Influence of Oxygen Consumption Rate Modulation on Bacterial Pattern Formation Models

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Introduction

Mathematical bacterial pattern formation models have been studied since the 1970s. Most models are based on Keller-Segel equations. In this approach, the dynamics of the bacteria population is modeled using a system of nonlinear reaction-diffusion-chemotaxis partial differential equations [1].

Escherichia coli exhibits attraction to self-excreted chemoattractant. It was also shown that the activity of *E. coli* depends on available oxygen [2]. The dynamics of oxygen consumption rate play an important part in the pattern formation. Multiple methods of oxygen consumption rate modulation have been used in different studies. The interactions between several active processes lead to very complex dynamic systems that are still poorly understood.

The model involving chemoattractant and oxygen dynamics is used to simulate the 2D patterns in bacterial populations near the inner lateral surface of a cylindrical micro-container.

The aim of this work

is to examine the effects of different functions modulating the oxygen consumption rate on the spatiotemporal pattern formation of luminous bacteria.

Governing equations

The dynamics of an *E. coli* population has been described by a system of three Keller-Segel type reaction-diffusion-chemotaxis equations, which in the dimensionless form read

$$\frac{\partial n}{\partial t} = D_n \Delta n - \chi \nabla (n \nabla c) + \alpha n f_n(n,o),$$

$$\frac{\partial c}{\partial t} = \Delta c + n\, f_c(n,o) - c,$$

$$\frac{\partial o}{\partial t} = D_o \Delta o - \lambda n\, f_o(n,o),$$

$n(x,y,t)$ – cell density,
$c(x,y,t)$ – chemoattractant concentration,
$o(x,y,t)$ – oxygen concentration,
D_n, D_o – diffusion coefficients,
χ – chemotactic sensitivity,
α – growth rate of the cell population,
λ – oxygen consumption rate,
$f_n(n,o)$, $f_c(n,o)$, $f_o(n,o)$ – rate modulation functions

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

$$(x,y) \in [0,l] \times [0,h], \quad l = 4.6\pi, \quad h = 0.45l$$

The initial values of the model:

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

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 finite difference technique.

A uniform discrete grid 250×112 was introduced in space directions and the constant dimensionless step size 5×10^{-4} was used in the time direction.

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

Rate modulation functions used

A. Oxygen-dependent carrying capacity [3,4]

$$f_n(n,o) = 1 - \frac{n}{o},$$
$$f_b(n,o) = \frac{o^p}{1+\beta n},$$
$$f_o(n,o) = o^p.$$

B. Saturating cell growth [5]

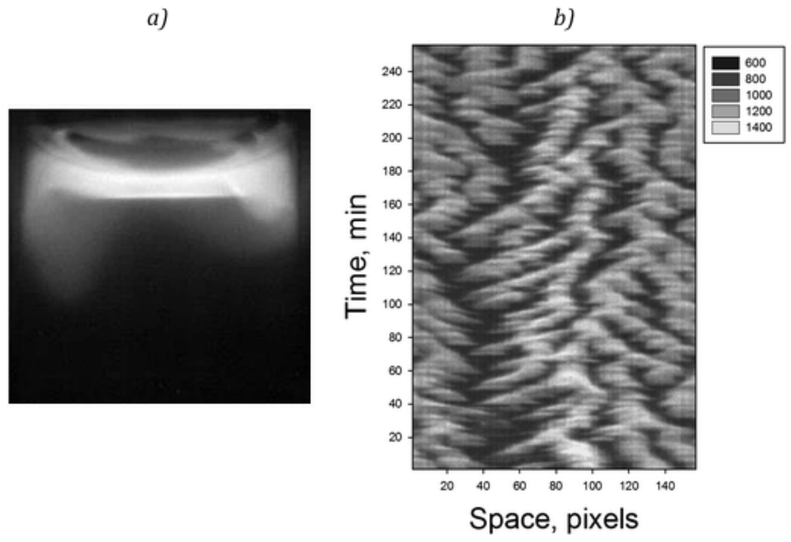
$$f_n(n,o) = \delta \frac{o^p}{1+\gamma o^p} - n,$$
$$f_c(n,o) = \frac{o n^{p-1}}{1+\beta n^p},$$
$$f_o(n,o) = \frac{o^p}{1+\gamma o^p}.$$

C. Cut-off approach [6]

$$f_n(n,o) = \theta(o - o^*) - n,$$
$$f_c(n,o) = \frac{\theta(o-o^*)}{1+\beta n},$$
$$f_o(n,o) = \theta(o - o^*).$$

p – influence of oxygen,
β – saturating chemoattractant production,
δ – optimal growth rate of the cell population,
γ – saturating cell growth,
$\theta(u)$ – Heaviside function,
o^* – oxygen consumption cut-off value.

