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Effect of Depth Length on Mixing in a Double-Diffusive Convection Two-Layer System

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Additional information is available at the end of the chapter

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1. Introduction

With the rapid development of industrial technologies within recent years, development of multi-function, high-performance materials that can survive harsh conditions is in demand. In regards to the materials manufacturing processes that accompany coagulation, it has been indicated that multilayer convection cell formation and amalgamation occurs due to double diffusive convection, and that this may exert an influence on material quality [1, 2]. When manufacturing this kind of material, solute elimination occurs on the coagulation interface during the multi-component solution coagulation process, and double diffusive convection occurs due to the gradient between temperature and concentration in the droplet phase. It is thought that multilayer cell structure formation and destruction occur due to this phenomenon in the droplet phase, and that this exerts a major influence over crystal growth speeds and material quality. However, many relevant details remain unexplained. As the phenomenon of convection cell amalgamation in particular is complex, the phenomenon of convection between low- and high-concentration layers has come to be considered as a system using experiments and mathematical simulations [3 - 10]. Bergman et al. [5] measured the speed of material passing through the diffusion interface at convection cell amalgamation and between convection cells. Subsequently, Nishimura et al. [7, 8] made broad-ranging changes to control parameters, and proposed a correlational formula for these issues. Hyun et al. [10] considered the amalgamation process in detail using 2-dimensional mathematical calculations, and showed that high-frequency component fluctuation occurs at the average Nu number.

Convection cell amalgamation is governed by the diffusion interface, where major gradients in concentration are present. As both thermally unstable diffusive-type double diffusive convection and opposing, sheer flows due to thermal convection co-exist in interface areas according to calculation results by Hyun et al. [10], it is anticipated that interface instability

can easily occur in these circumstances. Recently, Tanny et al. [9] focused on interface regions and investigated 2-dimensional structures using the Schlieren method. The team also reported that when initial buoyancy is low and thermal Rayleigh number is high, vortex arrays form above and below the interface, and convection cell amalgamation time is shortened. Considered in light of vortex structure, this phenomenon is thought to occur primarily due to shear current instability. However, while traditional research also leads us to anticipate interface instability due to double diffusive convection, characteristics of diffusive-type double diffusive convection in shear currents remain unknown.

Figure 1. Diffusive interface between the convective cell

As shown in Fig. 1, diffusion interface between convection cells is stable in terms of concentration in a gravitational field, but is thermally unstable due to the presence of a vertical temperature differential. Accordingly, it is clear that it takes the aforementioned diffusive state. It has been previously confirmed that non-flowing diffusive interfaces fall into oscillating modality. This is explained via the diffusive interface shown in Fig. 2. As heat diffusion is much faster than material diffusion, high-concentration lower fluid bodies rise due to thermal buoyancy. Afterwards, the fluid body is cooled rapidly while maintaining its concentration, and then proceeds to descend due to reversed buoyancy. The repeated occurrence of this phenomenon at the interface is known as oscillation modality. The diffusive interface between convection cells shown in Fig. 1 contains shear currents due to thermal convection caused by horizontal temperature gradients above and below the interface. As it is possible for 3-dimensional structures to form due to the presence of shear currents and the occurrence of oscillation modality at the interface in this sort of situation, a detailed investigation is seen as necessary. In actuality, Chen et al. [11] have reported 3-dimensional structures in cases of finger-type interfaces coexisting with shear currents.

Figure 2. Oscillatory modes

In order to investigate 3-dimensional structures in diffusive interfaces in this research, 3-dimensional mathematical calculations were conducted for diffusive interfaces occurring in an aqueous solution with density stratification into a linear state, which is heated and cooled as a system from both sides in a rectangular container. In addition, the computational domain in the direction of depth is changed, and the mixing process of each convection layer was examined.

