CFD Simulations of Fluid Dynamics Inside a Fixed-Bed Bioreactor for Sugarcane Vinasse Treatment

D.C.G. Okiyama[1(✉)], J.A. Rabi[1], R. Ribeiro[1], A.D.N. Ferraz Jr.[2], and M. Zaiat[2]

[1] Faculty of Animal Science and Food Engineering, University of São Paulo, Av. Duque de Caxias Norte 225, Pirassununga, SP 13635-900, Brazil
[2] São Carlos School of Engineering, University of São Paulo, Av. Trabalhador Sãocarlense 400, CP 359, São Carlos, SP 13566-590, Brazil

Abstract. Vinasse is a by-product from ethanol industry which can be exploited in ferti-irrigation after its treatment via APBR (anaerobic packed bed reactor). Comprehensive understanding of fluid dynamics within APBR is fundamental for its design and the goal of this work was to perform CFD (computational fluid dynamics) simulations of a laboratory-scale APBR by the use of commercial software. Tracer concentration patterns deviated from plain plug flow behaviour.

Keywords: Computational fluid dynamics · Agroindustrial effluent · Anaerobic packed bed reactor

1 Introduction

Resulting from the distillation of sugarcane juice, vinasse is a by-product of the sugar-ethanol industry. Large-scale exploitation of aforesaid agroindustrial effluent has long pointed to ferti-irrigation in sugarcane crops (Robertiello 1982). Nevertheless, due to high levels of organic matter, salt and nutrients usually found in vinasse, environmental issues have been raised towards its direct (i.e., untreated) long-term deposition onto crop soil (Madejón et al. 2001).

Anaerobic treatment of vinasse has been claimed as suitable practice prior to ferti-irrigation (Vlissidis and Zouboulis 1993) to mitigate both ground-water contamination and greenhouse effect gases emission (España-Gamboa et al. 2011). Anaerobic treatment can preserve the fertilising qualities (Moraes et al. 2014) while biogas can be recovered (Grisi et al. 2012).

Among anaerobic systems for high removal of biological oxygen demand (BOD), anaerobic packed bed reactor (APBR) is an attractive alternative thanks to its relatively simpler design and operation allied to its low cost and process stability (Ferraz Jr. 2013). Those engineering features are related to APBR ability to render higher solids retention time (SRT) with shorter hydraulic residence time (HRT) and toxicity tolerance (Satyawali and Balakrishnan 2008).

G. Mannina (ed.), *Frontiers in Wastewater Treatment and Modelling*,
Lecture Notes in Civil Engineering 4, DOI 10.1007/978-3-319-58421-8_107

Fluid dynamics in APBR has been studied by relying on ideal operation assumptions such as plug-flow or perfectly-mixed reactor (Levenspiel 1999) and single-parameter models have then been invoked such as longitudinal dispersion and continuous-flow stirred-tank reactor (CSTR) in series (Fazolo et al. 2006; Méndez--Romero et al. 2011; Fernandes et al. 2013). While helpful to identify eventual departure from ideal operation, aforesaid models might be relatively simple in view of current computer resources. In other words, APBR fluid dynamics can be more complex than CSTR in series so that computational fluid dynamics (CFD) may identify either dead zones or short-circuiting flows.

Comprehensive description of fluid patterns in APBR is vital for its design and performance analysis. By relying on fundamental conservation principles, the application scope of physics-based (also known as white-box) models is broader than data-driven (or black-box) models (Datta and Sablani 2007). All-inclusive APBR models are prone to be complex inasmuch as fluid flow and convective-diffusive species transport in porous medium must be concurrently combined with biochemical processes (e.g. acidogenesis, acetogenesis, methanogenesis, and hydrolysis). CFD indeed arises as helpful engineering tool to study fixed-bed systems for effluent treatment (Parco et al. 2007; Brannock et al. 2010; Głuszcz et al. 2011).

In the present work, time-dependent (i.e. dynamic) two-dimensional (2-D) CFD simulations were performed concerning the fluid dynamics inside an existing laboratory-scale cylindrical APBR for sugarcane vinasse treatment (Ferraz Jr. 2013). Specifically, the objective was to numerically simulate the upward flow of a tracer solution within a 2-D vertical cross-section of the APBR during three times the theoretical HRT (Okiyama 2014).

