

Numerical investigation of falling bacterial plumes caused by bioconvection in a three-dimensional chamber

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HIGHLIGHTS

- We investigate numerically the nonlinear dynamics of a 3D chemotaxis–fluid system without linearization and axisymmetry.
- We use an operator splitting–type Navier–Stokes solver to avoid a too strong restriction on the time step.
- We observe the formation of falling plumes and the convergence towards numerically stable stationary plumes.

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ABSTRACT

Oxytactic bacteria like *Bacillus subtilis* are denser than water and swim up an oxygen gradient as they require certain minimum concentration of oxygen to be active. Due to upswimming, bacteria accumulate in a layer below the water surface and the density of an initially uniform suspension becomes greater near the water surface than the water bottom. When the upper bacteria-rich boundary layer is too dense, it becomes unstable and an overturning instability develops, leading to the formation of falling bacterial plumes. Bioconvection in modestly diluted cell suspensions is described by equations for concentrations of bacteria and oxygen together with the Navier–Stokes equations and the continuity equation. In this paper, we investigate numerically falling bacterial plumes caused by bioconvection in a three-dimensional chamber by solving the full chemotaxis–fluid coupled system. In numerical simulations of the system, the admissible time step is restricted by stability criteria due to a high Schmidt number, which corresponds to highly viscous fluids or low diffusion rates of bacteria. In order to avoid a too strong restriction on the time step, we use an operator splitting–type Navier–Stokes solver: the advection term is solved using a semi-Lagrangian method and the diffusion term is solved using the backward Euler method. We present numerical examples showing the formation of falling bacterial plumes out of random initial data and the convergence towards stationary bacterial plumes. And the merging of neighboring plumes is observed for a specific parameter set.

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1. Introduction

In this paper, we consider the formation of falling plumes in a three-dimensional chamber that contains a suspension of oxytactic bacteria like *Bacillus subtilis* [1–3]. These bacteria are denser than water, consume oxygen, and swim up an oxygen gradient as they require certain minimum concentration of oxygen to be active. The upper surface of the chamber is open to the atmosphere and oxygen is replenished by diffusion from that surface. In a shallow

chamber, the oxygen concentration throughout the chamber is high enough to allow all bacteria to swim actively. But, if the chamber is deep, the oxygen concentration below a certain depth is very low (since the diffusivity of oxygen in water is very small and bacteria consume oxygen) and, therefore, bacteria in the lower region of the chamber become inactive. Due to upswimming, bacteria accumulate in the upper layer of water and the density of an initially uniform suspension becomes greater at the top than the bottom. When the upper bacteria-rich boundary layer is too dense, it becomes unstable and an overturning instability develops, leading to the formation of falling bacterial plumes. The plumes transport bacteria and oxygen from the upper boundary layer, which is rich in bacteria and oxygen, to the lower region of the chamber, which is depleted of both bacteria and oxygen.

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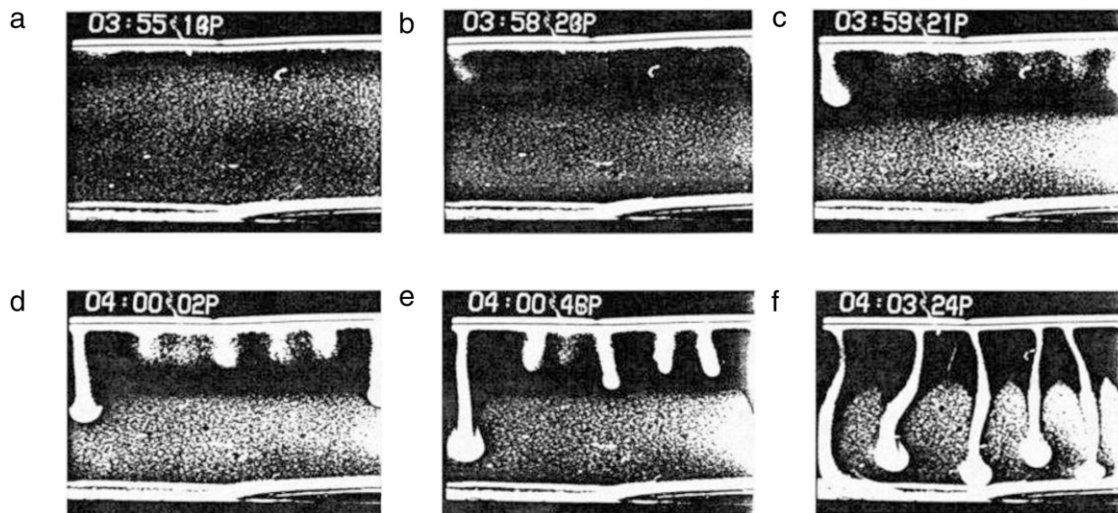


Fig. 1. Time sequence of photographs of a deep chamber containing a suspension of oxytactic bacteria like *Bacillus subtilis*. The successive times are shown at the upper left of each photograph.

