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A method for calculating the surface area of numerically simulated aggregates

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ABSTRACT

The success of many industrial processes largely depends on the structural characteristics of aggregates. In intensive aerobic digestion process for wastewater treatment applications, the structural characteristics namely aggregate shape, size and therefore the aggregate surface area strongly influence the transfer of dissolved oxygen from the aeration process to aggregates of harmful contaminants/microorganisms.

The aim of this study was to apply Discrete Element Modelling (DEM) techniques to the aggregation of suspended particles (microorganisms) to quantify the available surface area for convection and diffusion as a function of particles number concentration and surface charge. The simulation inputs included particle and fluid characteristics such as particle size and density, solid concentration, suspension pH and ionic strength. A post processing method based on the Go-chess concept was developed to quantify the surface area of aggregate structure. The simulation results showed that whilst an increase in connection points increases the total surface area of the aggregate, this does not necessarily translate into an increase in the surface area available for oxygen transfer as combinations of open and close pores are formed. Aggregate surface area was directly determined by aggregate structural characteristics, and increased rapidly when the coordination number was below 3.5 and the fractal dimension was less than 1.5. A correlation for prediction of aggregate external surface area was also proposed as a function of aggregate structural characteristics in terms of fractal dimension and coordination number.

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1. Introduction

The success of aerobic digestion process depends on sufficient transfer of oxygen to the microbes during the digestion process. Recent focus of the aerobic digestion process design is to increase the mother liquor suspended solids (MLSS) as much as possible to improve the volumetric efficiency of the digester. Higher MLSS implies sustaining larger population of microbes in a rather compact digester, which requires large enough oxygen transfer rate from water to the microbe sludge to sustain the digestion process.

The microbes have a tendency to stick together to form aggregates or 'flocks'. The formation of aggregates has implications for the surface area available to exchange oxygen from water. So far,

the surface area could not be measured directly from experiments. Modelling of the aggregate surface area is even more difficult, given the scarcity of experimental data. The surface area of aggregates is a complex parameter as the aggregate contains both the open and closed pores. In this study, a closed pore is defined as the space surrounded by some of the primary particles that comprise the aggregate. Closed pores do not contribute to the area available for mass transfer from bulk liquid. In summary, only a fraction of the total microbe area is available to exchange oxygen from the water. Calculation of the fraction of total aggregate surface area that is available for oxygen exchange is the cornerstone of mass transfer calculation in aerobic digestion process. Once perfected, the method can be extended to solid–liquid mass transfer process in general, e.g., water treatment and powder coating.

Experimentally, the interfacial area for two phases can be measured by a technique involving mass transfer and chemical reaction. The method involves finding a chemical reaction with rate of reaction that competes with the mass transfer in two different reaction/mass transfer rate ratios. However, it is extremely difficult

to find the reactants which will satisfy the criteria to exactly balance the solid–liquid reaction kinetics with mass transfer. Hence this method has enjoyed only a limited success in determination of gas–liquid interfacial area.

Generally, the fraction of total particle interfacial area available for mass transfer is assumed to be 1. The error arising out of using the total particle area is compensated by fitting the mass transfer coefficient values to the observed rate of mass transfer (the concentration gradient and the interfacial area being known).

An approximate approach to obtain aggregate surface area available for interphase mass transfer is via image processing. Perez et al. [1] estimated the morphological parameters of fractal aggregates by digital image analysis using commercial software Image-Pro Plus®. The relationships between the morphological parameters were analyzed and the results indicated that the highly porous aggregates are very irregular. Zartarian et al. [2] constructed a 3-D model of an aggregate from digitized microtome sections by the discrete smooth interpolation. Parameters of the aggregate such as size, surface area and volume were then measured on the 3D reconstructed object. However, the digital image processing approach can only provide rough approximation and may result in large errors especially in the 3-D analysis when dealing with wide size distribution of primary particles and complex aggregate structures [3].

In the present work, a methodology based on the concept of Go-chess was developed to accurately determine the external surface (or boundary) of a numerically simulated aggregate, outside which the interphase mass transfer is deemed as convection controlled (over the external surface area) and within which as diffusion controlled (through the porous structure). For this purpose, the code of Discrete Element Modeling (DEM) we developed earlier [4–6] was used for the simulation of aggregate formation of colloidal particles. The results of DEM simulations were then used as inputs to the Go-chess program to determine the external surface of each individual aggregate. The structure of fractal aggregates were also characterized in terms of equivalent size, longest dimension, coordination number and fractal dimension. The relationship between external surface area and the structural characteristics of aggregates were then investigated and correlated. The applicability of the Go-chess method in three dimensional situations has also been discussed.

2. Mathematical model

The mathematical model consists of two sequential parts: (i) DEM simulation of aggregate process; (ii) using DEM simulation results as input data to calculate quantities characterizing the fractal structure of aggregates.

