations $N_{uc} = N_{uh}$ with accuracy up to 8 digits after the comma. In previous 2D parametric studies, see e.g. [3], the flow organization was divided into five regimes according to the frequency ranges. Our 3D calculations in the cube do not follow this organization although our frequency range covers at least

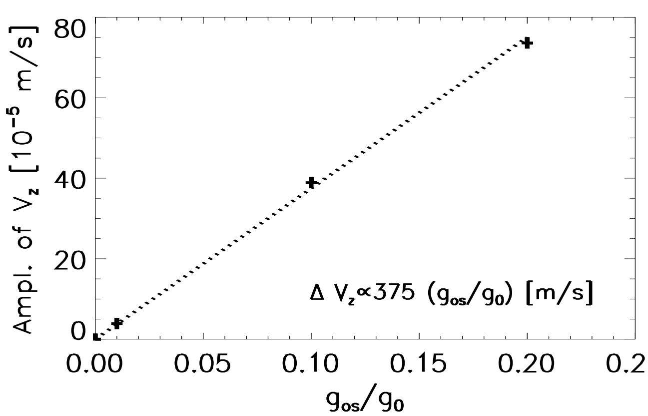

Fig.5: Amplitude of velocity V_z oscillationsv ersus the amplitude of g-jitter when =0.2Hz.

three indicated regimes. The Nusselt number oscillations are sinusoidal at all frequencies and the Fourier spectra display one clear maximum with negligible harmonics. Similar situation is also observed with increase of the oscillatory component, see Fig.3 when f =0.2*Hz*. The Nusselt number performs sinusoidal oscillations at the forcing frequency and only the amplitude of oscillations is increasing. Perhaps the external forcing (Ra=1.6·10^3 with g_{st} =10^{-2}) is too small to realize the 2D regimes. However, increasing the vibrational amplitude enhances the heat transfer rate significantly. One may find in the literature different empirical and semi-analytical dependencies of the Nusselt number on *Gr* (or *Ra*). For example, boundary layer theory predicts $Nu \sim Ra^{1/4}$ at large value of Rayleigh numbers which is not the case here. In the considered problem only small convective transport occurs and the results of Naumann [4], analytically obtained for parallel flow in a 2D extended cavity, is more suitable. He reports $Nu \sim Gr^2$ for steady accelerations as well as for g-jitter with zero mean. Our calculations with non-zero mean ($g_{st} \neq 0$) demonstrate the same tendency, although the defnitions of *Nu* are different. The evolution of $< N\,u_h >$, time averaged over several oscillation cycles, is shown in Fig.4 as function of g_{os}. The vertical lines near each point indicate the amplitude of oscillations, and the dotted line corresponds to the fit

$$< N\,u > = < N\,u_0 > + 3.2\ (g_{os} / g_0)^2.$$

Significant heat transfer enhancement occurs for $g_{os} > g_{st}$. Note, that in the absence of the steady component, g_{st} = 0, the heat transfer due to vibration is almost negligible: $<N_{uh}>-1 \approx 2.0 \cdot 10^{-5}$ when g_{os} =10^{-2} g_0 and f = 0.2Hz. Further comparison with parallel flows results reveals that the calculated maximal velocity in the bulk (mean value + amplitude) is also a linear function of g_{os} or *Gr* in the system, which is common for linear systems. The mean flow influence on the maximal velocity is relatively small. The increase of maximal velocity is mainly caused by the growth of oscillations amplitude, which is shown in Fig. 5. Hereafter the data are plotted at some fixed point near the hot

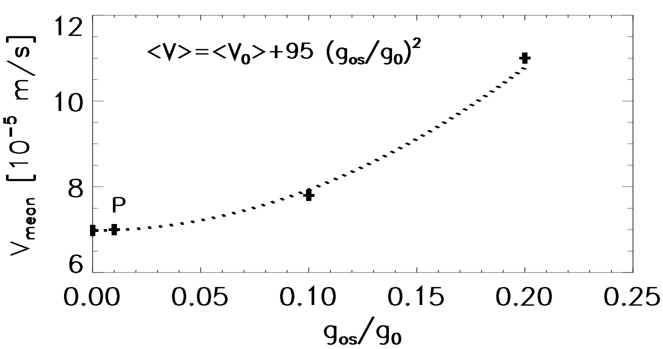

Fig. 6: Increase of mean velocity (at the same point near the hot wall as in Fig. 5) produced by vibrations; $g_{os} = g_{st} = 10^{-2} g_0$ *at point P.*

wall. The linear dependence ΔV_z ~375 (g_{os}/g_o) m/s is a good fit of the calculated points.

Non-linear effects are worth mentioning. Nonzero time-averaged fields arise from non-linear terms in the governing equations. The evolution of the steady mean velocity at f = 0.2Hz shown in Fig. 6 indicates that V_{mean} increases by 50% when g_{os} increases 20 times. Non-linear effects are small but non-negligible. Again, the power law for the mean velocity produced by vibrations $V_{mean} \sim (g_{os}/g_0)^2$ fits the numerical results well. We did not perform averaging of the equations according to Gershunis theory of TVC [5], although it is applicable. The theory states that a non-zero mean flow might be generated by vibrations when the period of oscillations is smaller than any characteristic time (viscous, thermal or diffusion) $\tau_{os} < [\tau_v, \tau_{th}, \tau_D]$. The frequency f =0.2Hz, for which the results are shown, fulfills these conditions. We note however that non-linear interactions of the static and vibrational components result in larger mean fields than in the pure oscillatory case (g_{st} = 0) at the same frequency.

5. Conclusions

Diffusion and Soret phenomena are influenced by convection in fluid mixtures. The simultaneous influence of low static gravity and g-jitter on heat and mass transfer in binary mixture was considered. Periodic oscillations normal to the density gradient significantly increase the heat and mass transfer when $g_{os} > g_{st}$. It is shown that non-linear interaction between the static and vibrational accelerations results in additional steady mean fields.

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