Computer Aided Chemical Engineering

Computational Fluid Dynamics Modelling of Phenol Oxidation in a Trickle-Bed Reactor using 3D Eulerian Model

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Abstract

Catalytic wet-air oxidation is an attractive solution to treating refractory wastewater. The process has been demonstrated at laboratory scale over a low-cost pillared clay catalyst in a trickle-bed reactor. However, complex interaction of fluid dynamics and reaction kinetics makes scaling up of laboratory reactors to industrial reactors very difficult. Changes in hydrodynamic parameters are significant when laboratory reactors are scaled up to commercial reactors. To understand the behaviour of fluids inside a trickle-bed reactor, a computational fluid dynamics model was developed from experimental data using an Euler–Euler model. A commercial software Fluent was used to study hydrodynamic behaviour, temperature distribution and oxidation process. The model indicated that a hot spot was formed near the centre of the reactor due to liquid mal-distribution. Moreover, incorporating monolithic structure in a reactor packing material helped to lower pressure drop due to low velocities inside monolith channels. Furthermore, when the reactor was modelled at 160 °C and 10 bar, phenol was completely oxidized to CO2.