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Multi-scale modelling of bioreactor–separator system for wastewater treatment with two-dimensional activated sludge floc dynamics

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ABSTRACT

A simple "first generation" multi-scale computational model of the formation of activated sludge flocs at micro-scale and reactor performance at macro-scale is proposed. The model couples mass balances for substrates and biomass at reactor scale with an individual-based approach for the floc morphology, shape and micro-colony development. Among the novel model processes included are the group attachment/detachment of micro-flocs to the core structure and the clustering of nitrifiers. Simulation results qualitatively describe the formation of micro-colonies of ammonia and nitrite oxidizers and the extracellular polymeric substance produced by heterotrophic microorganisms, as typically observed in fluorescence *in situ* hybridization images. These results are the first step towards realistic multi-scale multispecies models of the activated sludge wastewater treatment systems and a generic modelling strategy that could be extended to other engineered biological systems.

1. Introduction

Microbial communities play a vital role in the geochemical cycling both in the natural environment and engineered biological systems. Their enormous power emerges from the actions of very large numbers of individual bacteria (estimated to be on average 10^{29} in the seas and 10^{18} in a single wastewater treatment plant), divided between hundreds or thousands of species. However, most design and modelling approaches use macro-scale models that can consider the effect of micro-scale changed on performance. Bridging the gap between the macro and micro-scales would give engineers new tools that would enable them to better understand, design and optimize the novel and extant technologies.

Of all existing biotechnologies, arguably the most important biological processes are those being used for the treatment of municipal and industrial wastewaters. Of these, one of the most common is the activated sludge process. The floc,

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an aggregate of microorganisms and abiotic particles that comprise more than 70% of the bacterial biomass in such systems (Morgan-Sagastume et al., 2008), is central to this vital technology. The bacterial community composition, diversity and ecology of the activated sludge were extensively studied. Lately, the ecological processes that generate generic patterns in the community structure in lab scale bioreactors have also been addressed (Ayarza and Erijman, 2011).

However, most of the models in use describe only the one-dimensional layering of microbial communities within a floc and how these communities evolve and perform and, as a consequence, can predict in a limited extent how the environment affects the flocs characteristics and their dynamics. Spatial organization within the floc, as well as the floc size and morphology strongly influences the energy demands of activated sludge plant (Wilen et al., 2004) together with the removal efficiency of the bioreactor–separator system and quite possibly other properties as well. It is correspondingly desirable to construct mathematical models able to capture the multispecies interactions and to simulate the influence the floc morphology has on the activated sludge system (Ayarza and Erijman, 2011; Takacs and Fleit, 1995).

With few exceptions (for example, the studies of competition between floc-formers and filamentous microorganisms of Takacs and Fleit (1995) and Martins et al. (2004)), the models developed for the activated sludge floc consider the floc as an homogenous sphere (Abasaeed, 1999; Li and Bishop, 2003; Stenstrom and Song, 1991), some of them also consider the size distribution of flocs in the bioreactor (Biggs and Lant, 2002). The connection between the floc formation at micro-scale and the bioreactor–separator performance was not the aim of the previous models. Understanding the connections between these scales is an important and fundamental challenge. For the macro-scale characteristics of microbial systems are the emergent properties of micro-scale activities of hundreds, maybe thousands, of differing taxa.

Nevertheless, it is not clear what properties at the micro-scale (e.g., colony formation, microbial distribution, local inter-species interactions, floc shape, the extent of filamentous microorganisms, floc density and porosity distribution, solute transport properties, etc.) are important at the macro-scale, or how macro-scale changes in environment will affect micro-scale behaviour. This is however, strategically important information which would help us understand and predict how changes in the environment will affect microbial communities and how the communities themselves will impinge on the environment that could affect everything from global sinks and sources of green house gasses, other geochemical cycles, soil function or the sea, diseases and engineered biological systems.

Individual based modelling (IbM), developed initially for planar microbial colonies (Kreft et al., 1998), then extended to biofilms (Alpkvist et al., 2006; Kreft et al., 2001; Picioreanu et al., 2004) and granular sludge (Matsumoto et al., 2010), is well suited to capturing the dynamics of flocs. The IbM methodology allows a geometrically more realistic representation of the floc and this approach also permits the study of the growth of morphologically problematic filamentous bacteria (Martins et al., 2004). Moreover, IbM can facilitate the connection between the micro-scale of the floc phenomena and the macro-scale of the bioreactor performance, as shown in the model operating at different time scales (as well) in another "first generation multi-scale model" for granular sludge development by Xavier et al. (2007).

The goal of this study was to generate a relatively simple first generation multi-scale model of the activated sludge process to: (i) model the dynamics of the observed microbial structure and geometry of activated sludge flocs, in their interdependency with the bioreactor state variable and system operating conditions; (ii) integrate the faster micro-scale floc changes with the slower macro-scale bioreactor–separator system behaviour.

2. Materials and methods

2.1. Experimental

The microbial community structure within activated sludge flocs was analyzed in samples from a municipal wastewater treatment plant (Spennymoor, County Durham, UK) and from laboratory reactors, operated as described elsewhere (Bellucci et al., 2011), by the combined use of fluorescence *in situ* hybridization (FISH) and confocal laser scanning microscopy (CLSM). Samples (250 μl) were fixed within 4 h with 4% paraformaldehyde fixative solution (Hori and Matsumoto, 2010) and stored at −20 °C. Hybridization was performed according to the methodology described in Bellucci and Curtis (2011), with probes targeting the whole bacterial community (specific probes: Eub338i, Eub338ii, Eub338iii) (Daims et al., 1999), ammonia oxidizing bacteria (specific probes and competitors: Nso1225, Neu, CTE, 6a192, c6a192) (Wanner et al., 2006), and nitrite oxidizing bacteria (specific probes and competitors: Nit3, CNit3, Ntspa662, CNtspa662) (Daims et al., 2001). The hybridized biomass was then visualized by CLSM (Leica Microsystems Ltd., Milton Keynes, UK).

2.2. Model description

The overall scheme of the process considered for modelling is presented in Fig. 1. The system comprises a bioreactor in which the flocs are developing, a separator and a purge. Two parameters were defined for characterizing the bioreactor–separator system: hydraulic retention time (HRT – defined as the ratio between the reactor volume and the volumetric flow rate, V_R/Q) and solid dilution time (SDT – the average time spent by a floc inside the system before being eliminated through the purge). As defined here, SDT is related to HRT and the recycle and purge ratios, α and β, through the relationship (1):

$$\mathrm{SDT} = \mathrm{HRT}\frac{\alpha+\beta}{\beta(1+\alpha)} \quad (1)$$

For no recycle at all ($\alpha = 0$), SDT = HRT irrespective of the purge ratio β and the purge loses its meaning, becoming a simple outlet from the system. When $\alpha \to \infty$, SDT = HRT/β and the flocs will stay in the bioreactor the longest possible period for a constant β, which increases as β decreases. Thus, the difference between SDT and the traditionally used SRT (solids retention time) is that the SDT accounts for the number of flocs while SRT represents the total biomass.