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Three-dimensional numerical study on the effect of Schmidt and Rayleigh number on the flow patterns of bioconvection

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Abstract

We conduct a research on flow rate patterns of bioconvective model of microorganisms which are produced by swimming upward and gravity of the organisms using three dimensional numerical calculations. Simulation outcome shows that the Schmidt and Rayleigh number determine the fineness of the flow velocity. Moreover, it is shown that the best combination of these two parameters exists with which the finest flow velocity pattern realizes.

1. Introduction

Some kind of the flagellate forms a characteristic fluid motion called "bioconvection"(Kage et.al (2013)), which is caused by the density instability of microorganisms having the property of swimming upward (anti-gravitytaxis). Patterns of bioconvection are expected to vary with physical quantities, such as the swimming velocity of microorganisms and the density of microorganism. In order to find out the mechanism of bioconvection, numerical simulation is effective. Number of two-dimensional simulations using density model have been performed to find the most influential parameters to reproduce the experiment.

Nagata et al. (2016) compared bubble convection and bioconvection and showed that the Prandtl number differentiates between steady and unsteady states. At the same time, a crucial difference from bubbles was shown by numerical simulations; that was that the collapse pattern occurred. They concluded that the fact that microorganisms swimming upwards did not disappear at the top of the container unlike bubbles, and they possessed gravity caused the collapse pattern.

Meanwhile, Minakawa et al. (2018) conducted two-dimensional simulations under the constant Prandtl number and the several combinations of the Rayleigh and Schmidt numbers. According to them, the Schmidt number mainly formed the shape of the convection cell.

Furthermore, three-dimensional numerical attempts have been made in the past (Akaike et.al (2013)); however, realization of the reproduction was difficult. The reason for this is that, first, it required a large “machine-power” for three-dimensional numerical calculation, such as powerful calculators and a long simulation time; second, appropriate parameters were unknown to reproduce the steady state with fine convection pattern that had been found in the experiment.

In the present study, in order to surpass these hurdles, we prepare a simulation environment and investigate the effect of both the Schmidt and Rayleigh numbers applying the conditions of the past study carried out in two dimensions (Minakawa et.al (2018)).

2. Numerical methods

2.1 Basic equations of the density model

In this study, we use a density model in which microorganisms are expressed by volume density (Childress et al. 1975; Harashima et al. 1988). Basic equations of this model consist of Navier-Stokes equations and advection-diffusion equation for the volume density of microorganism. We employ Boussinesq approximation for the momentum equation, i.e. vertical direction of the Navier-Stokes equation has a gravity term that represents the gravity acts against the fluid element composed of the water and suspended microorganisms. Swimming speed of the microorganism appearing in the advection term in density equation is assumed to be constant.

The dimensionless basic equations are as follows:

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{\rho_w}\nabla p + \nu \nabla^2 \mathbf{v} + \boldsymbol{K}$$

$$\frac{\partial n_p}{\partial t} + u\frac{\partial n_p}{\partial x} + v\frac{\partial n_p}{\partial y} + \left(w + w_p\right)\frac{\partial n_p}{\partial z} = \kappa_h\left(\frac{\partial^2 n_p}{\partial x^2} + \frac{\partial^2 n_p}{\partial y^2} + \frac{\partial^2 n_p}{\partial z^2}\right) \tag{1}$$

where,

$\mathbf{v} = (u, v, w)$: velocity vector
t: time
ρ_w: fluid density
p: fluid pressure
ν: kinetic viscosity coefficient
$\boldsymbol{K} = (0, 0, -\frac{\Delta\rho}{\rho_0} g)$: external force per unit volume
$\Delta\rho_0$: density deviation caused by the presence of microorganisms
n_p: population density of microorganisms
g: gravitational acceleration
κ_h: diffusivity of microorganisms
w_p: swimming speed of microorganisms

