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Modeling granule development and reactor performance on anaerobic granular sludge reactors

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ABSTRACT

In this study, a dynamic model for up-flow anaerobic granular sludge reactors capable of simultaneously predicting the granule development (size and composition) and the reactor performance was developed, implemented and validated. The model couples the anaerobic digestion model No.1 (ADM1), slightly adapted, with the reactor hydrodynamics and the mass transfer processes within the granule for soluble and particulate components. Granular development prediction was achieved by considering the kinetic processes and the advective flux for particulate components inside the granular matrix and particulate detachment in the granule surface. The model was implemented in Matlab software. Simulations accurately predicted the methane production rate and the granular size distribution of a bench-scale expanded granular sludge bed (EGSB) reactor treating synthetic sucrose based wastewater. Additionally, the model was successfully implemented, not only considering a mean granule size, but also including a granule size distribution. Results showed that considering the granule size distribution only affected the particulate concentration in the reactor outlet stream at the expense of highly increasing the computational cost for simulation.

1. Introduction

Anaerobic digestion has become a competitive technology for wastewater treatment in the last decades [1–4]. The development of this technology was driven by the decoupling of hydraulic residence time (HRT) and cellular residence time; this was achieved by sedimentation, immobilization in fixed or moving bed or granulation process. Granular sludge reactors are the most currently used worldwide [3,5]. Mathematical modeling is a very useful tool for anaerobic systems design, as well as for optimizing already installed systems and for predicting the reactor performance under different operational conditions. Considerable effort has been expended on developing models that describe the performance of granular sludge reactors [6–12].

The anaerobic digestion is a complex multistep process performed by a community of microorganisms. Several mathematical models describing the processes involved in the anaerobic digestion have been developed over the years with an increasingly degree of complexity [13]. In 2002 the International Water Association (IWA) gather a group of international experts in anaerobic process analysis, modeling and simulation to develop a generalized model of anaerobic digestion (Anaerobic Digestion Model No.1, ADM1) published by Batstone et al. [14]. This model has been widely applied for different substrates [15–18]. It has also been applied to both completely mixed systems [15,17,19] and distributed parameters: semi-continuous tubular digester [13], up-flow anaerobic sludge bed (UASB) reactor with axial dispersion [20] and biofilms [9,10].

In fixed biomass systems the substrate utilization rate may be limited by mass-transfer resistance. Several researchers incorporated mass-transfer resistance by coupling diffusive and kinetic phenomena [6,7,9,21–23]. Although these researchers demonstrate the significant effect of diffusion on biofilm systems they all considered fixed biomass inside the biofilm and therefore a given granule diameter.

Growing interest in studying the composition of the biofilm, mainly in the study of the role of substrate kinetics on biofilm structure, has driven the development of models that consider the kinetics and mass transfer of the solid phase inside the biofilm in addition to the liquid phase behavior. Therefore researchers have proposed both unidimensional [8,9,12] and multidimensional models [10,11]. Although these multidimensional models are interesting tools to evaluate granulation theories and to visualize the heterogeneous structures in biofilms, they are complex models that increase the computational cost and require a high level of expertise of who implements them.

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Nomenclature

Abbreviations

COD	Chemical oxygen demand
EGSB	Expanded granular sludge bed
LCFA	Long chain fatty acids
ODE	Ordinary differential equations
UASB	Up-flow anaerobic sludge blanket
VFA	Volatile fatty acids
VSS	Volatile suspended solids