2 Materials and Methods

While the main objective of the present work was to perform CFD simulations, this section outlines some information about the experimental bioreactors for vinasse treatment, which are depicted in Fig. 1(a). Each laboratory-scale cylindrical APBR was assembled in acrylic tubes by comprising feeding module (FM), bed section (BS), effluent collection module (EC), and biogas collection module (BC), as sketched in Fig. 1(b).

Low-density polyethylene small cylinders were used as the supporting medium in BS as a compromise between organic matter removal, APBR stability and biogas production (Ferraz 2013). Figure 1(c) shows samples of aforesaid cylinders, whose approximate dimensions are 5.0 mm of length and 4.5 mm of diameter. Cylinders randomly filled up BS volume so that its packed-bed porosity ranged from 0.47 to 0.54 at start-up. Table 1 summarises the length, the inner diameter, the geometric volume and the volume occupied by the liquid phase at each APBR compartment. Biogas collection module (BC) is solely occupied by the gas phase.

In view of values in Table 1, the total APBR volume occupied by the liquid phase ranged from 2.1865 L for lower BS porosity up to 2.3625 L for higher BS porosity. The bioreactor was initially filled up with water and tracer solution was subsequently fed at

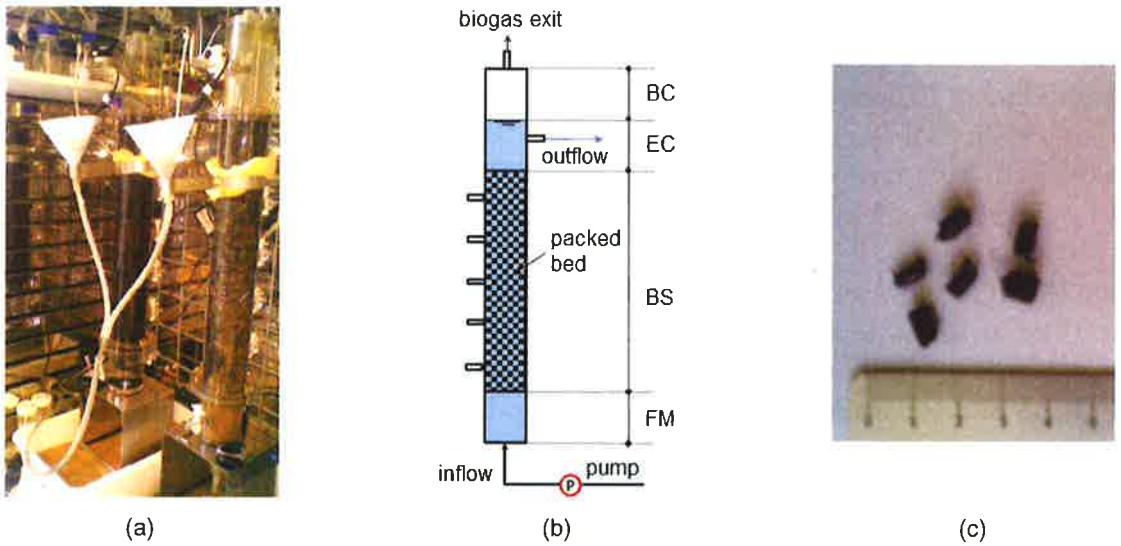

Fig. 1. Laboratory-scale cylindrical APBR for vinasse treatment: (a) picture of experimental bioreactors; (b) sketch depicting feeding module (FM), bed section (BS), effluent collection module (EC) and biogas collection module (BC); (c) picture of low-density polyethylene cylinders employed as supporting medium within BS

Table 1. Length, diameter, geometric volume and volume occupied by liquid phase of each APBR compartment

Compartment dimension	FM	BS		EC	BC
		Porosity = 0.47	Porosity = 0.54		
Length (m)	0.1	0.5	0.5	0.1	0.05
Diameter (m)	0.08	0.08	0.08	0.08	0.08
Geometric volume (10^{-3} m^3 = L)	0.5027	2.5133	2.5133	0.5027	0.2513
Volume with liquid (10^{-3} m^3 = L)	0.5027	1.1812	1.3572	0.5027	–

stepwise flow of 4.6 L/day, thereby yielding a theoretical HRT of approximately 12 h, namely 11.4 h for lower BS porosity and 12.3 h for higher BS porosity.