Rayleigh number, Ra, Prandtl number, Pr and Schmidt number Sc are defined as follows:

$$\mathrm{Ra} = \frac{\rho_p - \rho_w}{\rho_w}\frac{gH^2 n_0}{w_p \nu}$$

$$\mathrm{Pr} = \frac{\nu}{w_p H} \tag{2}$$

$$\mathrm{Sc} = \frac{\nu}{\kappa_h}$$

where,

ρ_p: mass density of single microorganisms
H: characteristic length (depth of the vessel)
n_0: characteristic number density of microorganism (average density)

The Rayleigh number represents the ratio of the generation of torque by buoyancy to the dissipation of torque by viscosity. The Prandtl number represents the viscous diffusion time divided by the time during which the microorganisms pass the fluid layer. The Prandtl number in this study also corresponds to the reciprocal of the Reynolds number. The Schmidt number represents the ratio of the diffusion of the microorganisms to the diffusion of the fluid.

2.2 Numerical setup

We use fractional step method that is one variation of MAC method to solve the equations numerically. All spatial derivatives are approximated by the central differences. First-order Euler explicit method is applied for time-integration.

We compute the flow in three-dimensional rectangular domain, consisting of (x, y, z) = (4cm, 4cm, 0.4cm), which has (120, 120, 24) grids. Grid intervals $(\Delta x,\ \Delta y,\ \Delta z,\ \Delta t)$ are set to (0.033cm, 0.033cm, 0.017cm,1×10^{-4}seconds).

Boundary conditions are set assuming “rigid” (no-slip condition). Population density and pressure of microorganism also are set to 0 on the bottom, liquid surface and side. The number of microorganisms in the domain conserves during the calculation; the number density N on the boundary is set to zero gradient.

Because the microorganisms are randomly distributed in the initial state and are assumed to be stationary, the initial condition is that (u, v, w) = (0, 0, 0) and the population density of microorganisms is assigned normal random number.

We simulate number of cases modifying the Rayleigh and Schmidt numbers and observe changes of the convection patterns during 1000 seconds. The number of convection cell was counted in the simulation domain at the height of H/2 and it was defined as the fineness of the pattern.

Table1 shows the spec of Windows Servers utilized in the present study. Each simulation takes one to three weeks.

Table 1 Server system utilized for the numerical simulation

Processor	Intel®Xeon® CPU E5-2640 v4 @2.40GHz (3 processors)
Memory	2.00 GB
System	64 bits operating system, x64 base processor

3. Results and discussions

3.1 The study on the Schmidt number

We observe the distribution of vertical fluid velocity modifying the Rayleigh and Schmidt numbers. Table 2 and 3 summarize the number of the distribution of vertical velocity observed on the simulation domain at the final time (1000s)[1]. In both tables the vertical and horizontal axis represent the Rayleigh and Schmidt number, respectively. While the red color appeared in the pattern shows the upward flow velocity, the blue one represents the downward one. In Table 2 and 3 observations are performed at the center of vertical and horizontal axis, respectively.

Numerical calculation in the present study is initiated based on real data used by the bioconvection experiment (Kage et.al (2013)). Simulation results in the past study (Akaike et.al (2013)) were not necessarily corresponding to the steady state having a fine pattern of the flow observed in the experiment.

In the present study referring to the report by two-dimensional numerical calculation (Minakawa et.al (2018)), we modify the Schmidt and Rayleigh number, and observe the change of flow patterns.

First, the Schmidt number is increased. This is realized by decreasing the diffusivity of microorganisms (equation (2)).

Rayleigh number 7.80E + 11 is actual parameter used in the experiment. As shown in Table 2 and 3, although it is a steady state, fine patterns are not reproduced when the Schmidt number is set to 10. When Schmidt number equals 100, maintaining the same Rayleigh number, a finer pattern can be realized at the center of the vertical axis, but it cannot be said that it is sufficiently fine. At the same time, it can be seen in the Table 3 that horizontal flows exist at the center of the horizontal axis.

