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# MODELING AND ANALYSIS OF ACTIVE AND PASSIVE PARTICLE SELF-FORMATIONS

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## **Abstract**

Growing bacteria populations form structured patterns. A lot of research has been focused on creating mathematical models accurately describing this formation. We give overview of several mathematical models describing bacteria growth using either Keller-Segel equations, or reaction-diffusion-advection equations.

**Keywords:** bacterial growth, Keller-Segel equations, reaction-diffusion-advection equations

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## 1 Introduction

It has been noticed in empirical experiments, that growing bacteria form downward facing structures, usually called plumes (see Fig. 1). Numerous mathematical models accurately describing surface layer structures of bacteria populations have been proposed [KS71, ZHCGG05]. Models explaining plume formation have been researched much more frequently recently [CFK<sup>+</sup>12, ADR19].

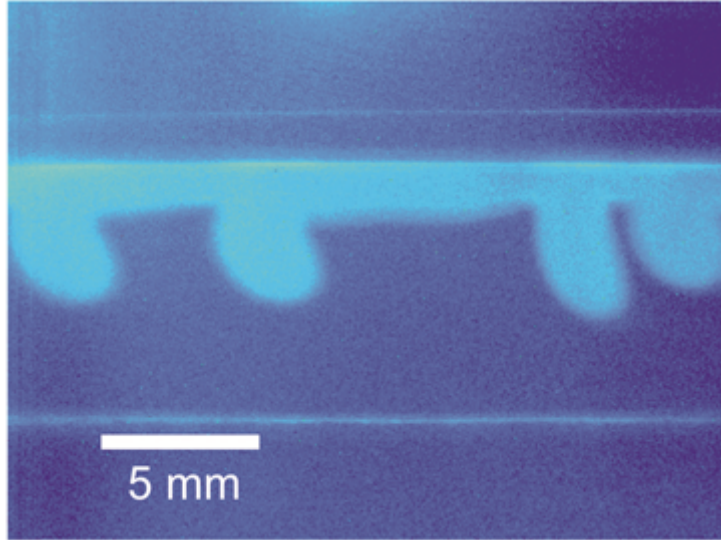


Figure 1: Bacteria plumes.

One of the objectives of doctoral thesis is to propose a two dimensional mathematical model describing plume formation in populations of bacteria.

## 2 Mathematical models for bacteria populations

*Copied from early draft of literature review section.*

### 2.1 Keller-Segel type models

Classical Keller-Segel model for chemotaxis introduced in 1971 [KS71] is composed by a set of two equations:

$$\begin{aligned}\frac{\partial u}{\partial t} &= \nabla(D_u \nabla u - \chi(u, v)u \nabla v) + f(u, v), \\ \frac{\partial v}{\partial y} &= \nabla(D_v \nabla v) + g_p(u, v)u - g_d(u, v)v,\end{aligned}\tag{1}$$

where  $x$  and  $t$  is space and time,  $u(x, t)$  is bacteria density,  $v(x, t)$  is chemical attractant concentration,  $D_u$  and  $D_v$  are diffusion coefficients,  $\chi(u, v)$  is chemotactic sensitivity,

$f(u, v)$  regulates bacteria growth and death,  $g_p$  and  $g_d$  regulate production and degradation of chemical attractant.

Keller-Segel type models remain some of the most frequently used models for chemotaxis in both 1-dimensional [Led16, PH11] and 2-dimensional [KOST12, CFK<sup>+</sup>12] modelling.

Important variants of this model: [Led16] (additional oxygen equation), [CFK<sup>+</sup>12] (plume formation).

## 2.2 Reaction-diffusion-advection equations

Another popular way to model chemotaxis is using reaction-diffusion-advection equations. General form of the equation is:

$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u) - \nabla \cdot (vu) + f(u), \quad (2)$$

where where  $x$  and  $t$  is space and time,  $u(x, t)$  is bacteria density,  $D$  is diffusion coefficient,  $v$  is velocity field, and  $f(u)$  represents chemical reactions.

Important variants of this model: [ADR19] (adds fluid dynamics using Navier-Stokes equations), [ZHCGG05].

## 3 Reproduction of experiments

As an introduction to numerical simulation of mathematical models, two experiments were reproduced.

### 3.1 One dimensional model

To simulate pattern formation of luminous *Escherichia coli* bacteria colony along the contact line of a circular container a dimensionless mathematical model using Keller-Segel equations was introduced [BŠ11]:

$$\begin{aligned} \frac{\partial u}{\partial t} &= D \frac{\partial^2 u}{\partial x^2} - \frac{\partial}{\partial x} \left( \frac{\chi u}{(1 + \alpha v)^2} \frac{\partial v}{\partial x} \right) + \gamma r u (1 - u), \\ \frac{\partial v}{\partial t} &= \frac{\partial^2 v}{\partial x^2} + \gamma \left( \frac{u^p}{1 + \beta u^p} - v \right), \quad x \in (0, 1), \quad t > 0, \end{aligned} \quad (3)$$

where  $u$  is dimensionless cell density,  $v$  is dimensionless chemical attractant concentration,  $D$  stands for diffusion coefficient,  $\alpha$  stands for the signal-dependent sensitivity,  $\beta$  stands for saturating of the signal production, and  $\gamma$  stands for the spatial and temporal scale.

