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CFD modelling of phenol biodegradation by immobilized *Candida tropicalis* in a gas–liquid–solid three-phase bubble column

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ABSTRACT

A three-dimensional transient model, combining three-phase fluid flow, interphase mass transfer and intrinsic bioreaction kinetics, was developed to simulate the dynamic behaviors of batch phenol biodegradation by immobilized *Candida tropicalis* in a gas–liquid–solid three-phase bubble column (BC). A computational fluid dynamics (CFD) method was used, with a multiple size group model adopted to determine the bubble size distribution, based on a previous three-phase BC hydrodynamic CFD model [1]. Current simulation results of phenol and oxygen concentration changes in the liquid phase were validated by corresponding experimental measurements under various operating conditions. Furthermore, local transient batch phenol biodegradation characteristics such as the oxygen concentration profiles in the gas, liquid and solid phases, the phenol concentration profiles in the liquid and solid phases, and the cell concentration profile in the solid phase were predicted. Comparisons between species interphase mass transfer and bioreaction rates were carried out to identify the rate-limiting step in the immobilized batch phenol biodegradation processes.

1. Introduction

Phenol is a common pollutant of industrial wastewaters from oil refineries, petrochemical plants, coking plants, brown coal distilling plants, wood manufacturing plants and phenolic-resin industries. Accumulation of phenol in an ecosystem can cause harmful effects so it is necessary to treat this waste before its safe discharge to water [2].

Biological treatment is a feasible method for removal of phenol from wastewater because of its low cost and avoidance of secondary pollution, especially at relatively low concentrations, compared with physicochemical methods [3]. Reactions with immobilized microbial cells are attracting more attention, as they may offer several advantages over processes with suspended biomass, including protecting cells from toxic substances and preventing suspended particles from joining the effluent stream [4]. Moreover, immobilized cells can be reused and can be easily separated from the reaction mixture [5]. Various types of solid matrices, such as polyacrylamide gels, alginate gels, porous glass, etc., have been used for immobilization of whole cells to maintain a high concentration of microorganisms in reactors [6–13]. Immobilization of cells with polyvalent salts of alginate has received the most attention because of the low cost and the mild conditions involved [14–17].

Bubble columns (BCs) have found wide applications over the years as cost-effective reactors for many industrial bioreactions [18]. Recently, numerous experimental investigations have indicated that BCs have very good performance in phenol biodegradation processes, both in gas–liquid (G–L) two-phase systems and in gas–liquid–solid (G–L–S) three-phase systems [19–26]. However, the understanding of this complex system, combining multiphase fluid flow, interphase mass transfer and intrinsic bioreaction, is rather limited, which prevents better optimization and scale-up of the process [27].

Computational fluid dynamics (CFD) has been adopted in the last decade as a useful tool to aid understanding of the multiphase hydrodynamics of BCs and, to a large extent, it can replace time-consuming and expensive experiments [28–33]. The current focus is on the modelling of multiphase bioreaction processes, for example, phenol biodegradation. However, most reports to date have been limited to the modelling of fluid hydrodynamics in G–L BCs [34–44] and only Feng et al. [45] in our lab have successfully developed a three-dimensional (3D) transient CFD model for simulating the local dynamic behaviors of phenol biodegradation in G–L BC using free cells. Until now, reports published on modelling of the fluid hydrodynamics of G–L–S BCs, let alone the G–L–S phenol biodegradation processes, have been very limited [46–48].

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Nomenclature

A	growth associated constant for phenol consumption
a	specific area (m^{-1})
B	non-growth associated constant for phenol consumption (s^{-1})
C	concentration ($kg\,m^{-3}$)
D	kinematic diffusivity ($m^2\,s^{-1}$)
d	diameter (m)
g	gravitational acceleration ($m\,s^{-2}$)
K	mass transfer coefficient ($m\,s^{-1}$)
K_i	phenol inhibition constant ($kg\,m^{-3}$)
K_o	oxygen half-saturation constant ($kg\,m^{-3}$)
K_s	phenol half-saturation constant ($kg\,m^{-3}$)
S	source term ($kg\,m^{-3}\,s^{-1}$)
Sc_T	turbulence Schmidt number
t	time (s)
$\mathbf{u}$	velocity vector ($m\,s^{-1}$)
x	mass fraction
$Y_{x/o}$	cell growth yield based on oxygen

Greek letters

α	volume fraction
ε	turbulence eddy dissipation ($m^2\,s^{-3}$)
Γ	mass transfer source term ($kg\,m^{-3}\,s^{-1}$)
μ	molecular viscosity (Pa s)
μ_{max}	maximum specific cell growth rate (s^{-1})
μ_T	turbulence induced viscosity (Pa s)
ρ	density ($kg\,m^{-3}$)