This work performed two sets of CFD simulations, one for each extreme porosity value at start-up (0.47 and 0.54) whose corresponding permeability was assessed through Kozeny-Carman correlation (Nield and Bejan 1992). For each numerically tested porosity (assumed to be uniform throughout BS compartment), Table 2 shows

Table 2. Porosity-dependent parameters used in CFD simulations of the laboratory-scale APBR

APBR porosity-dependent parameter	BS porosity = 0.47	BS porosity = 0.54
Bed total surface-to-volume ratio	683 m^{-1}	541 m^{-1}
Hydraulic radius	6.88×10^{-4} m	8.49×10^{-4} m
BS particle equivalent diameter	0.00275 m	0.0034
BS permeability	5.34×10^{-8} m^2	1.08×10^{-7} m^2

porosity-dependent parameters used in CFD simulations of the existing laboratory-scale APBR. Conversely, pipe-like flow (i.e. flow without porous medium) was assumed in both FM and EC compartments.

CFD simulations of the fluid dynamics in APBR were carried out with the help of COMSOL Multiphysics® by using the Chemical Species Transport module within the Chemical Reactor Engineering package. Specifically, transient 2-D (i.e. time-dependent two-dimensional) CFD simulations invoked the Transport of Diluted Species model in the Reacting Flow in Porous Media framework of the aforesaid commercial software.

The idea was to simulate upward fluid flow coupled with tracer (namely NaCl) transport in APBR compartments where tracer solution actually flows through, namely FM, BS and EC in Fig. 1(b). APBR was assumed to be initially filled up with clean water and stepwise tracer solution flow was fed in at FM inlet where Dirichlet boundary condition was imposed. Tracer concentration was assumed to remain constant at the experimental feeding value at FM inlet.

3 Results and Discussions

In order to set the number of finite elements for simulations, mesh-independence analysis was carried out by using 0.47 as BS porosity. Figure 2 depicts the finite-element meshes automatically generated by COMSOL Multiphysics® to APBR vertical cross-section. Used in subsequent simulations, normal mesh (with 12.352 elements) provided suitable compromise between computational effort and accuracy of numerical results. It is interesting to note that meshes are locally refined in transitions between APBR compartments as well as near walls, i.e. where steeper gradients (of tracer concentration and fluid velocity) are prone to occur.

For lower BS porosity (= 0.47), Fig. 3 shows tracer concentrations simulated in FM, BS and EC compartments for increasing time instants. CFD simulations pointed to plug-flow with some wall effects, which are noted (to some extent) along all vertical walls. Thereby, higher concentrations are observed around APBR centreline while lower concentrations occur near vertical walls. A somewhat parabolic profile prevails in the upward high concentration front, which deviates from plain plug flow behaviour. Relatively small dead zones are observed in the bottom of FM compartment. Simulations for higher BS porosity (= 0.54) yielded similar patterns, which are not shown here for the sake of brevity.

While tracer concentration at BS exit was numerically simulated as a function of BS radius, the experimental APBR actually referred to a single collection funnel at EC centroid. In view of that, two probing concentration profiles were screened: one at BS centreline and the other at BS half-radius. When compared to experimental data, the former yielded better results. Average concentration profile was evaluated through line-integral over the exiting fluid flow so that APBR features were assessed from both experimental and numerical concentration profiles. Experimental average HRT resulted as 11.6 h while CFD simulations rendered 10.6 to 11.4 h. As no preferential paths or relatively large dead zones were evidenced in CFD simulations, one may justify differences between average HRT values in terms of local variations in BS porosity, which was allegedly uniform in CFD simulations.