As the Schmidt number increases to 1000 and 10000, finer patterns than Sc = 100 can be seen at t = 50 to 100 seconds, but a pattern like “an explosion” occurs at t = 100 and 150 seconds, as Table 4 shows. Elucidation of the cause of this is the next challenge.

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[1] In this study, we do not calculate all combinations of Rayleigh and Schmidt number. Because we could not find the effectiveness of doing every single simulation as we proceed with the calculations. The omitted combinations are shaded in Tables 2 and 3.

Table 2 the state of the flow velocity at the center of the vertical axis (t=1000seconds)

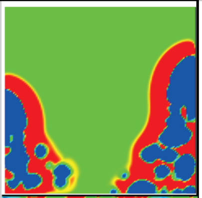
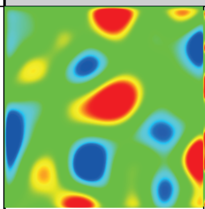
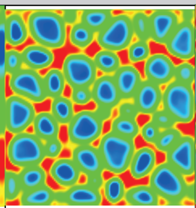
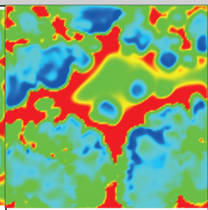
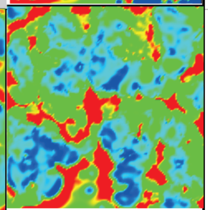
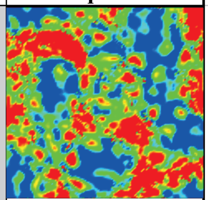
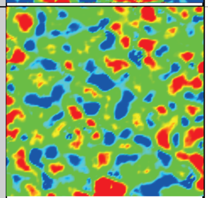
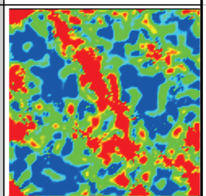
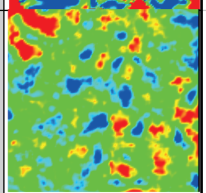
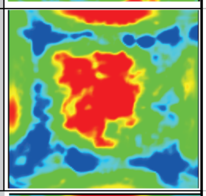
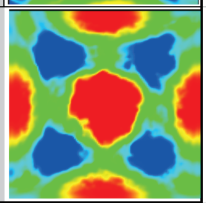
		Schmidt number			
		10	100	1000	10000
Rayleigh number	7.84E+10	no calculation			
	7.84E+11			 explosive	 explosive
	1.96E+12	no calculation			
	3.92E+12	no calculation			
	5.88E+12	no calculation			
	7.84E+12	no calculation			
	3.92E+13	no calculation			
	7.84E+13	no calculation			

Table 3 the state of the flow velocity at the center of the horizontal axis (t=1000seconds)

