

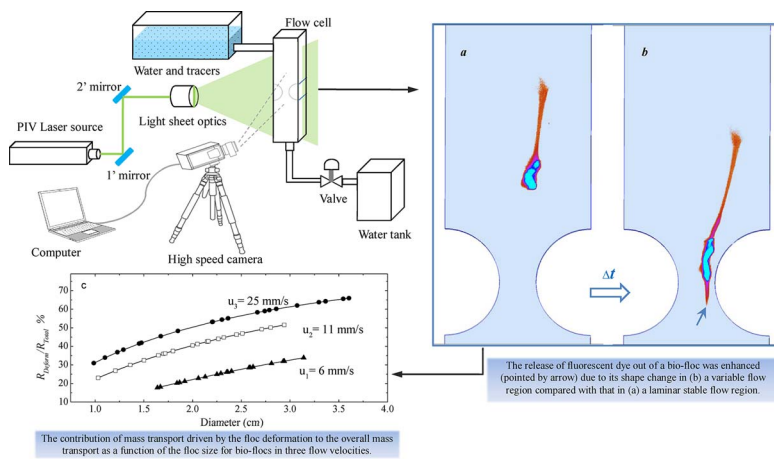
Effect of the shape change on the mass transport of bio-flocs in water

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GRAPHICAL ABSTRACT



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ABSTRACT

Molecular diffusion is regarded as the main mechanism of substrate transport in flocculant sludge in biological wastewater treatment. However, bio-flocs are highly porous and soft and are subject to frequent shape changes in a dynamic flow environment, which affect their mass transport mechanisms. In this study, the effect of shape deformation on the mass transport for individual bio-flocs was investigated, by employing the laser-induced fluorescence technique. The bio-flocs deformation was observed through a variable flow region, which enhanced the material (dyes) release from the interior of bio-flocs. Based on the experimental results, the rate of mass transport driven by flocs deformation could be more than an order of magnitude higher than diffusive rate. Over 50% of overall mass transport for single bio-floc was contributed by its shape deformation and the percentage would increase as the floc size increased. A comprehensive mass transport model was then developed for bio-flocs in a dynamic fluid environment, which took into account the deformation, intra-floc flow and molecular diffusion. The model indicated that shape deformation plays a dominant role in the material transport in larger bio-flocs, especially for larger chemical solutes with a lower diffusivity. The findings of this study provide new insights into the mechanisms of mass transport in bio-flocs in wastewater treatment facilities.

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1. Introduction

In biological wastewater treatment plants, microorganisms are normally suspended in the form of large aggregates, or bio-flocs, in bioreactors such as activated sludge aeration tanks and anaerobic digesters. The performance and capacity of wastewater treatment facilities in achieving organic degradation and nutrient removal is generally believed to be limited by the rate of mass transport in the bio-aggregates [1–4]. Mass transport has therefore been a central issue in studies of the role of bio-flocs in bioreactors for wastewater treatment. Conventionally, molecular diffusion is regarded as the predominant mechanism of the material transfer between the bulk fluid and the biological aggregates [5–8]. The microbial flocs are generally treated as a rigid object with a fixed shape and volume [9,10]. Owing to the slow rate of molecular diffusion, it is commonly expected that most bio-flocs will be subject to the mass transport limitations in bioreactors for wastewater treatment [2,11–13].

However, bio-flocs are highly porous and fractal, with a porosity of 99% or higher [14–16]. The open and permeable structure of microbial aggregates would allow for convective and diffusive mass transport of oxygen and organic matter within the aggregates [4,8]. Li and Yuan [14–17] studied the mass transfer mechanism of settling bio-flocs in quiescent flow, and they found that the fluid could penetrate the porous interior of the flocs. Xiao et al [18,19] further provided a visible evidence on the intra-floc flow by applying the particle imaging velocimetry (PIV) technique and CFD simulation, which tracked the flow streamlines passing through the interior of settling bio-flocs. This internal permeation can play a comparable or more important role than molecular diffusion in the overall mass transport through bio-flocs [11,17,20–22]. Moreover, unlike rigid objects, bio-flocs are soft and flexible and are thus likely to change their shape and structure to conform to the shear stress in the water flow [10,23–27]. In fact, the shape change or deformation of bio-flocs has been observed in turbulent flow by using the PIV technique [7,26]. During the shape deformation, solutes and particulate matter in the water enter the void volume of the bio-flocs. In other words, in a dynamic flow environment, the void pores within the bio-flocs expand and shrink according to the frequent shape changes. Consequently, chemicals in the water are forced into or out of the internal voids of individual bio-flocs, leading to much enhanced mass transport. However, the effect of the shape change on the material transport in bio-flocs in water has not been well verified.