The initial conditions for the model are:

$$u(x, 0) = 1 + \varepsilon(x), \quad v(x, 0) = 0, \quad x \in [0, 1], \quad (4)$$

where  $\varepsilon(x)$  is a 20% random uniform spatial perturbation.

The boundary conditions for the model are:

$$u(0, t) = u(1, t), \quad v(0, t) = v(1, t), \quad \frac{\partial u}{\partial x} \Big|_{x=0} = \frac{\partial u}{\partial x} \Big|_{x=1}, \quad \frac{\partial v}{\partial x} \Big|_{x=0} = \frac{\partial v}{\partial x} \Big|_{x=1}. \quad (5)$$

Numerical simulation was performed using numpy package for python programming language using explicit difference method. Results of the simulation were very similar to the results observed by the authors of the paper, so reproduction was deemed successful.

### 3.2 Two dimensional model

It has been noticed that cellulose-overproducing wrinkly spreader mutants of *Pseudomonas fluorescens* SBW25 grow in colonies that extend from the surface downwards. To model this behavior a model of 6 reaction-advection-diffusion and fluid dynamics equations was proposed [ADR19]:

$$\begin{aligned} \Delta \Psi &= -\omega, \\ \frac{\partial \omega}{\partial t} + (\vec{u} \cdot \vec{\nabla}) \omega &= \nu \Delta \omega - g \frac{\partial}{\partial x} \left( \frac{\rho}{\rho_0} \right), \\ \frac{\partial b}{\partial t} + (\vec{u} \cdot \vec{\nabla}) b &= D_b \Delta b + \delta b \left( 1 - \frac{b}{b_{sat}} \right), \\ \frac{\partial o}{\partial t} + (\vec{u} \cdot \vec{\nabla}) o &= D_o \Delta o - \gamma b \Theta(o), \\ \frac{\partial c}{\partial t} + (\vec{u} \cdot \vec{\nabla}) c &= D_c \Delta c + \alpha c (1 - c) \Theta(b - b^*) \Theta(o - o^*), \\ \frac{\partial p}{\partial t} + (\vec{u} \cdot \vec{\nabla}) p &= D_p \Delta p + \beta p (1 - p) \Theta(o - o^*), \end{aligned} \quad (6)$$

where  $\Delta$  is the Laplace operator,  $\Psi$  is the scalar field,  $\omega$  is vorticity,  $(\vec{u} \cdot \vec{\nabla})$  is the convective derivative,  $\nu$  is viscosity,  $\rho$  is mass density,  $\rho_0$  is density of the fluid medium,  $b$  is bacteria,  $o$  is oxygen,  $c$  is cellulose,  $p$  is pyoverdine,  $D_b$ ,  $D_o$ ,  $D_c$ , and  $D_p$  are diffusion coefficients,  $\delta$  is bacteria growth rate,  $b_{sat}$  is bacteria saturation value,  $\gamma$  is oxygen consumption rate,  $\Theta$  is Heaviside function,  $\alpha$  is cellulose production rate, and  $\beta$  is pyoverdine production rate.

Numerical simulation was performed using numpy and tensorflow packages for python programming language, however, due to some errors simulation was unsuccessful.

## 4 Conclusions

Model proposed by Ardre et al [ADR19] seems to describe plume formations in bacteria populations accurately, however, due to its complexity, numerical simulation of this model so far has failed.

## References

- [ADR19] Maxime Ardré, Djinthana Dufour, and Paul B Rainey. Causes and biophysical consequences of cellulose production by *Pseudomonas fluorescens* sbw25 at the air-liquid interface. *Journal of bacteriology*, 201(18):e00110–19, 2019.
- [BŠ11] Romas Baronas and Remigijus Šimkus. Modeling the bacterial self-organization in a circular container along the contact line as detected by bioluminescence imaging. *Nonlinear Anal. Model. Control*, 16(3):270–282, 2011.
- [CFK<sup>+</sup>12] A Chertock, K Fellner, A Kurganov, A Lorz, and PA Markowich. Sinking, merging and stationary plumes in a coupled chemotaxis-fluid model: a high-resolution numerical approach. *Journal of fluid mechanics*, 694:155, 2012.
- [KOST12] Kousuke Kuto, Koichi Osaki, Tatsunari Sakurai, and Tohru Tsujikawa. Spatial pattern formation in a chemotaxis–diffusion–growth model. *Physica D: Nonlinear Phenomena*, 241(19):1629–1639, 2012.
- [KS71] Evelyn F Keller and Lee A Segel. Model for chemotaxis. *Journal of theoretical biology*, 30(2):225–234, 1971.
- [Led16] Žilvinas Ledas. *Kompiuterinis švytinčių bakterijų struktūros formavimosi tirpale modeliavimas*. PhD thesis, Vilnius University, 2016.
- [PH11] Kevin J Painter and Thomas Hillen. Spatio-temporal chaos in a chemotaxis model. *Physica D: Nonlinear Phenomena*, 240(4-5):363–375, 2011.
- [ZHCGG05] M-P Zorzano, David Hochberg, M-T Cuevas, and J-M Gómez-Gómez. Reaction-diffusion model for pattern formation in *E. coli* swarming colonies with slime. *Physical Review E*, 71(3):031908, 2005.