2. Numerical analysis

2.1. Mathematical model

The model equations to describe the double diffusive natural convection consist of the continuity, the Navier-Stokes, the energy and the concentration equations in dimensionless forms as follows:

$$\nabla \cdot V = 0 \quad (1)$$

$$\frac{\partial V}{\partial \tau} + (V \cdot \nabla)V = -\nabla P + \text{Pr} \cdot \nabla^2 V + \text{Pr} \cdot \text{Ra}(\theta - N \cdot C)\kappa \quad (2)$$

$$\frac{\partial \theta}{\partial \tau} + (V \cdot \nabla)\theta = \nabla^2 \theta \quad (3)$$

$$\frac{\partial C}{\partial \tau} + (V \cdot \nabla)C = \frac{\nabla^2}{Le} \quad (4)$$

Dimensionless parameters Pr , Ra , Le , N and A are defined as follows:

$$\begin{aligned} Pr &= \frac{\nu}{\kappa}, Ra = \frac{g \cdot \alpha (T_{hot} - T_{cold}) b^3}{\kappa \cdot \nu} \\ Le &= \frac{\kappa}{D}, N = \frac{\beta (C_{max} - C_{min})}{\alpha (T_{hot} - T_{cold})}, A = \frac{h}{b} \end{aligned} \quad (5)$$

Here, the dimensionless variables are defined as follows:

$$\begin{aligned} X &= x/b, Y = y/b, Z = z/b \\ U &= u \cdot b/\kappa, V = v \cdot b/\kappa, W = w \cdot b/\kappa \\ \tau &= t \cdot \kappa/b^2, P = p \cdot b^2/(\rho \cdot \kappa^2) \\ \theta &= \frac{T - T_{cold}}{T_{hot} - T_{cold}}, C = \frac{C - C_{min}}{C_{max} - C_{min}} \end{aligned} \quad (6)$$

2.2. Boundary conditions

The boundary conditions in dimensionless form are illustrated in Fig.3. In the computational domain (see Fig.2), the aspect ratio is 1.25 and length of the direction of depth (Z) examined three kinds (1.0, 1.5 and 2.0). The initial temperature in the system is 0.0 and the initial concentration is linear profile: $C=f(Y)$

Figure 3. Boundary conditions

$$\begin{aligned}
 &\text{at } X=0, U=V=W=0, \theta=-0.5, \frac{\partial C}{\partial X}=0 \\
 &\text{at } X=1, U=V=W=0, \theta=+0.5, \frac{\partial C}{\partial X}=0 \\
 &\text{at } Y=0, U=V=W=0, \frac{\partial \theta}{\partial Z}, \frac{\partial C}{\partial Z}=0 \\
 &\text{at } Y=1.25, U=V=W=0, \frac{\partial \theta}{\partial Y}, \frac{\partial C}{\partial Z}=0 \\
 &\text{at } Z=0, U=V=W=0, \frac{\partial \theta}{\partial Y}, \frac{\partial C}{\partial Y}=0 \\
 &\text{at } Z=1.0, 1.5, 2.0, U=V=W=0, \frac{\partial \theta}{\partial Y}, \frac{\partial C}{\partial Y}=0
 \end{aligned}$$

2.3. Computation method

A fine difference method was employed to solve the model equations numerically. The calculation algorithm of pressure terms is the HSMAC method. To solve the mathematical model we developed a home-made code based on the HSMAC method [12,13] that utilizes the finite differences approximation: second order central finite differences for the viscous terms, third order up-wind finite differences (UTOPIA) [14] for the convective terms, and first order forward finite differences for the time derivative.

Details of the numerical algorithm are given next. The discrete form of eq. (2) is

$$\frac{{}^m(\tilde{v}_x)_{i,j,k}^{n+1} - {}^m(\tilde{v}_x)_{i,j,k}^n}{\Delta \tau} = \frac{{}^m(\tilde{p})_{i,j,k}^{n+1} - {}^m(\tilde{p})_{i+1,j,k}^{n+1}}{\Delta \tilde{x}} + (DSFX)_{i,j,k}^n \quad (7)$$

$$\frac{{}^m(\tilde{v}_y)_{i,j,k}^{n+1} - {}^m(\tilde{v}_y)_{i,j,k}^n}{\Delta \tau} = \frac{{}^m(\tilde{p})_{i,j,k}^{n+1} - {}^m(\tilde{p})_{i+1,j,k}^{n+1}}{\Delta \tilde{y}} + (DSFY)_{i,j,k}^n \quad (8)$$

