

Modeling the impact of fluid dynamics on biofilm activity in fixed-bed reactors

L. Prades*, J. Climent**, X. Guimerà*, S. Chiva**, Y. Bautista***, X. Gamisans* and A. D. Dorado*

* Department of Mining, Industrial and ICT Engineering, Universitat Politècnica de Catalunya, Bases de Manresa 61-73, 08240 Manresa, Barcelona, Spain (E-mail: lledo.prades@upc.edu; xavier.guimera@upc.edu; xavier.gamisans@upc.edu; toni.dorado@upc.edu)

** Department of Mechanical Engineering and Construction, Universitat Jaume I, Avd. Vicent Sos Baynat s/n, 12071 Castelló de la Plana, Castelló, Spain (E-mail: jcliment@uji.es; schiva@uji.es)

*** Instituto de Tecnología Cerámica, Asociación de Investigación de las Industrias Cerámicas, Avd. Vicent Sos Baynat s/n, 12071 Castelló de la Plana, Castelló, Spain E-mail: yolanda.bautista@itc.uji.es)

ABSTRACT

The influence of fluid flow dynamics in mass transfer and biokinetics was considered to develop a rigorous model for biofiltration processes in air pollution control. In particular, a 3D model has been developed employing CFD techniques to analyze the impact of hydrodynamics over mass transfer and to predict biofilm activity and space-time evolution of physical and biological phenomena involved. The rheology considered for the fixed biofilm has been experimentally characterized. The dynamic multiphase model describes biofilm and liquid phase interaction. Moreover, model predictions were corroborated with direct measurements in the interphase and within the biofilm by means of novel microsensors with high spatial resolution. Model predictions improved in comparison to conventional diffusional-reaction model and well-established modeling tools. Therefore, the developed and validated model becomes a valuable tool to characterize in detail main processes taking place in the interface and within the fixed-bed biofilm, and finally to optimize bioreactors operation.

Keywords

CFD modeling; fixed biofilm reactor; hydrodynamics; biofiltration; mass transfer

INTRODUCTION

In biofiltration systems, the gas/liquid interphase acts as a major medium for the transport of dissolved solutes into and out of the biofilm. Therefore, transfer processes can be affected by the reactor flow conditions, so an adequate characterization of this fluid flow is required in order to describe accurately the system, jointly with the biological behavior. Computational fluid dynamics (CFD) techniques have been employed as a useful tool for understanding multiphase hydrodynamics and biochemical reactions in the wastewater treatment field (Liotta et al. 2014), where the bioreaction behavior is associated to the liquid phase dynamics. Nevertheless, the complicated interactions between biofilm and fluid flow phases (gas and liquid), coupling hydrodynamics with mass transfer and bioreactions, have not been described using this type of techniques, being one of the keys to optimize biofilters performance.

The aim of this investigation is to develop more comprehensive models for biofiltration systems, by incorporating fluid flow dynamics, mimicking their hydrodynamics and behavior. In this work, a bioreactor models are developed employing CFD techniques and their performance are validated for both by experimental hydrodynamic characterization and comparing simulated result with experimental measurements recorded using DO microsensors. A fixed-bed biofilm reactor is used to characterize the biodegradation phenomena inside an aerobic heterotrophic biofilm, studying in detail the relevant phenomena in both liquid and biofilm phases. To confer a coherent identity models, the CFD simulation results are compared qualitative and critically with another results obtained from a well-established modeling tool, such as AQUASIM, and the results from using traditional

assumptions to model biological systems. Additionally, the multiphase model describes biofilm and liquid phase interactions, studying in detail the influence of fluid flow velocity. The developed 3D CFD models are used to study the influence of hydrodynamics over mass transport and to predict species presence anywhere in the bioreactor.

MATERIALS AND METHODS

Experimental set-up and biofilm characterization

Experimental measurements were conducted through an aerobic heterotrophic biofilm grown on a flat plate bioreactor (FPB). The FPB operation and the recording of microprofiles were performed as described in Guimerà et al (2015). Recorded DO profiles, obtained at different positions along the flat plate and recorded during both endogenous and substrate consumption conditions, were used to estimate the microbial consortium kinetic parameters (Expressions 1 and 2). The evaluation of the recorded microsensors profiles was performed using the methodology proposed by Wäsche et al. (2002).

$$R_B DO(i, j) \Big|_{\substack{i=1 \\ j=1}}^{\substack{i=n_L \\ j=n_B}} = q_{\max, DO} \cdot \frac{C_B DO(i, j)}{K_{S, DO} + C_B DO(i, j)} \cdot X(i, j) + k_d \cdot X(i, j) \quad (1)$$

$$R_B S(i, j) \Big|_{\substack{i=1 \\ j=1}}^{\substack{i=n_L \\ j=n_B}} = \frac{1}{Y_{DO/S}} \cdot q_{\max, DO} \cdot \frac{C_B DO(i, j)}{K_{S, DO} + C_B DO(i, j)} \cdot X(i, j) \quad (2)$$

The residence time distribution (RTD) was obtained in order to validate models hydraulic behavior. The measuring control point was located at the outlet of the bioreactor. Moreover, the obtained experimental data of mass transfer characterization study between liquid and biofilm phases were fitted with the correlation for FPB described by Zhang and Bishop (1994).

