Study of passive dye dispersion in convective hexagonal pattern

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Abstract. We study experimentally and numerically the dispersion of a passive molecular dye in a hexagonal pattern of Bénard-Marangoni (BM) convection (Prandtl number $\approx 900$). Indeed, it is not straightforward to estimate the effective (global) diffusion coefficient in such BM convection pattern, where the fluid flow is three-dimensional and periodical from cell to cell. The computations have been undertaken for two Peclet numbers ($Pe \approx 100-1000$) and constant fluid flow characteristics. One can distinguish two mechanisms of dispersion: inside a cell and from cell to cell. In the latter, only diffusion acts across the cell side in the horizontal direction, i.e. between symmetric facing streamlines with respect to the cell side. On the other hand, the dispersion inside a cell behaves streamwise depending on either the convective and diffusive fluxes add each other (low concentration gradient) or they oppose each other (high concentration gradient), while in the transversal direction by molecular diffusion.

1. Introduction
The diffusion of a passive matter in a convective flow has drawn a lot of interest from industrial applications (such as processes which require uniform mixing or impurity distributions) [1,2], plasmas [3,4], to environmental problems (spreading of pollutants) and astrophysics [5,6]. Indeed in all these problems, the passive tracer dispersion results from the combination of the molecular diffusion and the fluid flow convection, which can be quite complicated (turbulent, laminar but cellular or recirculating flows, etc.). Therefore, in such configurations one often observes an enhancement of the effective diffusion of impurities. The dispersion of a passive molecular dye in a convecting liquid has two physical origins: firstly the molecular diffusion from streamline to streamline, secondly, the transport of the tracer in the flow.

In recirculating flows such as Rayleigh-Bénard rolls, when advection is much greater than diffusion (high Peclet number), both mechanisms add each other to strongly enhance the tracer transfer. This phenomenon has been extensively studied theoretically [7-12] and experimentally [13,14]. On the
other hand there are some other convective cases in which regions of the fluid flow where advection
and diffusion act in opposite directions such as Bénard-Marangoni (BM) convection. This
phenomenon appears in a thin horizontal liquid layer uniformly heated from below and cooled
throughout its free upper surface. Close to the threshold, the convective flow is characterized by a
tessellation of hexagonal convective cells where the flow is upwards along the cell axis and
downwards along the cell edges. Inside each cell every streamline is closed and is set over a vertical
surface as it is well known. At the pattern level the dispersion of a passive molecular dye is not
straightforward to estimate because the fluid flow is three-dimensional, and furthermore despite it is
periodical from cell to cell the diffusion and advection act in various directions according to the
considered point. To our knowledge, only two works have been devoted to the anomalous diffusion in
Bénard-Marangoni convection, experimentally [15] and theoretically [16].

So the present work aims to complement the scarce previous results and broaden the understanding
of dye dispersion in a hexagonal pattern of Bénard-Marangoni convection.

2. Governing equations and numerical model
The modeling of the passive scalar dispersion in Bénard-Marangoni convection can be obtained in two
stages: first set-up the base fluid-flow; second keep frozen the obtained fluid flow and start the passive
dispersion process. The base flow is governed by the incompressible Navier-Stokes equations coupled
with the energy conservation equation and the passive dye dispersion obeys a standard advection-
diffusion equation.

2.1. The base Bénard-Marangoni fluid flow
Introducing dimensionless variables of space, time, velocity and temperature into the conservation
equations of mass, momentum and energy result in the following set:

\( \nabla \cdot \mathbf{u} = 0 \)  \hspace{1cm} (1)
\[
\frac{1}{Pr} \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \nabla^2 \mathbf{u} + Ra \theta e_z 
\]  \hspace{1cm} (2)
\[
\frac{\partial \theta}{\partial t} + (\mathbf{u} \cdot \nabla) \theta = \nabla^2 \theta 
\]  \hspace{1cm} (3)

supplemented with appropriate initial and boundary conditions. The fluid flow boundary
conditions are:

\( \mathbf{u} = 0 \)  \hspace{1cm} (4)

at all solid walls and the Marangoni condition at the free surface:

\( \mathbf{u} \cdot \mathbf{n} = 0 \quad \frac{\partial u}{\partial z} = -Ma \frac{\partial \theta}{\partial x} \quad \frac{\partial v}{\partial z} = -Ma \frac{\partial \theta}{\partial y} \)  \hspace{1cm} (5)

The associated heat transfer boundary conditions reduce to

\( \theta = 1 \)  \hspace{1cm} (6)

at the heated horizontal bottom wall,

\( \frac{\partial \theta}{\partial n} = 0 \)  \hspace{1cm} (7)

at all lateral walls, and finally at the free surface
\[ \frac{\partial \theta}{\partial n} = -Bi \theta \]  

(8)

The related physical parameters have been gathered into four non-dimensional numbers, namely the Biot number 
\[ Bi = \frac{d_l}{k_l} \frac{k_a}{d_a} \], the Marangoni number 
\[ Ma = \frac{\gamma d_l \Delta T}{\mu \kappa} \], the Rayleigh number 
\[ Ra = \frac{\beta g d^3 l}{\nu \kappa} \] and the Prandtl number 
\[ Pr = \frac{\nu}{\kappa} \].