Source: Photograph reproduced from Hillesdon et al. [1].

Fig. 1 shows time sequence of photographs of a deep chamber containing a suspension of bacteria reproduced from Hillesdon et al. [1]. The initial suspension is well mixed and quasi-homogeneous (Fig. 1(a)). First, a bacteria-rich upper boundary layer develops near the surface as bacteria swim up an oxygen gradient (Fig. 1(b)). Later, in Fig. 1(c)–(e), we can see the formation of falling bacterial plumes as the upper layer becomes unstable. The bacteria-rich plumes, which descend from the surface, carry oxygen from the surface and, in Fig. 1(f), some of the inactive bacteria in the lower region have been resuscitated by the oxygen carried by the descending plumes.

Bioconvection [4–7] in modestly diluted cell suspensions is described by equations for concentrations of bacteria and oxygen are coupled with the incompressible Navier–Stokes equations and the continuity equation. Hillesdon and Pedley [8] analyzed the linear stability for this chemotaxis–fluid coupled system and Metcalfe and Pedley [9] discussed the weakly nonlinear stability. Lorz [10] obtained a local existence result for the system and related systems. Duan et al. [11] proved global existence for the system with the simpler Stokes equations for weak potential or small initial oxygen concentration. Di Francesco et al. [12] investigated existence issues and asymptotic behavior of a model with nonlinear cell diffusion in the bacteria equation.

Harashima et al. [13] simulated gravitactic bioconvection in two dimensions and studied the evolution of bioconvection from an initially uniform state. Ghorai and Hill [14–16] investigated the structure and stability of two-dimensional gyrotactic plumes in tall, narrow chambers with either stress-free sidewalls or periodic sidewalls using a conservative finite-difference scheme. They also studied gyrotactic bioconvection in an axisymmetric chamber [17]. Chertock et al. [18] derived a high-resolution vorticity-based hybrid finite-volume finite-difference scheme to understand the interplay of gravity and chemotaxis in the formation of two-dimensional plumes. All the computations in [13–18] were based on continuum models. Hopkins and Fauci [19] simulated two-dimensional bioconvection using point particles rather than a continuum model and examined the general effects of a variety of different responses by the micro-organisms, including geotaxis, gyrotaxis, and chemotaxis.

Although there have been many numerical studies in two dimensions [13–19], bioconvection in three dimensions has not been well simulated due to computational difficulties, except the works of Ghorai and Hill [20] and of Karimi and Paul [21]. However,

they concerned with gyrotaxis only (not chemotaxis) and used a low Schmidt number ($= 20$), in which the Schmidt number is a dimensionless number defined as the ratio of viscosity and mass diffusivity. Note that a typical value of the Schmidt number for *Bacillus subtilis* in water is 500 [3,18].

Although it is relatively easy to solve the two-dimensional problem, bioconvection is intrinsically three-dimensional. In this paper, we therefore investigate a realistic three-dimensional bioconvection model. This work, for the first time to the authors' knowledge, considers the nonlinear dynamics of a three-dimensional chemotaxis–fluid system without linearization and axisymmetry. And, to avoid a too strong restriction on the admissible time step in numerical simulations of the system due to a high Schmidt number, we use an operator splitting-type Navier–Stokes solver: the advection term is solved using a semi-Lagrangian method and the diffusion term is solved using the backward Euler method.

The paper is organized as follows. In Section 2, we introduce the governing equations and perform the nondimensionalization of the governing equations. In Section 3, a numerical solution is given. We present numerical examples showing the formation of falling bacterial plumes out of random initial data and the convergence towards stationary bacterial plumes in Section 4. And the merging of neighboring plumes is observed for a specific parameter set. Finally, conclusions are drawn in Section 5.

2. Governing equations

Several related coupled chemotaxis–fluid model systems have been proposed and studied in [1–3,18] to describe bioconvection of a suspension of oxytactic bacteria in an incompressible fluid under the assumptions that the contribution of bacteria to the bacteria–fluid suspension is sufficiently small (since the density of the bacteria suspension is approximately equal to the density of the fluid) and that more detailed cell–cell interactions (such as hydrodynamic interaction) are neglected. The system, in which equations for concentrations of bacteria (n) and oxygen (c) are coupled with the incompressible Navier–Stokes equations (using the Boussinesq approximation) and the continuity equation, is as follows:

$$n_t + \mathbf{u} \cdot \nabla n = D_n \Delta n - \chi \nabla \cdot [nr(c)\nabla c], \quad (1)$$

$$c_t + \mathbf{u} \cdot \nabla c = D_c \Delta c - n\kappa r(c), \quad (2)$$

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