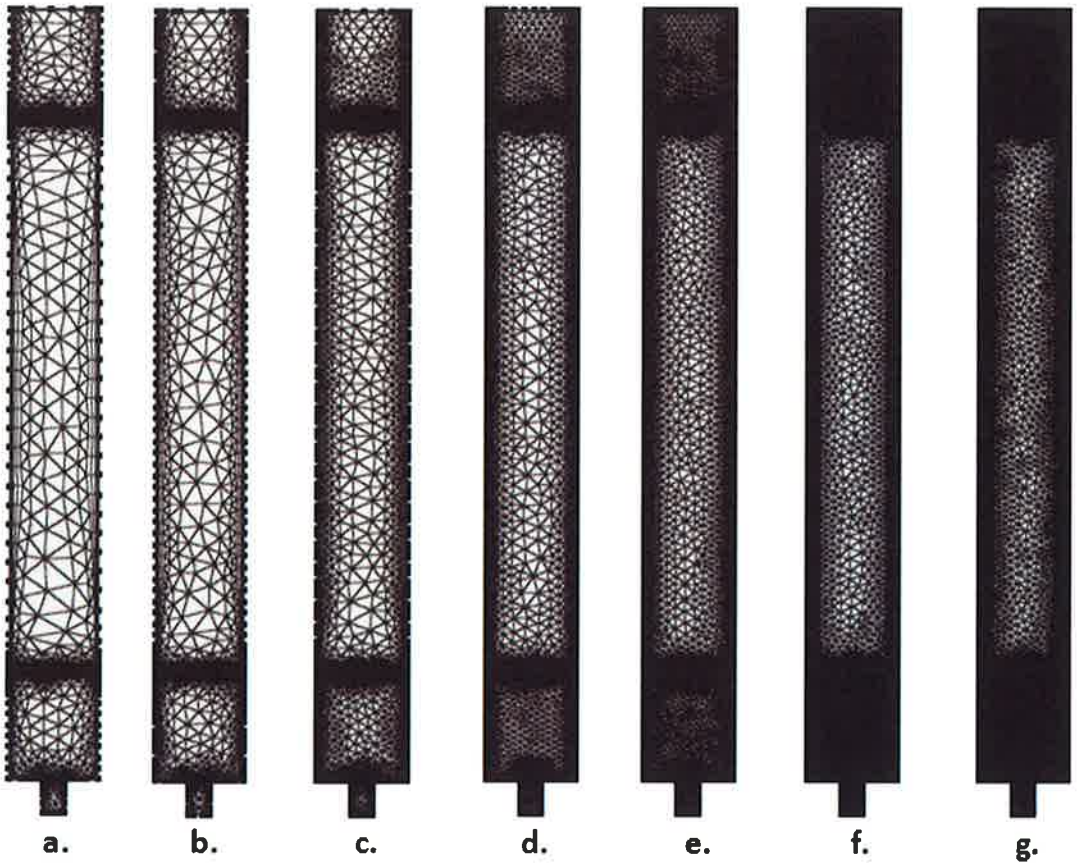

Fig. 2. Finite-element meshes automatically generated by COMSOL Multiphysics® for APBR vertical cross-section: (a) extremely coarse (4146 elements), (b) extra coarse (4.989 elements); (c) coarser (5.972 elements), (d) coarse (9.299 elements), (e) normal (12.352 elements), (f) fine (16.494 elements), (g) finer (27.811 elements)