2.1. DEM simulation of aggregation process

In aqueous solutions of suspended microorganisms, a single particle is interacting with the surrounding particles and fluid. By the DEM technique, the motion of each solid particle is tracked individually, accounting for the dynamics due to complex particle–particle and particle–fluid interactions. Detailed information on the particle is obtained at each time step. The governing equations for the translational and rotational motion of a single particle i are based on Newton's equation of motion, and read as,

$$m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{f}_{c,i} + \mathbf{f}_{s,i} + \mathbf{f}_{f,i} + \mathbf{f}_{b,i} + V_i(\rho_i - \rho_f)\mathbf{g} \tag{1}$$

and,

$$I_i \frac{d\mathbf{w}_i}{dt} = \mathbf{T}_i \tag{2}$$

where m_i, I_i, $\mathbf{v}_i$ and $\mathbf{w}_i$ are mass, moment of inertia, translational and angular velocities of particle i, respectively. ρ_i and ρ_f are the density of particle i and that of fluid, respectively. V_i is the volume of particle i. $\mathbf{f}_{c,i}$ is the total collision contact force, which is solved by the linear spring-dashpot model [7]. $\mathbf{f}_{s,i}$ are the total surface force between particle i and surrounding particles. $\mathbf{f}_{f,i}$ is viscous fluid force[4] and $\mathbf{f}_{b,i}$ is the Brownian random force [8]. $\mathbf{T}_i$ is the total torque, comprising the components caused by the tangential contact force and by the rolling resistance. The developed equations for the forces and torques have been detailed previously by Peng et al. [4–6]. For brevity, only the viscous fluid force and inter-particle forces are given below.

The viscous fluid force was considered to be,

$$\mathbf{f}_{f,i} = \frac{1}{8} \pi d_p^2 C_D \rho_f |\mathbf{v}_r| \mathbf{v}_r \tag{3}$$

where C_D is the steady drag coefficient and $\mathbf{v}_r$ is the relative velocity, i.e., $\mathbf{v}_r = \mathbf{v}_f - \mathbf{v}_p$. $\mathbf{v}_f$ is the ambient fluid velocity. The coefficient C_D is expressed as the function of the particle Reynolds number. As for a nano-size particle, most cases are in the Stokes regime due to the small particle size, thus C_D is calculated by [9],

$$C_D = \frac{24}{Re_p}, \ Re_p < 2 \tag{4}$$

where

$$Re_p = \frac{\rho_f |\mathbf{v}_r| d_p}{\mu_f} \tag{5}$$

Substituting Eqs. (5) and (4) into Eq. (3), the viscous fluid force is simplified as,

$$\mathbf{f}_{f,i} = 3\pi \mu_f d_p \mathbf{v}_r \tag{6}$$

Two types of major long range forces, namely van der Waals and electrical double layer (EDL) forces have been considered as the dominant forces in colloidal suspensions in the absence of additives such as polymeric dispersants and coagulants. The effect of these forces is commonly modelled using the well-known DLVO theory [10,11], which is the algebraic summation of van der Waals attractive force, $\mathbf{f}_{vdw}$ and electrostatic repulsive force, $\mathbf{f}_{ele}$.

For two spherical particles, i and j, these forces can be expressed as:

$$\mathbf{f}_{vdw,i} = \sum_{j=0}^{N_c} \left[-\frac{A_H(4r_i r_j)^3}{6} \left[\frac{s_{ij}}{[s_{ij}^2 - (r_i + r_j)^2]^2 \times [s_{ij}^2 - (r_i + r_j)^2 + 4r_i r_j]^2} \right] \right] \tag{7}$$

and,

$$\mathbf{f}_{edl,i} = \sum_{j=0}^{N_c} \left[64\pi \varepsilon_r \varepsilon_0 \kappa \left(\frac{RT}{zF_c} \right)^2 \times \tanh\left(\frac{zF_c \zeta_i}{4RT} \right) \times \tanh\left(\frac{zF_c \zeta_j}{4RT} \right) \times \frac{r_i r_j}{r_i + r_j} e^{-\kappa h_{ij}} \right] \tag{8}$$

where h_{ij} is the surface separation distance, s_{ij} the centre-to-centre distance between the two particles, A_H the Hamaker constant, κ the Debye–Huckel parameter, F_c the Faraday constant, z the valence of the background electrolyte, ε_r the dielectric constant of the medium, ε_0 the permittivity of vacuum, and R the gas constant; ζ_i and ζ_j denote the zeta-potentials of the particles.

When two particles approach to each other and are close to contact (less than 4 nm approximately to physical contact) [12], the Johnson–Kendall–Robert's adhesive model [13] is commonly applied to calculate the surface adhesion and avoid numerical singularity in Eq. (7):

$$\mathbf{f}_{JKR} = \frac{3\pi r_i r_j}{2(r_i + r_j)} W_{iLj} \tag{9}$$