Variables

$C_{B,i}$	Concentration of component i in the bulk liquid (kgCOD/m^3 [1])
$C_{G,i}$	Concentration of component i per unit of granule liquid phase (kgCOD/m^3 [1]) [2]
C_i	Carbon content of component i (kmole$_C$/kg$_{COD}$)
$C_{in,i}$	Concentration of component i in the influent (kgCOD/m^3 [1])
d_p	Granule diameter (m) [2]
$D_{e,i}$	Diffusion coefficient of component i within the granule (m^2/s)
D_R	Reactor diameter in the fluidization zone (m)
$D_{w,i}$	Molecular diffusion coefficient of a component i in water (m^2/s)
E_i	Input function (kgCOD/m^3/day [1])
$f_{COD,i}$	Theoretical chemical oxygen demand for particulate material i (kgCOD/kg)
$f_{D,i}$	Correction factor for diffusion in granule relative to diffusion in pure water for a component i ($f_{D,i} = D_{e,i}/D_{w,i}$)
F_{obj}	Objective function (for parameter estimation)
$f_{p,i}$	Product p on substrate i yield
f_{Rp}	Fractional distribution of granule sizes inside the reactor (MS model)
g	Gravitational acceleration (g = 9.8 m/s^2)
$j_{r,i}$	Mass flux of the component i in the radial direction (kgCOD/m^2/s)
K_{a,CO_2}	Acid–base equilibrium coefficient ($CO_{2,ac}/HCO_3^-$)
k_d	First order decay rate (1/day)
k_{dt}	Detachment rate coefficient (m s^2/kg)
$K_{H,i}$	Henry's law coefficient for component i (kgCOD/m^3/bar [1])
$K_{I,k,j}$	Concentration of inhibitor k giving 50% inhibition of the rate for process j (kgCOD/m^3)
k_j	First order reaction rate coefficient for process j (1/day)
k_La	Gas–liquid transfer coefficient (1/day)
$k_{m,j}$	Monod maximum specific uptake rate for process j (1/day)
$K_{s,j}$	Monod half saturation constant for process j (kgCOD/m^3)
$M_{pulse,j}$	Pulse input mass of component i (kgCOD [1])
N_G	Number of granules inside the reactor
N_i	Net flux from granule to bulk liquid for component i (kgCOD/s [1])
n_j	Number of transformation processes
n_R	Number of replicates (for parameter estimation)
n_{Rp}	Number of granules with different d_p inside the reactor (MS model)
n_S	Number of soluble components
n_X	Number of particulate components
n_Y	Number of observations (for parameter estimation)
p_{gas}	Gas pressure (bar)
$p_{gas,i}$	Gas i partial pressure (bar)
Q	Volumetric flow rate (m^3/day)
r	Granule radial distance in spherical coordinates (m)
R	Universal gas constant (0.082 m^3 atm/kmol/K)
Re	Reynolds number
$r_{dt,i}$	Specific detachment rate for particulate component i (kgCOD/m^3/s) [2]
$r_{G,i}$	Reaction rate for component i (kgCOD/m^3/day [1]) [2]
R_p	Granule radius (m) [2]
S_i	Concentration of soluble component i in the granule (kgCOD/m^3 [1]) [2]
$S_{B,i}$	Concentration of soluble component i in the bulk liquid (kgCOD/m^3 [1])
$S_{step,i}$	Concentration of soluble component i in the feed during step experiments (kgCOD/m^3 [1])
$S_{I,k}$	Concentration of inhibitory component k (kgCOD/m^3)
$S_{in,i}$	Concentration of soluble component i in the influent (kgCOD/m^3 [1])
t	Time (s)
t_c	Time conversion factor (86400 s/day)
t_{step}	Time when step change is initiated (day)
t_{Final}	Final integration time (s)
tol_c	Tolerance for granular growth (m/s)
tol_R	Relative tolerance for concentration of all components (%)
t_{pulse}	Time when impulse is injected (d)
T	Operational temperature (K)
u	Liquid up-flow velocity (m/s)
u_{des}	Advective velocity of particulate components in the granule (m/s) [2]
u_{dt}	Global detachment velocity (m/s) [2]
u_g	Gas superficial velocity (m/s)
V_M	Blanket volume (m^3)
V_R	Reactor volume (m^3)
X_i	Concentration of particulate component i in the granule (kgCOD/m^3) [2]
$X_{B,i}$	Concentration of particulate component i in the bulk liquid (kgCOD/m^3)
$X_{in,i}$	Concentration of particulate component i in the influent (kgCOD/m^3)
Y_i	Yield coefficient of biomass on substrate i
$y^e_{p,r}$	Experimental observation p, replicate r (for parameter estimation)
y^m_p	Simulated observation p (for parameter estimation)

Greek letters

ε	Gas (ε_g), liquid (ε_l) and solid (ε_s) holdups
ε_L	Volume fraction of liquid phase in the granule
$\varepsilon_{s,k}$	Volid holdup for $R_p(k)$ size granules (MS model)
ΔR_p	Increase/decrease in the granule radius for one iteration (m) [2]
Δt_c	Time increase for one iteration (s)
Δt_{pulse}	Injection time for impulse (s)
$\upsilon_{i,j}$	Stoichiometric coefficients of component i in process j
$\rho_{B,j}$	Rate of process j in the bulk liquid (kgCOD/m^3/day [1])
ρ	Gaseous (ρ_g), liquid (ρ_l) and solid (ρ_s)[2] phases density (kg m^{-3})
ρ_j	Kinetic and liquid–gas transfer rate equations of process j (kgCOD/m^3/day [1])
$\rho_{s,i}$	Density of particulate component i (COD per cell volume) (kgCOD/m^3)