Superscripts

*	saturated state
–	dimensionless state

Subscripts

0	initial state
a	alginate gel
g	gas phase
l	liquid phase
m	mineral salt medium
n	nitrogen
o	oxygen
p	phenol
s	solid phase
sup	superficial
x	cell

Until recently, bubbles were usually considered to be uniformly distributed in the multiphase reactor but with progress in model development, the evolution of bubble size distribution (BSD) and bubble–bubble interactions can now be taken into account, both of which play very significant roles in calculation of the G–L specific interfacial area [49–54]. With the so-called multiple size group (MUSIG) model, bubble sizes result directly from the population balance equation and bubble–bubble interactions are controlled by bubble coalescence and breakup laws [55,56].

The objective of this study was to develop a 3D transient CFD model for simulating the dynamic behaviors of batch phenol biodegradation with immobilized *Candida tropicalis* in alginate gel beads in a G–L–S three-phase BC. This required coupling of three-phase fluid flow, interphase species mass transfer and intrinsic bioreaction kinetics, with the BSD determined by applying the MUSIG model. Model simulation results of phenol and oxygen concentration changes in the liquid phase were validated by corresponding experimental measurements under various operating conditions. Local transient phenol biodegradation behaviors, such as hydrodynamic characteristics and species distributions, were predicted by the model and the rate-limiting step was determined through comparisons between interphase mass transfer and bioreaction of species.

2. Model development

In the immobilized batch phenol biodegradation process, solid carriers are suspended in the liquid phase. Oxygen is transferred from the gas phase into the liquid phase and both phenol and oxygen are transferred from the liquid phase into the solid phase, where they are consumed by cells. The solid particles are assumed to be spherical, with a single, constant radius during the biodegradation process, while cells are distributed uniformly within the alginate gel beads. Substrate degradation and cell growth within the alginate gel beads are both limited by phenol and oxygen concentrations, while all other nutrients are in excess. The influence of free cells in the liquid phase on phenol biodegradation is negligible because they are present only in very small amounts [57].

Based on the above considerations, a 3D transient CFD model was developed to simulate the batch phenol biodegradation dynamic behaviors by immobilized *C. tropicalis* in a G–L–S three-phase BC, combining three-phase fluid flow, interphase species mass transfer and intrinsic bioreaction kinetics. An Eulerian approach was adopted to describe the flow behavior of each phase. The liquid phase, composed of mineral salt medium, phenol and oxygen, was considered to be the continuous phase, while the gas phase, composed of nitrogen and oxygen, and the solid phase, composed of alginate gel, phenol, oxygen and cells, were considered to be the dispersed phases. A turbulence model, simulating the local transient hydrodynamics as well as the MUSIG model describing the BSD, were previously presented in detail [1] so is not repeated here.

2.1. Species transport equations

The following provides a detailed description of the species transport equations and the corresponding model parameters:

$$\frac{\partial}{\partial t}(\rho_g\alpha_g x_{o,g}) + \nabla\cdot(\rho_g\alpha_g x_{o,g}\mathbf{u}_g) = \nabla\cdot\left[\alpha_g\left(\rho_g D_{o,g} + \frac{\mu_{T,g}}{Sc_{T,g}}\right)(\nabla x_{o,g})\right] - \Gamma_{o,gl} \quad (1)$$

$$\frac{\partial}{\partial t}(\rho_l\alpha_l x_{o,l}) + \nabla\cdot(\rho_l\alpha_l x_{o,l}\mathbf{u}_l) = \nabla\cdot\left[\alpha_l\left(\rho_l D_{o,l} + \frac{\mu_{T,l}}{Sc_{T,l}}\right)(\nabla x_{o,l})\right] + \Gamma_{o,gl} - \Gamma_{o,ls} \quad (2)$$

$$\frac{\partial}{\partial t}(\rho_l\alpha_l x_{p,l}) + \nabla\cdot(\rho_l\alpha_l x_{p,l}\mathbf{u}_l) = \nabla\cdot\left[\alpha_l\left(\rho_l D_{p,l} + \frac{\mu_{T,l}}{Sc_{T,l}}\right)(\nabla x_{p,l})\right] - \Gamma_{p,ls} \quad (3)$$

$$\frac{\partial}{\partial t}(\rho_s\alpha_s x_{o,s}) + \nabla\cdot(\rho_s\alpha_s x_{o,s}\mathbf{u}_s) = \nabla\cdot\left[\alpha_s\left(\rho_s D_{o,s} + \frac{\mu_{T,s}}{Sc_{T,s}}\right)(\nabla x_{o,s})\right] - S_{o,s} + \Gamma_{o,ls} \quad (4)$$