In this study, an advanced fluid visualisation technique, laser-induced fluorescence (LIF), was used to investigate the mass transport driven by the shape change of bio-flocs in a variable water flow. Bio-flocs saturated with a tracer dye were observed individually through a flow chamber to determine their shape changes and related mass transport rates. The objectives of the LIF-based experimental investigation included (i) to directly track the material (dye) transported from the bio-flocs into water under different flow conditions, (ii) to quantify the rates of material transport driven by molecular diffusion, internal permeation and shape change for individual bio-flocs, (iii) to evaluate the importance of the shape changes of individual bio-flocs for the overall mass transport in comparison to molecular diffusion and (iv) to develop a comprehensive model to describe the dynamics of material transport through bio-flocs that accounts for their permeable and deformable features and the hydrodynamic condition of the flow field. The experimental findings provided new insights into the mechanisms of the mass transport in bio-flocs in wastewater treatment bioreactors.

2. Materials and methods

2.1. Numerical simulation

2.1.1. Mass transport for individual bio-flocs

Bio-flocs have a soft and permeable structure and, thus, their

continuous change of the shape in a sheared flow can be an important driving force for mass transport [7,26]. For a non-degradable substance within a floc with an enclosed volume, V , the mass flow rate in a controlled volume without chemical reactions can be written as $\frac{d(VC)}{dt} = V\frac{dC}{dt} + C\frac{dV}{dt}$, where $\frac{dV}{dt}$ signifies the rate of the effective volume change caused by the shape deformation of the floc in the flow. When the deformable and permeable features of the floc are both taken into account, the equation can be specified as:

$$\frac{d(VC)}{dt} = V\left(\left(\frac{dC}{dt}\right)_{MD} + \left(\frac{dC}{dt}\right)_{Iflow}\right) + C\frac{dV}{dt} \quad (1)$$

where $\left(\frac{dC}{dt}\right)_{MD}$ and $\left(\frac{dC}{dt}\right)_{Iflow}$ denote the rates of mass transport driven by the molecular diffusion and internal flow, respectively.

2.1.2. Mass transport by molecular diffusion (R_{MD}) and internal flow (R_{Iflow})

The rate of mass transport by molecular diffusion for a bio-floc can be written as $V\left(\frac{dC}{dt}\right)_{MD} = D_m\frac{dC}{dr}|_r=A$, where r is the radius of the enclosed spherical volume of the floc and D_m is the diffusion coefficient of the chemical concerned [18]. For material transport inside the floc, the chemical concentration gradient through the floc surface can be approximated by a linear form of $\frac{dC}{dr}|_r = \frac{\Delta C}{\delta}$, where ΔC is the chemical concentration gradient through the surface layer of the floc with a thickness of $\delta = qr$, and $q (< 1)$ is a fraction factor. Thus, the rate of molecular diffusion through the surface of the floc can be written as:

$$R_{MD} = \frac{4\pi r D_m \Delta C}{q} \quad (2)$$

For a fractal and permeable bio-floc, the rate of mass transport brought about by the internal flow through the floc can be written [11,28–30] as:

$$R_{Iflow} = V\left(\frac{dC}{dt}\right)_{Iflow} = \pi r^2 \eta \Delta v \Delta C \quad (3)$$

where Δv is the relative velocity of the flow toward the bio-floc and η is the fluid collection efficiency of the floc, which is determined by comparing the terminal settling velocities of impermeable and permeable flocs (detailed procedures are provided in Supplementary Information, SI 1).

2.1.3. Mass transport due to shape change (R_{Deform})

The fluid shear or instable flow can force the porous and deformable structure of a floc to change its shape and volume to conform to the hydrodynamic stress [26,27,31,32]. During the shape change, liquid can be forced out of the compressed void space or into the expanded void space of the bio-floc, resulting in considerable liquid and material exchange. The rate of mass transport due to the continuous shape change of the floc can be described by:

$$R_{Deform} = \frac{4\pi}{3} k f \xi r^3 \Delta C \quad (4)$$

where ξ is the ratio of the volume of the deformed floc to its initial volume, k is an effectiveness factor for the consequential material exchange caused by the shape deformation and f is the frequency of shape change in the flow, which can be related to the velocity gradient of the flow by $f = 1/\Delta t = dv/dz$, where Δt is the duration of a shape change of the floc in the flow. Overall, the mass transport within individual bio-flocs, accounting for molecular diffusion, internal flow and shape deformation, can be written as follows,

$$R_{Total} = R_{Deform} + R_{Iflow} + R_{MD} = \pi r \Delta C \left(\frac{4}{3} k f \xi r^2 + \eta \Delta v r + \frac{4 D_m}{q} \right) \quad (5)$$

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