$$\frac{{}^m(\tilde{v}_z)_{i,j,k}^{n+1} - {}^m(\tilde{v}_z)_{i,j,k}^n}{\Delta \tau} = \frac{{}^m(\tilde{p})_{i,j,k}^{n+1} - {}^m(\tilde{p})_{i+1,j,k}^{n+1}}{\Delta \tilde{z}} + (DSFZ)_{i,j,k}^n \quad (9)$$

$$\frac{\theta_{i,j,k}^{n+1} - \theta_{i,j,k}^n}{\Delta \tau} = (DSEN)_{i,j,k}^n \quad (10)$$

Here n is the time step and m is the iteration index. $DSFX$, $DSFY$, $DSFZ$ and $DSEN$ stand for the convection and viscous terms. The grid nodes have the indices (i, j, k) in X , Y and Z directions, respectively.

The mass balance (1) provides an equation for pressure. Introducing the discrete derivative

$$D_{i,j,k}^{n+1} = \frac{(\tilde{v}_x)_{i,j,k}^{n+1} - (\tilde{v}_x)_{i-1,j,k}^{n+1}}{\Delta \tilde{x}} + \frac{(\tilde{v}_y)_{i,j,k}^{n+1} - (\tilde{v}_y)_{i,j-1,k}^{n+1}}{\Delta \tilde{y}} + \frac{(\tilde{v}_z)_{i,j,k}^{n+1} - (\tilde{v}_z)_{i,j,k-1}^{n+1}}{\Delta \tilde{z}} \quad (11)$$

The grid pressure $\tilde{P}_{i,j,k}$ may be calculated by Newton method

$${}^{m+1}(\tilde{p})_{i,j,k}^{n+1} = {}^m(\tilde{p})_{i,j,k}^{n+1} - {}^m D_{i,j,k}^{n+1} \left[\frac{\partial D_{i,j,k}}{\partial \tilde{p}_{i,j,k}} \right]^{n+1} = {}^m(\tilde{p})_{i,j,k}^{n+1} + \delta(\tilde{p})_{i,j,k}^{n+1} \quad (12)$$

The velocity is given by

$${}^{m+1}\tilde{v}_{x(i,j,k)}^{n+1} = {}^m\tilde{v}_{x(i,j,k)}^{n+1} + \left(\frac{\partial \tilde{v}_{x(i,j,k)}}{\partial \tilde{p}_{(i,j,k)}} \right)^{n+1} \delta \tilde{p}_{x(i,j,k)}^{n+1} \quad (13)$$

$${}^{m+1}\tilde{v}_{y(i,j,k)}^{n+1} = {}^m\tilde{v}_{y(i,j,k)}^{n+1} + \left(\frac{\partial \tilde{v}_{y(i,j,k)}}{\partial \tilde{p}_{(i,j,k)}} \right)^{n+1} \delta \tilde{p}_{y(i,j,k)}^{n+1} \quad (14)$$

$${}^{m+1}\tilde{v}_{z(i,j,k)}^{n+1} = {}^m\tilde{v}_{z(i,j,k)}^{n+1} + \left(\frac{\partial \tilde{v}_{z(i,j,k)}}{\partial \tilde{p}_{(i,j,k)}} \right)^{n+1} \delta \tilde{p}_{z(i,j,k)}^{n+1} \quad (15)$$

The calculation procedure is then:

1. Use eqs. (7), (8),(9) to compute the velocities $\{{}^{m+1}(\tilde{v}_x)_{i,j,k}^{n+1}, {}^{m+1}(\tilde{v}_y)_{i,j,k}^{n+1}, {}^{m+1}(\tilde{v}_z)_{i,j,k}^{n+1}\}$ for ${}^{m+1}\tilde{p}^{n+1} = {}^m\tilde{p}^n$.
2. Repeat the calculation until ${}^{m+1}D^{n+1} \leq \varepsilon$ is satisfied, eq. (10)-(15) [in this study $\varepsilon = 10^{-3}$]; report $(\tilde{v}_x)^{n+1}, (\tilde{v}_y)^{n+1}, (\tilde{v}_z)^{n+1}, \tilde{p}^{n+1}$.
3. Calculate θ^{n+1} using eq. (10).
4. Repeat the cycle 1-3, until the final time.