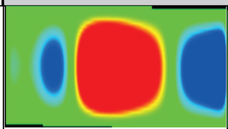
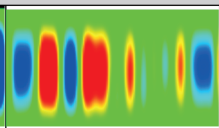
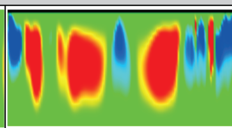
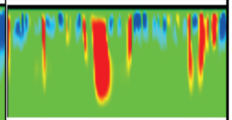
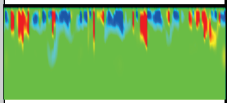
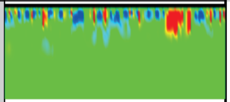
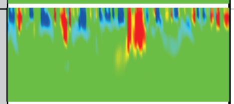
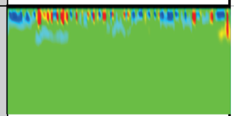
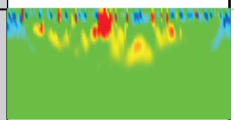
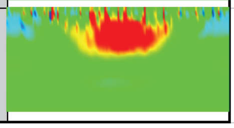
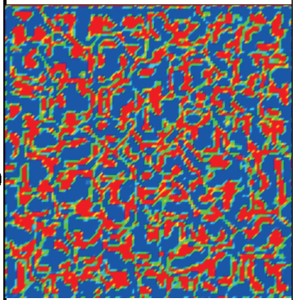
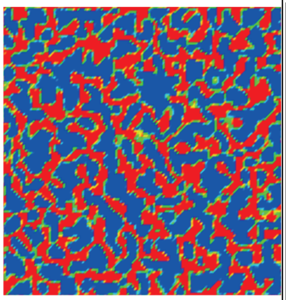
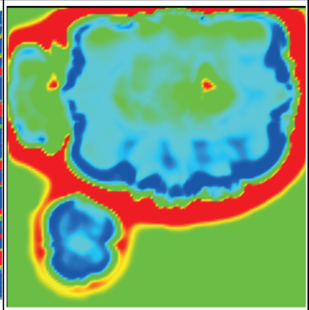
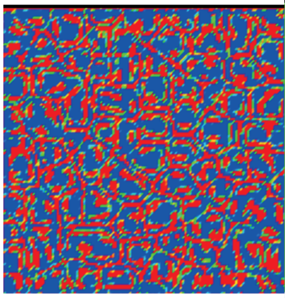
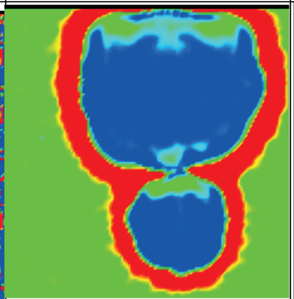
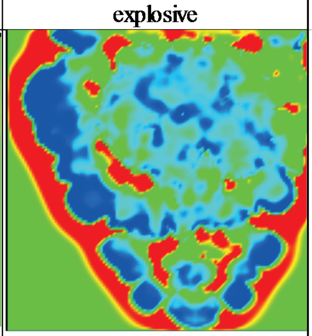
Rayleigh number		Schmidt number			
		10	100	1000	10000
	7.84E+10	no calculation			
	7.84E+11			 explosive	 explosive
	1.96E+12	no calculation			
	3.92E+12	no calculation			
	5.88E+12	no calculation			
	7.84E+12	no calculation			
	3.92E+13	no calculation			
	7.84E+13	no calculation			

Table 4 Flow velocity pattern changing with time transition at the center of the vertical axis (the Rayleigh number = 7.84E+11)

		time (seconds)		
		50	100	150
Schmidt number	1000			 explosive
	10000		 explosive	 explosive

3.2 The study on the Rayleigh number

Next, the Rayleigh number is changed. Since one of the objectives of this research is reproduction of fine patterns appeared in the experiments, we attempt to reproduce these patterns by changing the Rayleigh number with Schmidt number fixed to 10000.

At the same time, we look for the Rayleigh numbers so that the explosion pattern discussed in 3.1 would not occur. We modify Rayleigh numbers by changing the characteristic density of microorganism to the average density (equation (2)).

As summarized in Table 2, when the Rayleigh number is changed, the steady state of the flow velocity pattern also changes. It can be said that Rayleigh number = 3.92 E + 12 realizes the finest pattern.

In this case, no explosion pattern can be observed; furthermore, as shown in Fig. 1, the number of convection cell also becomes steady with the lapse of time.

