Modelling pattern formations of bacteria: influence of gravity

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Introduction

In microcontainers, growing bacterial colonies of various species self-organize and form patterns. Often during physical experiments, the formation of plumes can be observed: vertical structures descending from the larger aggregate of bacteria near the top of the microcontainer. The mechanism of plume formation is still poorly understood, but the use of mathematical modelling can help fill the gaps of knowledge.

Studies of mathematical models for bacterial pattern formation have intensified since the introduction of Keller–Segel partial differential equations model for chemotaxis in 1971 [1]. When modelling *Escherichia coli*, experiments have shown that the dynamics of oxygen have to be taken into account [2]. Hillesdon et al. have shown that by coupling the Keller–Segel model with the fluid flow equation, plume formation can be modelled in colonies of *Bacillus subtilis* [3].

The aim of this work

is to investigate the effects of gravity on the modelled *Escherichia coli* plume formation, and to investigate the influence of these dimensionless model parameters: Schmidt number, Rayleigh number, and oxygen cut-off threshold [4].

Governing equations

The dynamics of an *E. coli* population are described by a system of Keller–Segel type equations coupled with Navier–Stokes incompressible fluid equations in the stream-vorticity formulation:

$$\frac{\partial n}{\partial t} + \mathbf{u}\cdot\nabla n = D_n \Delta n - \chi \nabla(n \nabla c) + \alpha n\left(1 - \frac{n}{o}\right),$$

$$\frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = \Delta c + \frac{n}{1+\beta n}\Theta(o_{max} - o) - c,$$

$$\frac{\partial o}{\partial t} + \mathbf{u}\cdot\nabla o = D_o \Delta o - \lambda n,$$

$$\frac{\partial \omega}{\partial t} + \mathbf{u}\cdot\nabla \omega = \nu \Delta \omega - \kappa \nu \frac{\partial n}{\partial x},$$

$$\Delta \Psi = -\omega$$

$n(x,y,t)$ – cell density,
$c(x,y,t)$ – chemoattractant concentration,
$o(x,y,t)$ – oxygen concentration,
$\omega(x,y,t)$ – vorticity vector,
$\Psi(x,y,t)$ – stream function,
$\mathbf{u} = \left(u_x(x,y,t), u_y(x,y,t)\right)$ – velocity field of the water,
D_n, D_o – diffusion coefficients,
χ – chemotactic sensitivity,
α – cell population growth rate,
β – saturating chemoattractant production rate,
λ – oxygen consumption rate,
o_{max} – maximal oxygen concentration for activity,
ν – Schmidt number,
κ – Rayleigh number.

Vorticity function ω and stream function Ψ are defined as follows:

$$\omega = \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y}, \quad u_x = \frac{\partial \Psi}{\partial y}, \quad u_y = -\frac{\partial \Psi}{\partial x}.$$

Modeling domain

The spatiotemporal pattern formation was modeled in the liquid cultures of luminous *E. coli* near the inner latter surface of a circular micro-container.

The 2D domain of the dimensionless model is

$$(x,y) \in [0,l] \times [0,h], \quad l = 5.6\pi, \quad h = 0.45l$$

The initial values of the model:

$$n(x,y,0) = 1 + \xi(x,y), \;\; c(x,y,0) = 0, \;\; o(x,y,0) = o_0,$$

ξ is a 10% random perturbation, o_0 is the oxygen concentration near the upper contact surface.

The boundary conditions for n and c are no-penetration at the bottom and the top of the domain, for o are no-penetration at the bottom and fixed at the top of the domain. The boundary conditions at the sides of the domain are periodic.

Numerical simulation

Because of nonlinearity, the initial value problem was solved numerically using hybrid implicit-explicit finite difference technique.