The third order upwind scheme (Utopia scheme) for the inertial terms of Eqs. (2)-(4) was applied to the calculation. The local Nu number on the hot wall was calculated from a Taylor series for the temperature field and the average Nu number was computed by integration over the hot wall. The time step width $\Delta \tau$ was 1×10^{-6} .

2.4. Computational meshes

Figure 4 indicates computational domain ($Z=1.0, 1.5, 2.0$). The computational meshes used the uniform grid, and the finite difference grid points in the X-, Y- and Z-directions were $80 \times 100 \times 80$, $80 \times 100 \times 120$, $80 \times 100 \times 160$.

Figure 4. Computational domain

3. Result and discussion

3.1. Overall system behaviour

Figure 5 shows change over time to flow distribution, temperature distribution, and concentration distribution for an X–Y plane at system depth coordinates $Z=0.5$. As density is stratified linearly under initial concentration conditions in these calculations, density strata interface behavior shows major changes over a short time when compared to standard density stratification. At $\tau=0.002$ (Fig. 5 (a)), immediately after calculation starts, currents appear in the previously-still solution, and a large-scale vortex rotating in a counter-clockwise direction is present near the center. Accompanying this, vortices form at opposed upper and lower corners of the system. As heating and cooling is conducted from left and right wall surfaces, influence on temperature distribution gradually becomes apparent in the solution. The initial linear state of concentration distribution strata can be confirmed as decaying from the system's central region. At $\tau=0.005$ (Fig. 5 (b)), the vortex near the center decays, and an inclined interface appears in contrast near the center. This formation is shaped largely in parallel to concentration and flow distributions, and heating and cooling areas from wall areas spread toward the center. Concentration distribution changes in a form similar to temperature distribution, and a concentration plume forms near the interface. Each condition becomes pronounced at $\tau=0.008$ (Fig. 5 (c)). Of the multiple plumes formed along concentration distribution lines in Fig. 3

(b), one plume is present in both the upper and lower high- and low-concentration sides. At $\tau=0.015$ (Fig. 5 (d)), currents have become extremely complex and 3-dimensional. In terms of temperature distribution, a higher temperature stratum is present at the top, and a low temperature stratum is present at the bottom. Furthermore, the inclined interface becomes vertical in terms of concentration distribution, disorder is present near the interface, and an unstable state can be seen.

Figure 5. Velocity vector, concentration and temperature distribution for $Z=2.0$ in depth length at $Z=0.5$.

3.2. Heat transfer characteristics

Figure 6 shows the variation of the average Nu number in the heated wall. Furthermore, during the figure show $Z=1.0, 1.5$, and 2.0 results. Overall changes in the Nu number are different with

pure convection as shown in Figure 6, uneven distribution. Minimum Nu number (position 1) to transition from thermal to thermal convection is less than pure convection. It is in due to the vertical density stratification. Then the Nu number increased with time and repeat the development layer, Nu number refers to the maximum value (position 2). However, for changing vertical from horizontal surface as shown in Fig. 5 (d), from heated wall heat transfer of cooling wall will be suppressed. As a result the Nu number is reduced again. Since then each layer blends Nu number increases again. And completely mixed, Nu number indicating steady-state value.

Note changes in the depth direction Z : increases the value of Z , and minimum value of the Nu number is even smaller. Also the Nu Max value has not been observed difference. The Nu number becomes a steady state value of time becomes shorter with increasing Z .

