

SIMULATION OF ACTIVE TURBULENCE FOR ENHANCED METHANE-TO-METHANOL CONVERSION PERFORMANCE IN METHANOTROPHIC COMMUNITIES

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ABSTRACT

Rapid climate change driven by global warming poses serious threats to both natural ecosystems and human society. Methane, one of the major greenhouse gases, has a global warming potential more than 20 times higher than that of carbon dioxide, making its mitigation critically important.

Methanotrophs have recently attracted attention for their ability to convert methane into methanol, a valuable alternative fuel. In this study, the collective swimming behavior of methanotrophs is investigated by analyzing two-dimensional active turbulent flows using computational fluid dynamics (CFD). The parameters of the Toner-Tu equation are systematically identified through comparison with experimental observations of methanotroph suspensions.

Key flow characteristics, including mean velocity, integral length scale, characteristic time scale, and energy spectrum, are quantitatively evaluated as functions of optical density (OD). Based on these analyses, Toner-Tu parameters corresponding to OD are derived. In addition, the energy transfer characteristics associated with activity are analyzed to elucidate the underlying mechanisms of active turbulence.

This study provides physical insights into active turbulence induced by methanotrophs and offers a predictive framework for understanding their collective behavior under varying experimental conditions.

INTRODUCTION

Global warming has led to significant changes in the Earth's climate system, with profound impacts on both natural ecosystems and human society. The rising frequency of extreme weather events, including droughts, heatwaves, and floods, has led to ecosystem degradation, reduced agricultural productivity, and significant risks to human health and safety. These impacts are widely attributed to the accumulation of greenhouse gases resulting from anthropogenic activities, highlighting the urgent need for effective mitigation strategies.

Among greenhouse gases, methane accounts for a significant fraction following water vapor and carbon dioxide and is reported to have a global warming potential more than 20

times greater than that of carbon dioxide (Ross and Rosenzweig, 2017). Recently, considerable efforts have been made to mitigate methane while simultaneously converting it into methanol, a valuable alternative fuel, using genetically engineered methanotrophs that metabolize methane.

To maximize the methane-methanol conversion efficiency of methanotrophs, it is essential to understand the flow that arise during their collective swimming behavior. In bacterial suspensions, active turbulence is observed, characterized by vortex structures and energy spectra similar to those in inertial turbulence despite operating at low Reynolds numbers ($Re < 1$). To describe such phenomena, Toner and Tu proposed a continuum equation governing the collective motion of active particles (Toner and Tu, 1998). Subsequently, extended models incorporating a Swift-Hohenberg term have been used to analyze the flow of *Bacillus subtilis* suspensions under high-density conditions (Dunkel et al., 2013; Wensink et al., 2012; Mukherjee et al., 2023).

However, a universal governing equation capable of describing active turbulence has not yet been established (Alert et al., 2022), and systematic studies on the collective behavior of methanotrophs remain limited.

In this study, the collective swimming behavior of methanotrophs is investigated by analyzing a two-dimensional active turbulent flow field using CFD, and by modeling the parameters of the Toner-Tu equation through comparison with methanotroph suspension experiments. This work extends the physical understanding of active turbulence induced by methanotrophs and provides a foundation for predicting collective behavior under various conditions, thereby contributing to the optimization of methane to methanol conversion processes.

METHODS

2.1. Experimental data

The methanotrophs used in this study were cultured and provided by the NanoBio Engineering Laboratory at Kyung Hee University. The samples were subsequently centrifuged at the Soft Interface Laboratory at Kyung Hee University, and

experimental images were acquired under different optical density (OD) conditions. The OD, defined as the absorbance of the medium, is given by

$$OD = \log_{10} \left(\frac{\Phi_e^i}{\Phi_e^t} \right) \quad (1)$$

where Φ_e^i and Φ_e^t denote the incident and transmitted radiant flux, respectively.

The images were recorded at a resolution of 1024×1024 pixels and a frame rate of 100 fps, corresponding to a spatial resolution of $50 \mu\text{m}$ per 158 pixels.

The velocity fields were obtained using particle image velocimetry (PIV), implemented in the open-source software PIVlab (Thielicke et al., 2021). A multipass FFT algorithm was employed with a total of three passes. In the first pass, the interrogation window size was set to 128 pixels with a step size of 32 pixels. In the second and third passes, the interrogation window sizes were reduced to 64 pixels and 32 pixels, respectively, with a 50% overlap applied. Additionally, each interrogation window was configured to include at least five bacteria to ensure reliable velocity estimation.

The observation domain was $324.05 \mu\text{m} \times 324.05 \mu\text{m}$, and PIV analysis was performed for OD values of 34, 68, 101, 135, 152, and 202.

