WATER RESEARCH 47 (2013) 4739–4751

Available online at www.sciencedirect.com

SciVerse ScienceDirect

journal homepage: www.elsevier.com/locate/watres

Multidimensional modeling of biofilm development and fluid dynamics in a hydrogen-based, membrane biofilm reactor (MBfR)

Kelly J. Martin [a], *Cristian Picioreanu* [b], *Robert Nerenberg* [a,*]

[a] Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, 156 Fitzpatrick Hall, Notre Dame, IN 46556, USA

[b] Department of Biotechnology, Faculty of Applied Sciences, Delft University of Technology, Julianalaan 67, 2628 BC Delft, The Netherlands

ARTICLE INFO

Article history:
Received 22 January 2013
Received in revised form
16 April 2013
Accepted 18 April 2013
Available online 9 May 2013

Keywords:
MBfR
Hollow fiber membrane reactor
Denitrification
Biofilm model
Spiral-wound

ABSTRACT

A two-dimensional, particle-based biofilm model coupled with mass transport and computational fluid dynamics was developed to simulate autotrophic denitrification in a spiral-wound membrane biofilm reactor (MBfR), where hydrogen is supplied via hollow-fiber membrane fabric. The spiral-wound configuration consists of alternating layers of plastic spacer net and membrane fabric that create rows of flow channels, with the top and bottom walls comprised of membranes. The transversal filaments of the spacer partially obstruct the channel flow, producing complex mixing and shear patterns that require multidimensional representation. This study investigated the effect of hydrogen and nitrate concentrations, as well as spacer configuration, on biofilm development and denitrification fluxes. The model results indicate that the cavity spacer filaments, which rest on the bottom membranes, cause uneven biofilm growth. Most biofilm resided on the bottom membranes, only in the wake of the filaments where low shear zones formed. In this way, filament configuration may help achieve a desired biofilm thickness. For the conditions tested in this study, the highest nitrate fluxes were attained by minimizing the filament diameter and maximizing the filament spacing. This lowered the shear stress at the top membranes, allowing for more biofilm growth. For the scenarios studied, biomass limitation at the top membranes hindered performance more significantly than diffusion limitation in the thick biofilms at the bottom membranes. The results also highlighted the importance of two-dimensional modeling to capture uneven biofilm growth on a substratum with geometrical complexity.

1. Introduction

The membrane biofilm reactor (MBfR) is a drinking water and wastewater treatment technology based on membranes that supply a gaseous substrate to biofilm that grows on the membrane exterior (Martin and Nerenberg, 2012). The MBfR has been studied extensively with oxygen/air supporting aerobic processes (Syron and Casey, 2008) and hydrogen gas,

* Corresponding author. Tel.: +1 574 631 4098; fax: +1 574 631 9236.
E-mail addresses: kmartin9@nd.edu (K.J. Martin), C.Picioreanu@tudelft.nl (C. Picioreanu), nerenberg.1@nd.edu (R. Nerenberg).
0043-1354/$ – see front matter
http://dx.doi.org/10.1016/j.watres.2013.04.031

an electron donor, supporting autotrophic denitrification and other reductive bioprocesses (Celmer-Repin et al., 2010; Ergas and Reuss, 2001; Martin and Nerenberg, 2012; Nerenberg and Rittmann, 2004). With complete consumption of hydrogen gas possible within the biofilm layer, hydrogen utilization efficiencies can approach 100 percent (Lee and Rittmann, 2002). Hydrogen-based denitrification is the application studied in this research.

Among biofilm reactors, MBfRs are unique because of counter-diffusional substrate delivery, where substrates (e.g., hydrogen and nitrate) diffuse into the biofilm from opposing sides. Excessively thick MBfR biofilms can experience dual substrate limitation, where both the inner and outer regions of the biofilm become substrate limited due to diffusional resistance. This results in reduced biological activity and lower nitrate fluxes (Semmens and Essila, 2001). Biofilms with insufficient thickness may also exhibit low nitrate fluxes because of biomass limitation. Considering the sensitivity of the MBfR biofilm to biofilm thickness, biomass management is especially critical to the maintenance of satisfactory denitrification rates. However, difficulty in controlling biofilm detachment makes biomass management the most significant challenge in the scale-up of the MBfR (Syron and Casey, 2008).