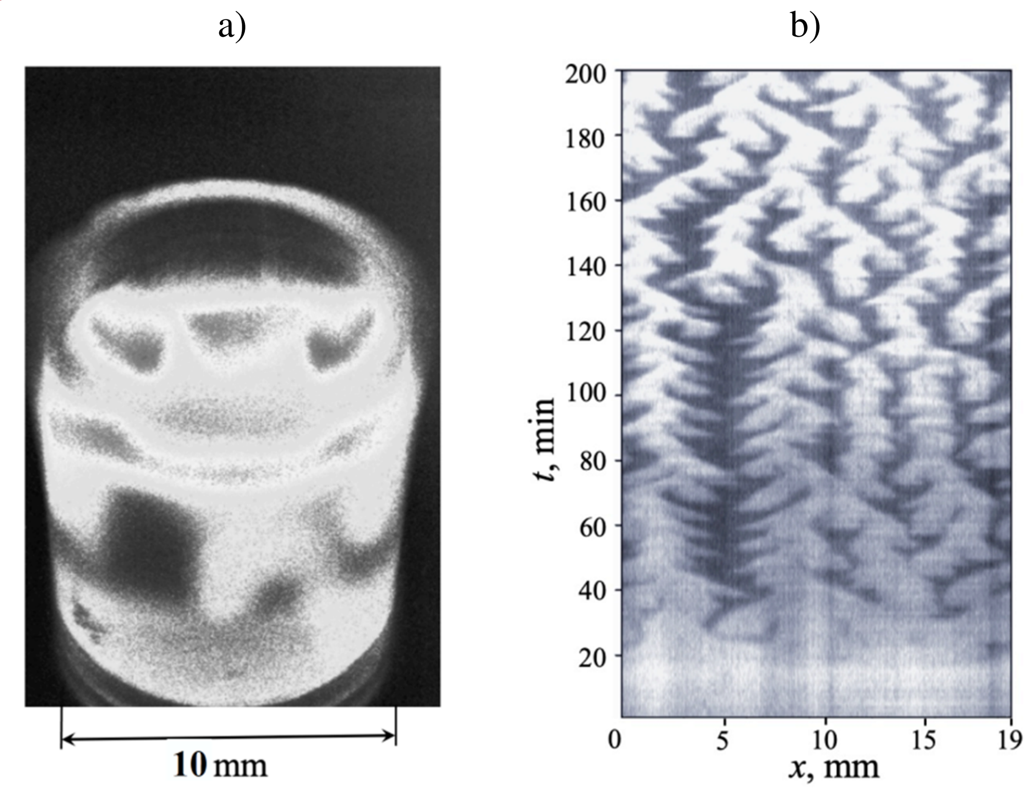
A uniform discrete grid 250×112 in space dimensions, and a constant dimensionless time step in the interval $[2 \cdot 10^{-4}, 5 \cdot 10^{-4}]$ was used.

Simulator was programmed in Python programming language using the NumPy package, and the results have been visualized using Matplotlib library.