Experimental data

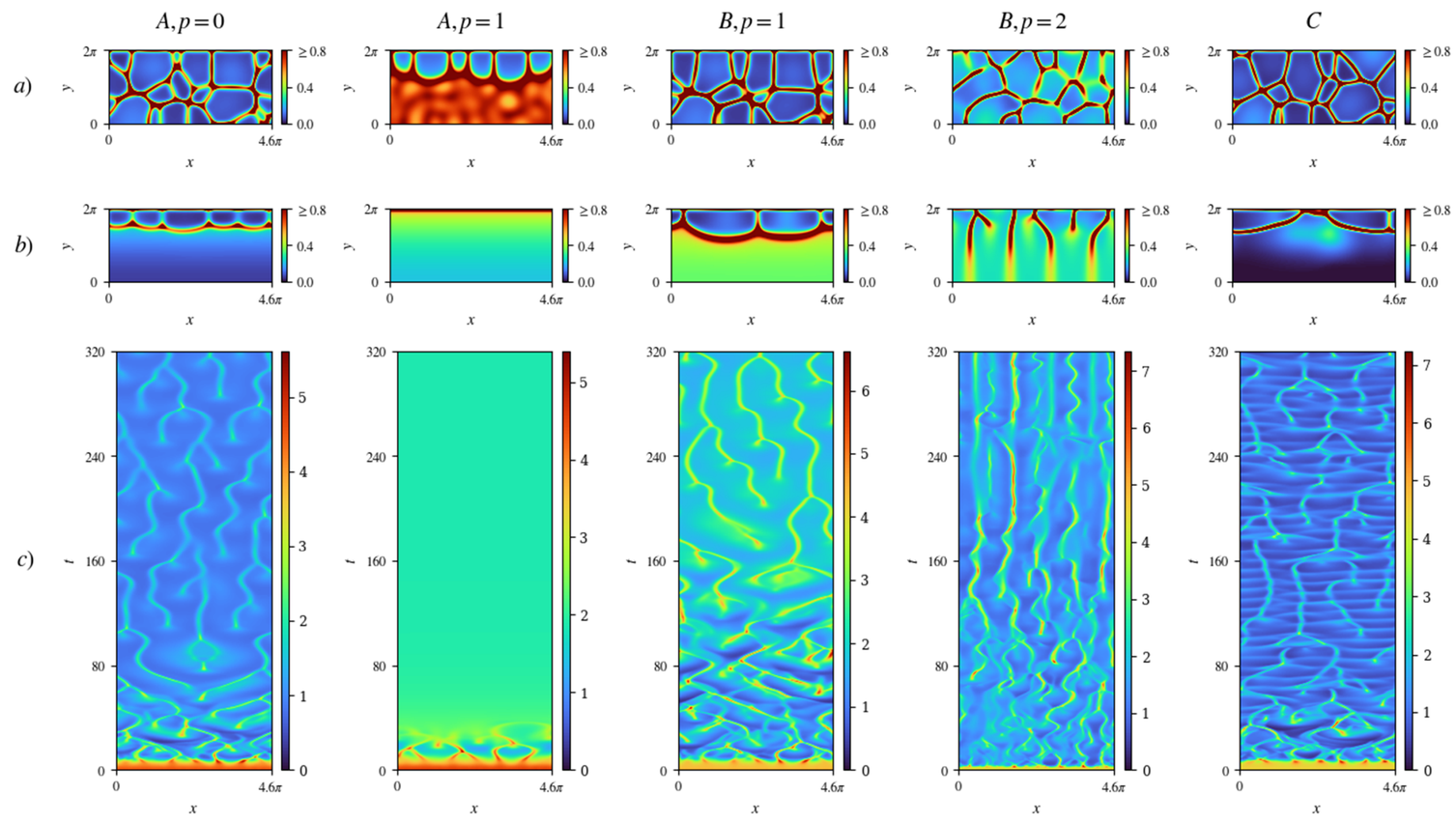


Experimental data examples: a) bioluminescence as seen from the side of a cylinder tube [7], b) spatiotemporal plot of bioluminescence near the contact line [2]

Model parameters

$\alpha = 1$, $\beta = 0.73$, $\lambda = 0.048$, $\chi = 8.3$,
$D_n = 0.04$, $D_o = 0.12$, $\delta = 2.4$, $\gamma = 1.5$,
$o_0 = 1$, $o^* = 0.2$

Simulation results



Visualization of cell density. a) and b) is cell density at time T=10 and T=320 respectively. c) Spatiotemporal plot showing dynamics of cell density.

Conclusions

The developed computational model can be used to investigate the effect of the modulation of the oxygen consumption rate on the bacterial self-organization in liquid unstirred cultures.

The form of the rate modulation functions is of crucial importance to the bacterial pattern formation.

Different forms of the modulation functions allow to simulate different features of experimentally observed patterns more adequately.

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