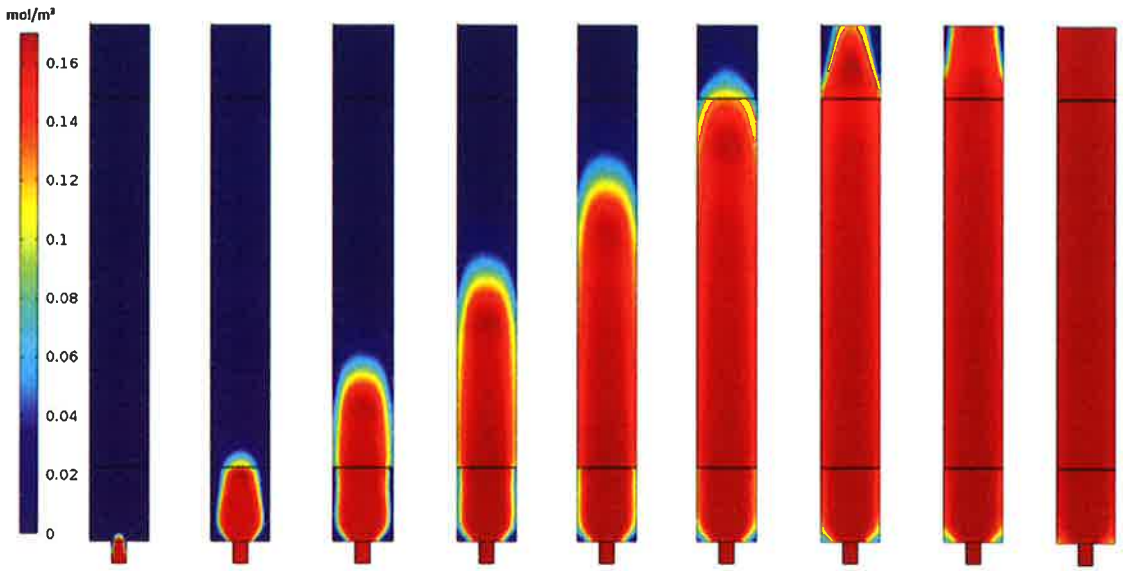

Fig. 3. Tracer concentrations simulated in FM, BS (porosity = 0.47) and EC compartments at increasing time instants (from left to right): 702 s (= 0.195 h), 7020 s (= 1.95 h), 10044 s (= 2.79 h), 21060 s (= 5.85 h), 28080 s (= 7.8 h), 35100 s (= 9.75 h), 42606 s (= 11.835 h), 50130 s (= 13.925 h), and 84330 s (= 23.425 h)

Care should then be exercised when performing CFD simulations while assuming constant porosity. User-defined routines, for instance, should be added to the simulator to account for biofilm on the carriers as well as suspended solids in the medium. Accordingly, as part of our ongoing research to develop in-house simulators of bioreactors for wastewater treatment, lattice Boltzmann method (LBM) has been considered as alternative route (van der Sman 2007). Known to yield relatively simpler computational codes (Mohamad 2011), LBM may numerically simulate either suspended solids in multiphase flow (Ladd and Verberg 2001) or biofilm formation and detachment (Picioreanu et al. 2001), in addition to biogas bubbles generation and transport (Chen 2010).

4 Conclusions

If compared to long-standing models for non-ideal bioreactors for wastewater treatment, CFD can be an efficient engineering tool as it is able to thoroughly depict the APBR in terms of its internal fluid dynamics as well as species concentration profiles. As far as design of up-flow APBR for sugarcane vinasse treatment is concerned, such comprehensive knowledge is strategic for not only scale-up procedures but also operation under distinct scenarios. Future developments may point to surrogate computational methods such as LBM so as to simulate biofilm on the carriers as well as suspended solids and/or biogas in the medium.

Acknowledgements. Authors thank FAPESP São Paulo Research Foundation (Brazil) for research grants (project 11/51902-9). First author thanks FAPESP for MSc scholarship (project 12/23459-6) as well.

References

Brannock M, Leslie G, Wang Y, Buetehorn S (2010) Optimising mixing and nutrient removal in membrane bioreactors: CFD modelling and experimental validation. Desalination 250 (2):815–818

Chen X (2010) Simulation of 2D cavitation bubble growth under shear flow by lattice Boltzmann model. Commun Comput Phys 7(1):212–223

Datta AK, Sablani SS (2007) Mathematical modeling techniques in food and bioprocess: an overview. In: Sablani SS, Rahman MS, Datta AK, Mujumdar AR (eds) Handbook of food and bioprocess modeling techniques. CRC Press, Boca Raton, pp 1–11