2.2. Numerical simulation

To model the collective flow behavior of bacterial suspensions, an active turbulence continuum equation was employed.

$$\frac{\partial u}{\partial t} + \lambda_0 u \cdot \nabla u = -p + \lambda_1 \nabla u^2 - \Gamma_0 \nabla^2 u - \Gamma_2 \nabla^4 u - (\alpha + \beta |u|^2) u \quad (2)$$

$$\nabla \cdot u = 0 \quad (3)$$

Here, λ_0 and λ_1 are defined in terms of the parameter s , which represents the contribution of the active stress as follows,

$$\lambda_0 = 1 - s, \quad \lambda_1 = -\frac{s}{2} \quad (4)$$

The incompressible condition is valid for dense suspensions where density fluctuations are sufficiently small to be neglected. Here, p denotes the pressure, and the sign of s depends on the swimming mechanism of the bacteria, which can be classified as pushers or pullers. Based on previous studies, methanotrophs are classified as pushers; therefore, a negative value of s was adopted.

The coefficients α and β form a Landau-type velocity potential. When $\alpha < 0$, energy is injected into the flow field from the active particles, while $\beta > 0$ is required to ensure stability. In addition, to sustain a self-organized turbulent state, the conditions $\Gamma_0 < 0$ and $\Gamma_2 > 0$ were imposed.

To numerically solve the active turbulence flow field, a customized solver was developed based on OpenFOAM. Since energy transfer driven by active stress plays a dominant role in active turbulence, it is essential to minimize numerical dissipation. For this purpose, a fractional step method was employed to couple the momentum equation with the mass conservation equation.

For validation of the developed solver, the Navier-Stokes equations were first applied to benchmark problems. The velocity profile of lid-driven cavity flow (Kuhlmann, 2018) and the energy dissipation characteristics of decaying two-

dimensional homogeneous isotropic turbulence (Sallam, 2024) were compared with previously reported results. The governing equation was then replaced with the active turbulence formulation, and additional validation was performed by comparing the energy spectra with the results of Mukherjee et al. (2023).

All simulations were conducted in a computational domain of size 10×10 using a 256×256 grid with periodic boundary conditions. Statistical quantities were computed using velocity fields obtained after the energy spectrum reached statistical convergence.

The integral length scale (L) and the velocity autocorrelation function (C) is defined as follows,

$$L = \int_0^{r_0} C(r) dr \quad (5)$$

$$C(r) = \overline{\langle u(t, r) \cdot u(t, r + R) \rangle} \quad (6)$$

where r_0 denotes the first zero-crossing point of the normalized velocity autocorrelation function $C(r)/C(0)$. The integral length scale is calculated by integrating up to this point.

RESULTS

The PIV analysis shows that the root-mean-square (rms) velocity $\sqrt{\langle u_x^2 + u_y^2 \rangle}$ increases with increasing OD. Linear regression indicates that, within the range $34 \leq OD \leq 202$, the relationship follows

$$u_{rms} = 0.014OD + 3.1 \quad (7)$$

The integral length scale also increases with OD and follows

$$L = 0.033OD + 5.8 \quad (8)$$

In contrast, the integral time scale exhibits a nonlinear behavior, showing a sharp increase beyond $OD \approx 135$.

Analysis of the energy spectra reveals that the energy in the low-frequency region increases with OD. In addition, the slope in the high-wavenumber region becomes steeper, changing from -2.0 to -3.5 , suggesting enhanced dissipation of small-scale structures with increasing density.

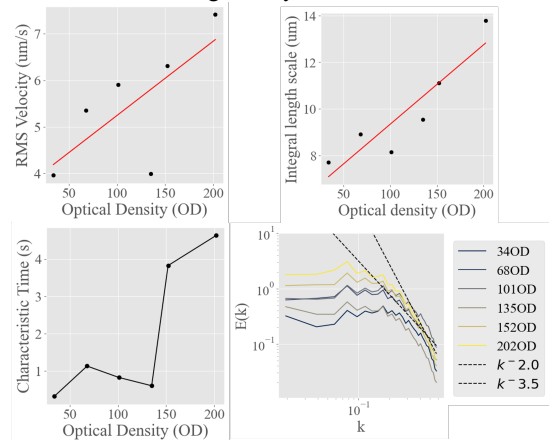


Figure 1. Physical characteristics of methanotrophic bacteria dynamics at different OD: root-mean-square velocity, integral length scale, integral time scale, and energy spectra.

Since the active turbulence continuum equation includes phenomenological parameters that depend on the system, previously reported parameter sets for other bacterial species cannot accurately reproduce the collective flow of methanotrophs. This necessitates a systematic identification of model parameters tailored to methanotroph suspensions. To this end, a parametric study is performed to investigate the effects of α , β , Γ_0 , Γ_2 , and s on the flow characteristics.

To reproduce the OD-dependent collective flow of methanotrophs, parameter estimation was performed. The simulation results were rescaled to match the physical domain, where the domain length scale was fixed and velocity scaling was applied based on the rms velocity for comparison with experimental data.

Based on vortex structures, energy spectra, and velocity probability density functions, optimal parameters were determined for each OD condition. As a result, by fixing $\beta = 0.1$, $s = -2.5$, $\Gamma_0 = -0.040$, and $\Gamma_2 = |\Gamma_0^3|$, the experimental results were successfully reproduced by varying α within the range of -2 to -4 .