Figure 6. Average Nu number on the hot wall with time for $Z=1.0, 1.5$ and 2.0 in depth length

3.3. Influence of computational domain (depth length: Z)

Figure 7 shows $\tau=0.01$ at depths of $Z=1.0, 1.5$, and 2.0 for X - Y plane ($Z=0.5$) and Y - Z plane ($X=0.5$) and a 3-dimensional contour diagram of concentration. Overall concentration structure

near the interface can be confirmed as symmetrical along vertical and horizontal axes. For X–Y plane concentration distribution of $1.0 \times 1.25 \times 1.0$ (Fig. 7 (a)), the interface is inclined and interface between high and low concentrations is extended near the center. When Z is increased, it is clear that high and low concentration interface extension increases further near the center as shown in Fig. 7 (b) and (c). On the Y–Z plane, the same patterns form horizontally and vertically at the center as Z rises. In the 3-dimensional contour diagram, at $1.0 \times 1.25 \times 1.0$ (Fig. 7 (a)), a concentration distribution with significant curvature appears near the center of the interface. Additionally, concentration distribution is unstable vertically along the Y axis. When Z is increased even further, the curved interface near the center disappears, and the center changes to an extremely smooth interface as shown in Fig. 7 (b) and (c). Disorder near the center decreases in Y axis vertical concentrations as Z increases.

Figure 7. Concentration profile at $\tau = 0.01$

Similarly, Figure 8 shows the result of the concentration distribution in the $\tau=0.015$. Overall concentration distribution, as can be seen in the interface of the X-Y plane than in Figure 5, has the left and right opposite slope. In addition, the interface near it changes to a very complex structure. Further, when Z is large, as can be seen in the contour diagram, toward the center of the interface ($Z=0.5$) from the wall direction ($X=0, 1.0$) unevenness appeared on the structure of the interface, resulting in three-dimensional structure.

Figure 8. Concentration profile at $\tau=0.015$

4. Conclusions

We studied three-dimensional numerical calculations of double-diffusive convection in a rectangular parallelepiped enclosure filled with salt-stratified fluid under a horizontal

temperature difference for realistic values of parameters ($A=1.25$, $Ra=2.7\times10^7$, $N=0.882$, $Pr=7.15$ for an NaCl-H₂O system). The initial salt concentration linear profile was examined.

Three-dimensional numerical result with a high spatial resolution can capture the fine structures such as salt fingers and traveling plumes. In the linear profile, near the interface, vertical motion is dominant due to salt fingers in each layer. In addition, when the computational domain changes, it has a big influence on the behaviour of plume that appears on the diffusive interface. As a result, the mixing state of the entire faction is greatly different.

Nomenclature

A	aspect ratio $=h / b$
b	width of the system m
B	dimensionless width of the system
C	dimensionless concentration $=(c-c_{min}) / (c_{max}-c_{min})$
c	concentration kgm^{-3}
c_{max}	initial maximum concentration (initial concentration in a linear profile) kgm^{-3}
c_{min}	initial minimum concentration (initial concentration in a linear profile) kgm^{-3}
D	diffusion coefficient m^2s^{-1}
g	acceleration due to gravity ms^{-2}
h	height of the system m
H	dimensionless height of the system
Le	Lewis number $=\kappa/D$
N	buoyancy ratio $=\beta(c_{max}-c_{min}) / \{\alpha(T_{hot}-T_{cold})\}$
Nu_{ave}	average Nusselt number
p	pressure Pa
P	dimensionless pressure
Pr	Prandtl number $=\nu/k$
Ra	Rayleigh number $=g \cdot \alpha(T_{hot}-T_{cold}) \cdot b^3 / (\kappa \cdot \nu)$
T	temperature K
T_{cold}	temperature on the cold wall K
T_{hot}	temperature on the hot wall K
t	time s
U, V, W	dimensionless velocity

X, Y, W	dimensionless coordinate
<i>Greek symbols</i>	
α	volumetric coefficient of thermal expansion K^{-1}
β	volumetric coefficient of expansion with concentration m^3kg^{-1}
$\Delta\tau$	dimensionless time step
θ	dimensionless temperature $= (T - T_{cold}) / (T_{hot} - T_{cold})$
κ	Thermal diffusivity m^2s^{-1}
ν	Kinematic viscosity m^2s^{-1}
ρ	Density kgm^{-3}
τ	dimensionless time

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