España-Gamboa E, Mijangos-Cortes J, Barahona-Perez L, Dominguez-Maldonado J, Hernández-Zarate G, Alzate-Gaviria L (2011) Vinasses: characterization and treatments. Waste Manag Res 29(12):1235–1250

Fazolo A, Pasotto MB, Foresti E, Zaiat M (2006) Kinetics, mass transfer and hydrodynamics in a packed bed aerobic reactor fed with anaerobically treated domestic sewage. Environ Technol 27(10):1125–1135

Fernandes BS, Saavedra NK, Maintinguer SI, Sette LD, Oliveira VM, Varesche MBA, Zaiat M (2013) The effect of biomass immobilization support material and bed porosity on hydrogen production in an upflow anaerobic packed-bed bioreactor. Appl Biochem Biotechnol 170 (6):1348–1366

Ferraz ADN Jr (2013) Anaerobic digestion of sugar cane vinasse in acidogenic fixed bed reactor followed by methanogenic reactor sludge blanket type. Ph.D. thesis (in Portuguese), São Carlos School of Engineering, University of São Paulo, São Carlos, Brazil

Głuszcz P, Petera J, Ledakowicz S (2011) Mathematical modeling of the integrated process of mercury bioremediation in the industrial bioreactor. Bioproc Biosyst Eng 34(3):275–285

Grisi EF, Yusta JM, Dufo-López R (2012) Opportunity costs for bioelectricity sales in Brazilian sucro-energetic industries. Appl Energ 92:860–867

Ladd AJC, Verbeg R (2001) Lattice-Boltzmann simulations of particle-fluid suspensions. J Stat Phys 104(5):1191–1251

Levenspiel O (1999) Chemical reaction engineering, 3rd edn. Wiley, New York

Madejón E, López R, Murillo JM, Cabrera F (2001) Agricultural use of three (sugarbeet) vinasse composts: effect on crops and chemical properties of a Cambisol soil in the Guadalquivir river valley (SW Spain). Agric Ecosyst Environ 84(1):55–65

Méndez-Romero DC, López-López A, Vallejo-Rodríguez R, León-Becerril E (2011) Hydrodynamic and kinetic assessment of an anaerobic fixed-bed reactor for slaughterhouse wastewater treatment. Chem Eng Process 50(3):273–280

Mohamad AA (2011) Lattice Boltzmann method: fundamentals and engineering applications with computer codes. Springer, London

Moraes BS, Junqueira T, Pavanello LG, Cavalett O, Mantelatto PE, Bonomi A, Zaiat M (2014) Anaerobic digestion of vinasse from sugarcane biorefineries in Brazil from energy, environmental, and economic perspectives: profit or expense? Appl Energ 113:825–835

Nield DA, Bejan A (1992) Convection in porous media. Springer, New York

Okiyama DCG (2014) Numerical simulation of hydrodynamics within fixed-bed biorreactor for vinasse treatment. M.Sc. thesis (in Portuguese), Faculty of Animal Science & Food Engineering, University of São Paulo, Pirassununga, Brazil

Parco V, Du Toit G, Wentzel M, Ekama G (2007) Biological nutrient removal in membrane bioreactors: denitrification and phosphorus removal kinetics. Water Sci Technol 56(6): 125–134

Picioreanu C, van Loosdrecht MCM, Heijnen JJ (2001) Two-dimensional model of biofilm detachment caused by internal stress from liquid flow. Biotech Bioeng 72(2):205–218

Robertiello A (1982) Upgrading of agricultural and agroindustrial wastes: the treatment of distillery effluents (vinasses). Agric Wastes 4(5):387–395

Satyawali Y, Balakrishnan M (2008) Wastewater treatment in molasses-based alcohol distilleries for COD and color removal: a review. J Environ Manag 86(3):481–497

van der Sman RGM (2007) Lattice Boltzmann simulation of microstructures. In: Sablani SS, Rahman MS, Datta AK, Mujumdar AR (eds) Handbook of food and bioprocess modeling techniques. CRC Press, Boca Raton, pp 15–39

Vlissidis A, Zouboulis AI (1993) Themophilic anaerobic digestion of alcohol distillery wastewaters. Biores Technol 43(2):131–140