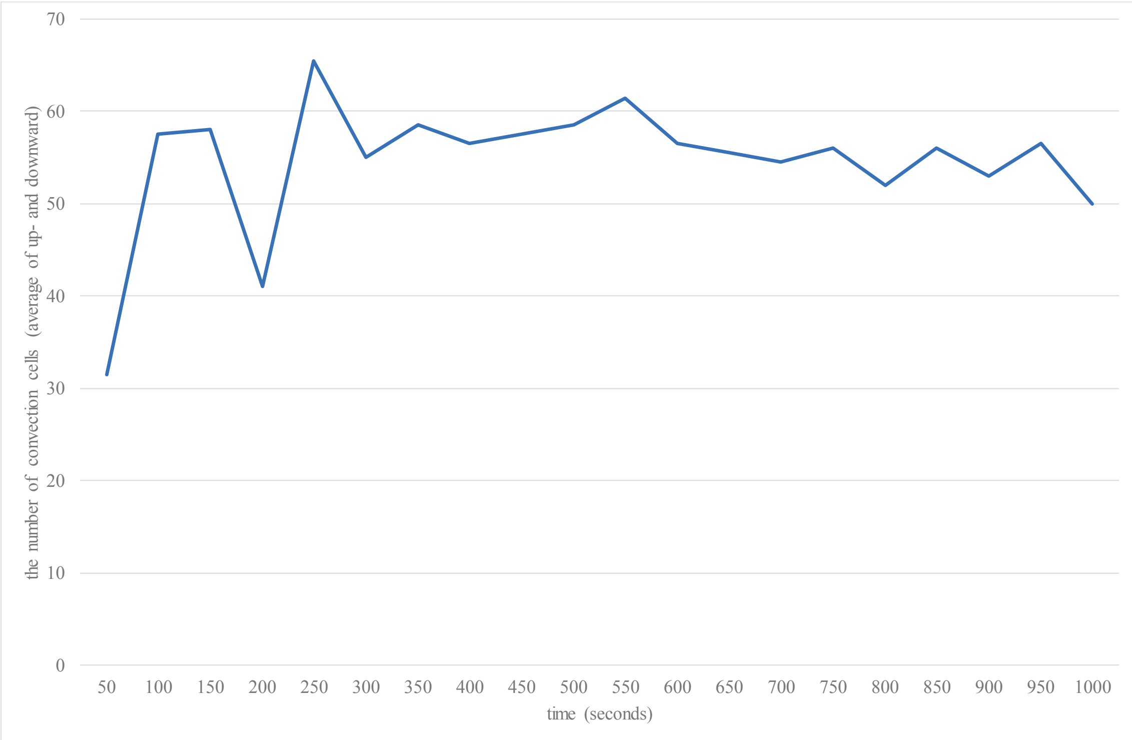


Figure 1 The number of convection cells as the time lapses (Sc=10000, Ra=3.92 E + 12)

3.3 Discussions

We perform three-dimensional numerical simulation on bioconvection patterns, and find that both the Schmidt and the Rayleigh numbers clearly have influence on the flow velocity pattern. A combination of both numbers exists to make the flow velocity pattern finer: that is the Schmidt and the Rayleigh number equal 10000 and 3.92E+12, respectively.

In the past research using two-dimensional numerical calculation, we could observe the steady state flow, but in the three-dimensional calculation, the steady state is closer to turbulent flow pattern. From this, we presume that it becomes unstable due to the increase of the degree of freedom.

We have tried to find the parameters that make finer convection pattern, but the steady pattern obtained in the experiment does not occur in this simulation. Considering this, we would like to refine simulation results further by introducing a motion model of microorganisms.

4. Summary and future work

In this research a three-dimensional numerical simulation of microorganism model is conducted.

In reproducing the fine pattern observed in the experiment, the Schmidt and Rayleigh number proved to be effective parameters. The pattern becomes finer as the Schmidt number increases; nevertheless, when Schmidt number = 1000 or more, explosion patterns are recognized at the early stage (100 secs) of simulation.

Furthermore, as the Rayleigh number is increased, this explosion pattern disappears and the finest pattern is obtained with the Rayleigh number = 3.92 E + 12. However, if the Rayleigh number is further increased, the pattern becomes coarser.

Future research topics include the following:
1. Consider further the Rayleigh number at the Schmidt number = 100
2. Identify the cause of the explosion
3. Perform more sophisticated calculations by increasing the number of grids
4. Apply a petri dish domain to match the experiment
5. Modify density instability model

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