Model parameters

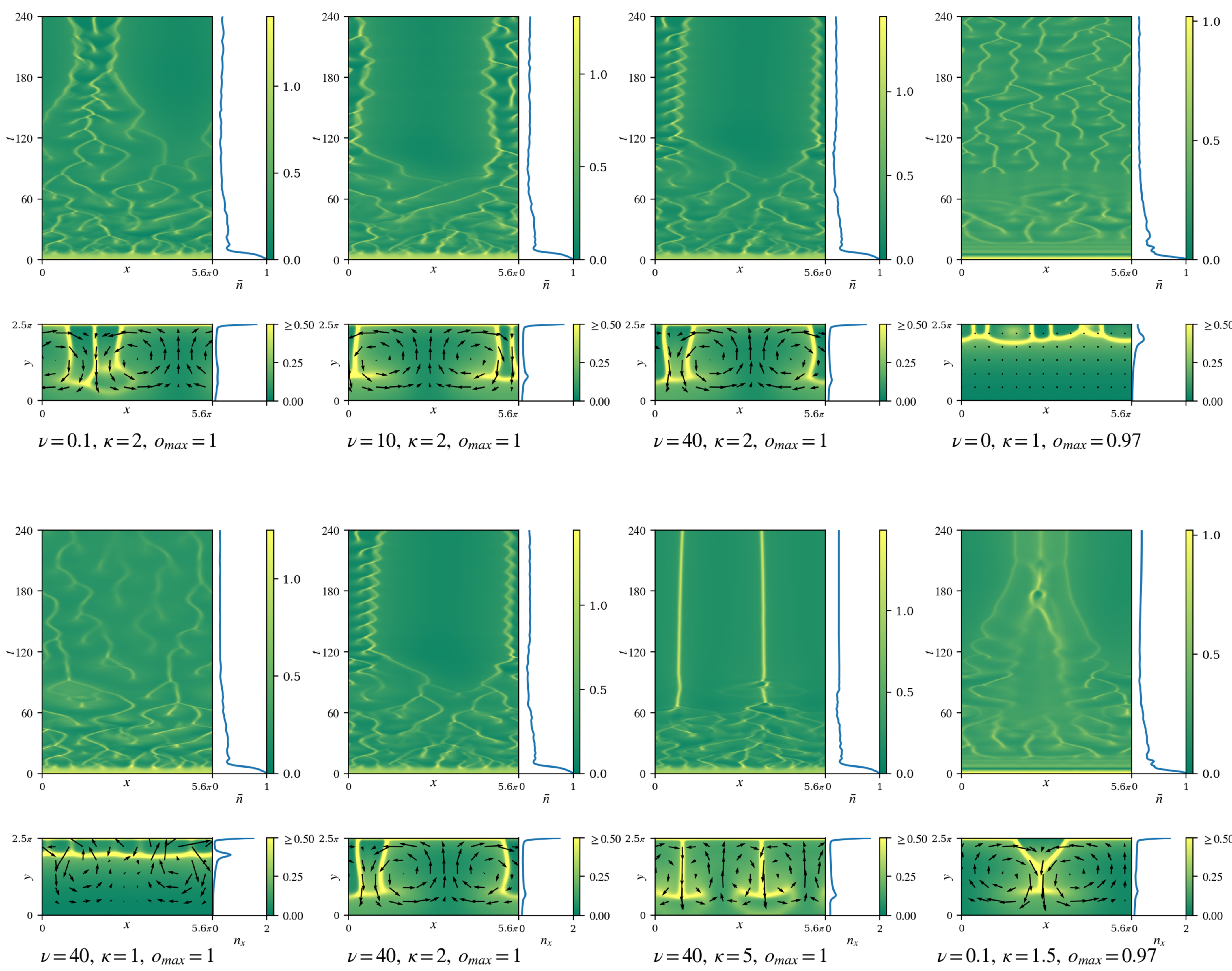
$\alpha = 1, \quad \beta = 0.73, \quad \lambda = 0.048, \quad \chi = 8.3,$
$D_n = 0.04, \quad D_o = 0.12, \quad o_0 = 1$

Experimental data



Experimental data examples: a) perspective view of the bioluminescent culture [5], *b) spatiotemporal plot of bioluminescence near the contact line* [2]

Simulation results



Visualization of cell density: spatiotemporal plots showing dynamics of cell densities, and cell densities at dimensionless time moment t=240, simulated using parameters shown.

Conclusions

Reaction–diffusion–chemotaxis model, coupled with the incompressible Navier–Stokes equations and a cut-off mechanism, can simulate mushroom-shaped plume-like patterns resembling bioluminescence patterns.

Plumes form in simulated bacterial patterns only when the Rayleigh number κ exceeds a critical value, which depends on the Schmidt number. As the Schmidt number ν increases, plumes form earlier.

Once the simulation reaches a quasi-stable state, the Schmidt number has only a small effect on the plume form, even for large differences in parameter ν values.

References

1. E.F. Keller, L.A. Segel, Model for chemotaxis, *J. Theor. Biol.*, 30(2):225–234, 1971
2. R. Šimkus, R. Baronas, Ž. Ledas, A multi-cellular network of metabolically active *E. coli* as a weak gel of living Janus particles, *Soft Matter*, 9(17):4489–4500, 2013.
3. A.J. Hillesdon, T.J. Pedley, O. Kessler, The development of concentration gradients in a suspension of chemotactic bacteria, *Bull. Math. Biol.*, 57:299–344, 1995.
4. B. Dapkūnas, R. Baronas, R. Šimkus, Effect of gravity on the pattern formation in aqueous suspensions of luminous *Escherichia coli*, *Nonlinear Anal.-Model. Control*, 30(2):346–365, 2025.
5. R. Šimkus, R. Baronas, Metabolic self-organization of bioluminescent Escherichia coli, *Luminescence*, 26(6):716–721, 2011.