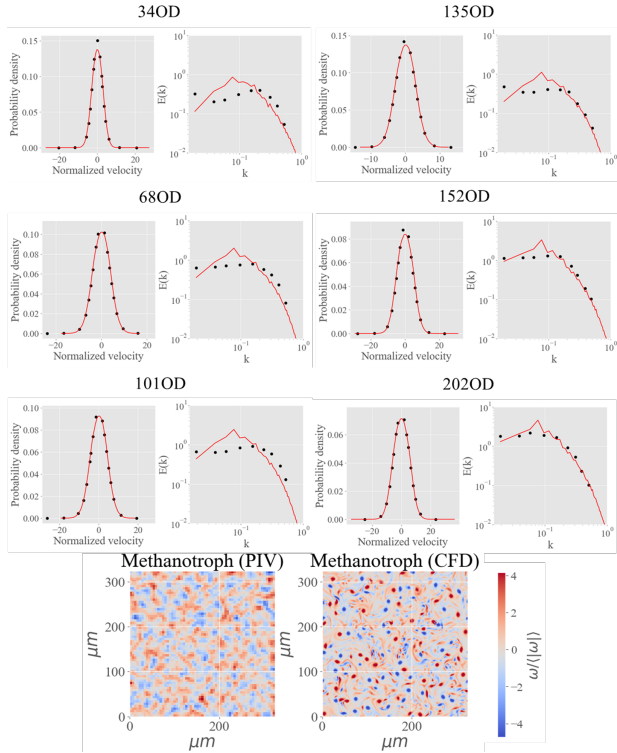


Figure 2. (Top) Velocity probability density functions and energy spectra obtained from simulations using optimized equation parameters for each methanotrophic bacterial density. (Bottom) Normalized vorticity fields of methanotrophic bacteria at OD 202 from PIV and CFD.

In particular, α shows a decreasing trend with increasing OD. By modeling this relationship linearly, a regression coefficient of $R^2 = 0.64$ was obtained, yielding the following expression:

$$\alpha = -0.013OD - 0.17 \quad (9)$$

demonstrating that the density-dependent collective swimming behavior can be effectively reproduced using this parameterization.

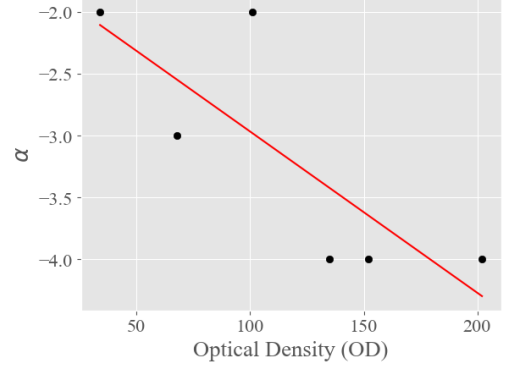


Figure 3. α parameter for modeling the active turbulent flow field of methanotrophic bacteria as a function of density, with β , Γ_0 , and s fixed at 0.1, -0.040 , and -2.5 , respectively.

Finally, to investigate the energy transfer mechanism in active turbulence, the energy transfer function derived from the Karman-Howarth equation in Fourier space was evaluated. The results show that a two-dimensional inverse energy cascade occurs, in which energy is transferred from smaller to larger scales, as confirmed by a negative energy flux. Energy is injected at high wavenumbers, and the energy transfer becomes more active as the value of α increases.

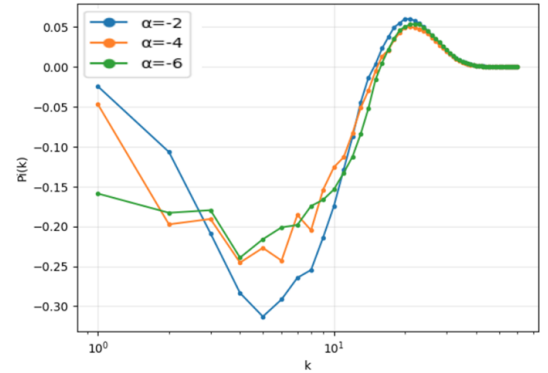


Figure 4. Energy transfer function as a function of α . Energy is injected at high wavenumbers, and an inverse energy cascade is observed. As α decreases, energy transfer becomes more active.

CONCLUSION

In this study, a Toner-Tu-based framework was introduced to model active turbulence in high-density methanotroph suspensions, and a customized active turbulence solver was developed and validated using OpenFOAM. By comparison with experimental PIV results, parameter estimation was performed as a function of optical density, and Toner-Tu model parameters capable of reproducing the collective flow of methanotrophs were established.

The results demonstrate that methanotroph-induced active turbulence exhibits distinct characteristics compared to both inertial turbulence and *Bacillus subtilis*-based active turbulence,

particularly in terms of energy dissipation and velocity distributions. These findings highlight the importance of system-specific parameterization in describing active turbulent flows.

This study provides a quantitative understanding of the physical characteristics of methanotroph-induced active turbulence and establishes a predictive framework for describing their collective behavior under varying density conditions. Future work will focus on a more detailed investigation of energy transfer mechanisms to further elucidate the physics of active turbulence driven by methanotrophs.

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