Rheological characterization

In order to characterize the biofilm as a non-newtonian flow, analyses in the steady shear mode were performed. The flow curve measurements were conducted with control shear stress, raising shear stress stepwise. The data results were fitted with Herschel-Bulkley model to describe shear-thinning behavior with a yield stress (Mezger, 2006).

CFD modelling

The commercial CFD software ANSYS® Academic Research, Release 16.2, was used to solve the equations of continuity and momentum. Firstly, a single-phase model was used to validate the implementation of the biological kinetics into the CFD code, introducing hydraulic pressure loss model in the momentum equation in order to model physical characteristics of biomass. Secondly, a multiphase model was used to characterize the bioreactor performance, including two different fluids inside this domain (the liquid phase and the biofilm phase). This biofilm phase was characterized as a pseudoplastic fluid. In both models the bioreactor was defined by a single domain, and the region of the biological system was introduced as a subdomain in the lower part of the flat plate. The implementation of biological reactions in the CFD software was performed using the methodology described by Climent et al (2014), in which variables on kinetic expressions were defined as additional variables in the computational space, including an extra transport equation for each of them. In addition, the expressions for the biodegradation kinetics (Expressions 1 and 2) were included as source terms. Related to define mass transfer phenomena, a dimensionless Sherwood number based on empirical correlation was defined for the additional variables.

RESULTS AND DISCUSSION

Validation of the CFD models performance

Three different modeling tools (AQUASIM, MATLAB and CFD software ANSYS) were used for

modeling the bioreactor performance and compare the results. A first set of simulations was carried out using 2D steady-state models. The results of the simulations performed are presented in Figure 1A. Qualitatively, AQUASIM, MATLAB and CFD simulated profiles present the same behavior and the same trend throughout the biofilm, reaching the anaerobic limit at similar depths for all the studied biofilm densities. Therefore, fitting the kinetic constants and their implementation into CFD software can be stated as successful. For a more quantitative comparison with the experimental results, the normalized root mean square errors (NRMSE) between the experimental DO profiles and the simulated DO profiles were determined. The deviations obtained using AQUASIM, MATLAB and CFD software are 5.36%, 4.35% and 3.47% respectively, reproducing with great accuracy the biological behavior. Hence, comparing AQUASIM and MATLAB simulated profiles with the CFD ones, in which a detailed simulation of mass transport phenomena in the liquid has been considered, the fact of including hydrodynamics models improves the simulations results, reducing the NRMSE around 2% for the studied conditions.

CFD simulation results

A new set of CFD simulations was carried out, describing the bioreactor performance using a 3D model in transient conditions. From the results, it was possible to analyze fluid flow characteristics, mass transport mechanism and biodegradation phenomena along the bioreactor in unsteady state. At first stage, the hydrodynamics characterization of bioreactor was studied from streamlines, velocity profiles and RTD analysis. Streamlines and velocity profiles are shown in Figure 2 along the bioreactor. The streamlines (Figure 2A) show that the liquid phase was correctly (evenly) distributed over the bioreactor, contacting the overall of the biomass (specified in brown). Moreover, the velocity profiles (Figure 2B) identified bioreactor zones which support the highest and lowest velocities. The bioreactor zones which supported lower velocities were mainly in the biofilm section, thus the diffusive phenomena were predominant over the mass transport in these zones. Finally, the velocity profiles in the liquid phase (represented by L1 line in the cross section of the bioreactor in Figure 2B) match satisfactory the velocity distribution of a laminar flow regime (Figure 2D). To perform the RTD analysis, both experimental and simulated $E(t)$ curves were obtained and presented in Figure 1B. As it can be seen, defined CFD model reproduced correctly the experimental data obtained in the control point, located at outlet of the bioreactor. Then, it was concluded that the bioreactor hydrodynamics model was equivalent to plug-flow reactor in series with a continuous stirred-tank reactor. At second stage, the study of DO profiles inside in the FPB was detailed. Figure 2 shows an example of DO profiles at final stage of the simulation in a section of the bioreactor. At initial stage, oxygen concentration was null in the biofilm and it was saturated in liquid phase. At final stage, after running the simulation (Figure 2C and 2D), oxygen had been transferred from the liquid to the biofilm phase and DO profiles were formed due to transformation and diffusivity phenomena inside the biofilm, which were implemented previously into CFD code. Moreover, the experimental and simulated DO profiles obtained at other different flow velocities (data not shown) presented the same behaviour and the same trend throughout the biofilm, reaching the anaerobic limit at identical depths, for all the studied flow conditions. Therefore, the developed CFD model could be used to determine the effective thickness of biofilm and to differentiate between aerobic and anaerobic zones in the biofilm region under a wide range of conditions.

