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Simulation of a bubble column reactor using CFD approach. Application: ferrous biooxidation

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Extended abstract

Understanding the complexity of the fluid dynamics in bubble column and airlift reactors is important due to their application in the chemical and bioprocess industries. So the objective of this research was to develop a fundamental understanding of the hydrodynamics and interactions with the chemistries involved in the bubble column reactor to maximize overall efficiency for the ferrous biooxidation according to the following reaction:

$$2Fe^{2+} + 2H^{+} + \tfrac{1}{2}O_2 \xrightarrow{A.\,ferrooxidans} 2Fe^{3+} + H_2O \qquad (1)$$

In the present attempt bacterial oxidation of Fe^{+2} to Fe^{+3} in a bubble column reactor was simulated using a commercially available computational fluid dynamics package (FLUENT). Gas-liquid interactions were modeled using an Eulerian model implemented in the software [1]. The finite volume method is adopted to solve three dimensional governing equations. The solver specifications for the discretization of the domain involve the first-order upwind for momentum and phase coupled SIMPLE [2] for velocity–pressure coupling, respectively. For the volume fraction and concentration of species in the liquid phase, first-order discretization scheme was used.

The initial ferric concentration was set to zero. At the walls, no-slip boundary condition was applied (Dirichlet boundary condition). For inlet flow, constant fluid velocity with given phase concentrations, and for the outlet flow, the pressure were specified as boundary conditions.

The superficial gas velocity was adjusted between 0.01 and 0.5 m s^{-1}, and results showed that at velocities higher than 0.1 m/s the biological rate was decreased. The reason is that in very high velocities bacteria will damage and therefore the bacterial activity will be decreased.

Gas holdup is an important factor that affects on interfacial surface area and also activity of microorganisms and therefore the reaction rate. For the ferrous biological oxidation, air volume fraction in the bioreactor is one of the variables that needs to be maximized to have a high reaction rate. The velocity and air volume fraction at normalized radial distance in three different cross sections of 15, 30 and 45 cm from the bottom of the column at t=120 s are presented in Fig. 1. As it expected the parabolic profiles observed in the simulation results.

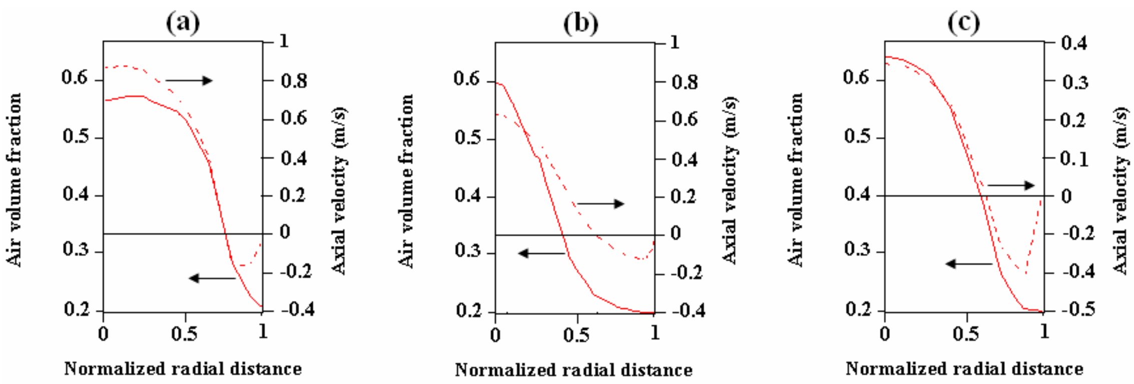

Figure 1: 2D plots of velocity and air volume fraction versus normalized radial distance in (a) 15 cm, (b) 30 cm and (c) 45 cm from the bottom of the column at t=120 s.

The measured oxygen concentration in the gas outlet stream at inlet air velocity of 0.1 m/s was higher than 15%, so the biooxidation process was limited by the availability of oxygen in the liquid medium. Fig. 2 shows that at any time the ferrous biological oxidation rate in the column increases from the bottom to top of the reactor. On the other hand, during the air bobbles moving up through the column because of coalescence, their diameters will increase. Therefore, the ferrous biooxidation depends strongly on the gas–liquid interfacial area, and so, gas–liquid mass transfer dominates.

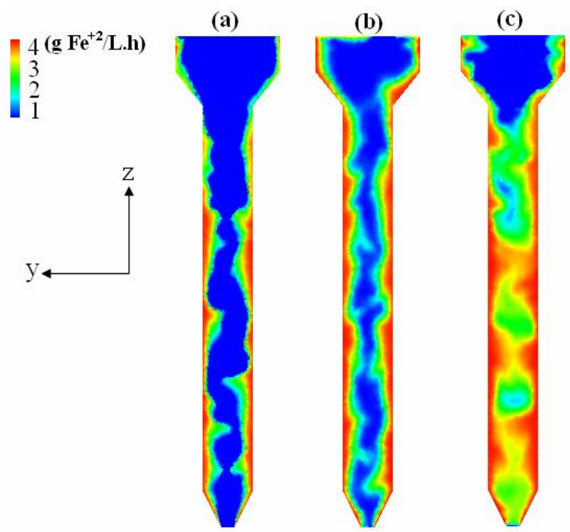

Figure 2: (a-c) Snapshots of ferrous bioxidation rate in the bioreactor at t=60, 120 and 180 s. Here the inlet air velocity is 0.1 m/s and initial ferrous concentration set to 6.7 g/L. The figure was plotted in the plane (z-y) passing through the center of the column.

Conclusion

The simulation results indicate that the Eulerian formulation is a successful approach to predict the hydrodynamics of column bioreactor. The superficial air velocity of 0.1 m/s and initial ferrous concentration of 6.7 g/L determined as optimum values. According to the simulation results maximum ferrous biological oxidation rate was obtained 4 and 3.7 g/L.h at optimum conditions, respectively.

References

[1] Fluent, (2006), *Fluent 6.2 Users Guide*, Fluent Inc., Lebanon.

[2] Vasquez, S.A., Ivanov, V.A., (2000), A Phase Coupled Method for Solving Multiphase Problems on Unstructured Meshes. In Proceedings of ASME FEDSM'00: ASME 2000 Fluids Engineering Division Summer Meeting, Boston, USA.