2.2. The dispersion of a passive molecular dye

The time evolution of the passive dispersion dye obeys the standard advection-diffusion equation:

\[ \frac{\partial C}{\partial t} + (u \cdot \nabla) C = Pe \nabla^2 C \]  

(9)

where \( C \) designates the passive dye concentration in the convective fluid flow and \( Pe \) stands for the Peclet number. This conservation equation is supplemented with the boundary condition (constant concentration at center of the vessel)

\[ C(x^2+y^2<0.1, 0 \leq z \leq 1, t > 0) = 1 \]  

(10)

and a non absorbing (zero flux) condition along the solid walls and free surface

\[ \frac{\partial C}{\partial n} = 0 \]  

(11)

In the present Bénard-Marangoni convection problems the Peclet Number is defined as

\[ Pe = \frac{\gamma d_l \Delta T}{\rho \kappa K_c} \], (where \( K_c \) is the passive dye diffusivity into the liquid).

2.3. Numerical model

A finite element model has been developed to numerically solve the governing equations (1-11) on computational domains of arbitrary shape and numerous validations have been performed for the Bénard-Marangoni convection class of flows [17]. In the present work, a steady state hexagonal convection pattern is first computed and then one computes the transient passive dye dispersion in the liquid layer assuming the fluid flow to be insensitive to the dye.

3. Results

3.1. Experiments

The experimental set-up is essentially made up of a cylindrical container (8 cm diameter) surrounded by Perspex lateral wall. The vessel bottom is horizontal and made of copper. It is supplemented with a regular hexagonal array of small copper cones to maintain a steady convective hexagonal pattern. The wave number of the array is that of the naturally selected pattern just above the threshold. The1 mm depth silicon oil layer (\( Pr \approx 900 \) at 20°C) is uniformly heated from below and cooled from above thanks to a thermally regulated water flow.

In the experimental process, one first establishes a steady convective hexagonal pattern for \( Ma = 1.1Mac \) (critical Marangoni number). Then the dye is injected into the centre of a cell located in the middle of the pattern and dispersion takes place.
A temporal sequence of snapshots is presented in figure 1 in the vicinity of this central cell. Owing to the symmetry of the hexagonal pattern, only one quarter of the plane is displayed. It is noteworthy that the dispersion first takes place along the apothems (the lines joining adjacent cell centers) of the first neighboring cells defining a wedge centered at the cell center (figure 1a). Then the dye spreads out towards the corners of this cell (figure 1b-1e). In figure 1f the dye progressively invades the second neighboring cell. In figures 1g-1i the contamination of the second neighbors goes on and that of the third neighbors begins. On can notice that the dye never goes through the cell axis but circumvents it by both sides.

**Figure 1.** Time evolution of the dye diffusion in a regular hexagonal Bénard-Marangoni convection (the black dots located at the centre of the cells are the metallic cones).

3.2. Computations and discussion

Owing to the problem symmetries the computational domain represents only one quarter of the actual experimental container. The steady hexagonal Bénard-Marangoni convective pattern is computed for $Ma = 85$, $Ra = 0$, $Bi = 0.1$ and $Pr = 900$. Then the time evolution of the dye dispersion is computed with the obtained steady velocity field for $Pe = 1000$. Some computed results are depicted in figure 2, both from an isometric view centered on the dye injection (left) and top view of the liquid layer (right). The velocity field (figure 2a) and dye concentration one are presented at $t=25s$ (figure 2b), $t=50s$ (figure 2c), $t=75s$ (figure 2d), respectively.
Figure 2. Isometric and top views of the velocity and dye concentration fields in BM convection.
From the isometric views of the dye concentration field at different instants (figure 2b-d) one can distinguish basically two mechanisms of dispersion: inside a cell and from cell to cell. In the latter, only diffusion acts across the cell side in the horizontal direction, i.e. between symmetric facing streamlines with respect to the cell side. On the other hand, the dispersion inside a cell behaves very differently whether the convective and diffusive fluxes add each other (low concentration gradient) or they oppose each other (high concentration gradient). So dispersion inside a convective cell is highly location dependent: convective dominated in streamwise direction or molecular diffusion dominated otherwise (transversal directions with respect to the cellular fluid flow or in counter flow locations).

4. Conclusion

The dispersion of dye in Bénard-Marangoni convection has been experimentally and numerically investigated. A fair agreement can be observed between these two kinds of results. The numerical model enables us to get a more detailed insight of the mechanism compared to the experiments which provides global results across the liquid thickness. The present study has confirmed that the boundary tubes around the axis of the hexagonal cells are regions of great diffusive resistance whereas the regions where the fluid flow acts in the same direction as the diffusion are of high global transfer. So it is undoubtedly a quite different dispersion mechanism as compared as in Rayleigh-Bénard configurations where convection plays the dominant role. In a forthcoming work we will be able to determine the effective diffusion coefficient and the influence of several physical parameters.

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