Recently, a hydrogen-based MBfR became commercially available for the treatment of nitrate and other oxidized contaminants from compromised drinking water sources (Martin and Nerenberg, 2012). The MBfR module employs a spiral-wound configuration, where layers of inert, plastic spacer net separate layers of hollow-fiber membrane fabric, creating narrow flow channels that guide the water past walls of biofilm-covered fibers. The narrow flow channels provide excellent ratios of membrane surface area to reactor volume. The plastic spacer net partially obstructs the flow channel, producing complex fluid dynamic and mass transport schemes that are highly influential in biofilm development. The spiral-wound configuration is frequently used by filtration modules, such as reverse osmosis (RO) units, and modeling studies have investigated the impact of spacer design on the magnitude and distribution of shear stress and (bio)fouling (Schwinge et al., 2004; Picioreanu et al., 2009; Radu et al., 2010). However, the conclusions of these studies are not transferrable to MBfR systems. In contrast to filtration systems, the MBfR provides a substrate at the membrane surface and supports biofilms that exhibit unique behavior due to counter-diffusion. It is important to specifically study MBfR biofilm development in the spiral-wound flow channel and the impact of spacer design on biofilm management and contaminant removal fluxes.

Modeling brings an understanding of the biofilm microenvironment (e.g., chemical gradients and structural heterogeneity) and ultimately a better understanding of macroscale process performance (e.g., denitrification fluxes). Furthermore, modeling allows for evaluation of design and operational parameters with the results identifying the most important parameters to explore experimentally. In the past, MBfRs have been modeled by pseudo-analytical (Casey et al., 1999) and one-dimensional (1-d) numerical models (Debus and Wanner, 1992; Downing and Nerenberg, 2008a; Lackner et al., 2008; Pavasant, 1996; Shanahan and Semmens, 2004; Syron and Casey, 2008). However, the spiral-wound MBfR requires multi-dimensional modeling for correct representation. The complex geometry of the woven membrane fabric and spacer net create complicated fluid dynamics and mass transfer patterns that influence biofilm morphology and activity. Moreover, heterogeneity in the biofilm surface morphology (i.e., variability in biofilm thickness) may significantly impact reactor performance, due to the sensitivity of the counter-diffusional biofilm to thickness. There is, however, very limited research addressing the effect of the two-dimensional (2-d) biofilm structure on counter-diffusional biofilms. Matsumoto et al. (2007) simulated the community structure of nitrifying and denitrifying bacteria in an oxygen-based MBfR using a 2-d hybrid approach: small clusters of bacteria were represented as individual entities, and the extracellular polymeric substance was described with a continuum field. For simplicity, however, the model only simulated biofilm growth on a flat surface without consideration of fluid flow and shear patterns.

Cellular automata (CA) models were the first to simulate biofilm growth on a substratum with complicated irregular geometry including packed bed porous media with support grains (Kapellos et al., 2010) and RO feed channels with spacer (Picioreanu et al., 2009; Radu et al., 2010). Later, particle-based biofilm models were introduced for biofilms in packed bed porous media (Graf von der Schulenberg et al., 2009; Picioreanu et al., 2010; Pintelon et al., 2012). Particle-based representation of the biomass is known to create more realistic biofilm morphology than CA models (Wanner et al., 2006).

The main objective of this study was to develop a 2-d, particle-based biofilm model that simulates a spiral-wound MBfR treating nitrate in drinking water or treated wastewater. An existing 2-d, CA biofilm model used to study biofouling in RO feed channels with spacer (Radu et al., 2010) was modified to accommodate: 1) counter-diffusional biofilm growth on a geometrically complex substratum considering the fluid dynamics and mass transport of multiple substrates and 2) particle-based biofilm representation with biomass attachment, division, spreading and detachment. The model was used to evaluate the effect of substrate concentration and spacer filament configuration on spiral-wound MBfR biofilm development, the biofilm microenvironment, and macroscale reactor performance.

2. Methods

The spiral-wound MBfR model consists of two main parts: 1) a biofilm submodel, which considers biomass as individual rigid spheres undergoing attachment, growth, division, spreading, and detachment and 2) a physical submodel, which calculates hydrodynamics and mass transport with reaction for multiple substrates.

2.1. Model geometry

The spiral-wound MBfR is comprised of alternating layers of woven membrane fabric and spacer net. The longitudinal fibers of the spacer net, oriented parallel to the main flow