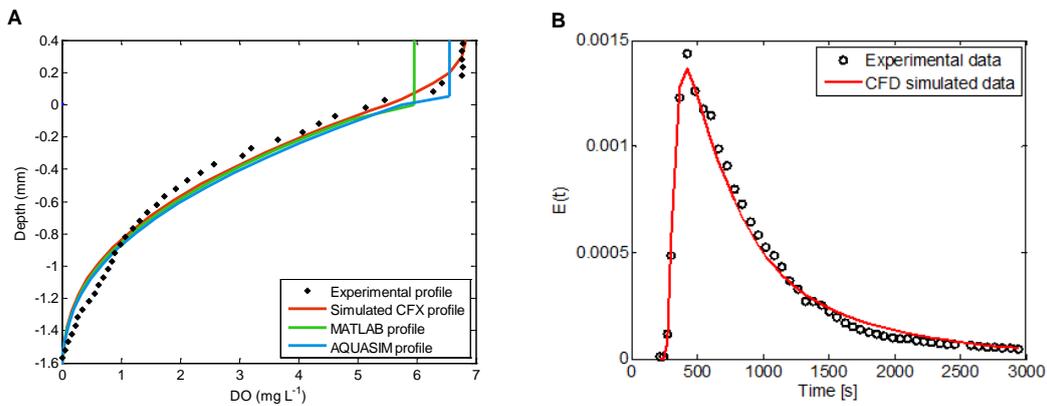


Figure 1. Validation of the developed CFD model. (A) Experimental DO profiles (symbols) and simulated DO profiles (solid lines) measured in depth at liquid and biofilm phases. (B) Comparison between experimental (symbols) and simulated results (solid line) of RTD analysis.

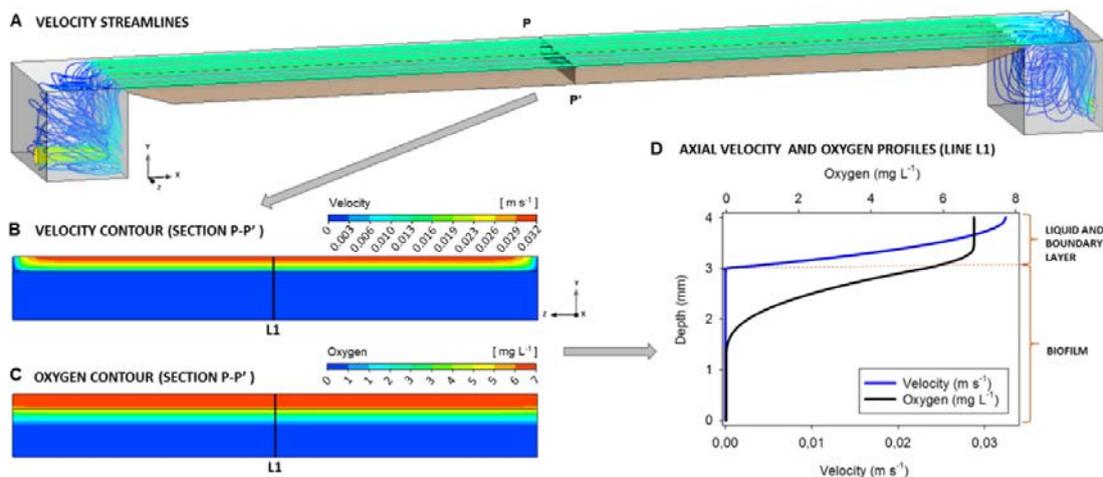


Figure 2. Results of CFD simulation of fixed-biofilm reactor. (A) Velocity streamlines inside the bioreactor, (B) velocity contours in section P-P', (C) oxygen contours in section P-P', and (D) axial velocity and oxygen profiles in line L1.

REFERENCES

- Climent, J., Martínez-Cuenca, R., Berlanga, J. G., Julián-López, B. and Chiva, S. (2014) CFD simulation of hydrodynamics and biological reactions in an activated sludge process of WWTP. *World Water Congress Exhibition (IWA 2014) Proceedings*, IWA, Ed.
- Liotta, F., Chatellier, P., Esposito, G., Fabbricino, M., Van Hullebusch, E. D. and Lens, P. N. L. (2014) Hydrodynamic Mathematical Modelling of Aerobic Plug Flow and Nonideal Flow Reactors: A Critical and Historical Review, *Critical Reviews in Environmental Science and Technology*, **44**, 2642–2673.
- Guimerà, X., Moya, A., Dorado, A.D, Villa, R., Gabriel, D., Gabriel, G. and Gamisans, X. (2015), Biofilm dynamics characterization using a novel DO-MEA sensor: mass transport and biokinetics. *Applied microbiology and biotechnology*, **99**, 55–66.
- Mezger, T. G. (2006). The rheology handbook: for users of rotational and oscillatory rheometers. Vincentz Network GmbH & Co KG.
- Wäsche, S., Horn, H. and Hempel, D. C. (2002) Influence of growth conditions on biofilm development and mass transfer at the bulk/biofilm interface. *Water Research*, **36**, 4775–4784.
- Zhang, T. and Bishop, P. (1994) Experimental determination of the dissolved oxygen boundary layer and mass transfer resistance near the fluid-biofilm interface *Water Science and Technology*, **30**, 47–58.