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Computational Fluid Dynamics of Ethylene Dichloride Production by Oxychlorination Reaction in a Fluidized Bed

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Extended Abstract

The flow behavior of three dimensional gas-solid fluidized bed reactors is investigated. Computational Fluid Dynamics (CFD) based on the Eulerian—Eulerian flow model is simulated for ethylene dichloride production in an oxychlorination unit as an industrial case study. The simulated riser portion is 3.9 m in diameter and 15.5 m in height. The simulation is separated into 2 models; constant catalyst volume fraction and catalyst load variation. The effects of the operating parameters are studied [1]. The ethylene molar feed fraction is varied from 0.17 to 0.3 with the constant mole ratio of hydrochloric acid to oxygen at 3.6. The result shows that the ethylene conversion gradually decreases when the ethylene mole fraction of the feed is more than 0.22. With the outlet pressure rising from 200 to 450 kPa, the ethylene conversion increases from 96.39 to 98.46%. The ethylene conversion significantly increases in the pressure range from 200 to 400 kPa and stays constant at over 400 kPa. The increase of cooling medium temperature from 320 to 420 K drives the ethylene conversion from 96.9 to 98.8% and the gas outlet temperature from 422 to 565 K. The gas feed temperature is varied from 400 to 500 K. The simulation shows that the gas feed temperature is varied from 400 to 500 K. The simulation shows that the gas outlet temperature also increases from 476 to 527 K but the ethylene conversion has a minor effect. Variation of catalyst quantity from 19,500 to 78,000 kg is carried out to study gas-solid flow behavior and transport phenomena. The simulation of 78,000 kg of catalyst shows the blowing out effect [2]. The developed CFD model has the potential of being applied as a tool to predict the effect of the operating parameters and the gas-solid behavior in the reactor.

References

- [1] S. M. Al-Zahrani, A. M. Aljodia, and K. M. Wagialla, "Modeling and simulation of 1,2-dichloroethane production by ethylene oxychlorination in fluidized-bed reactor," *Chemical Engineering Science*, vol. 56, pp. 621-626, 2001.
- [2] M. M. El-Hawagi, and M. A. El-Rifai, "Mathematical modeling of catalytic fluidized-bed reactors-I. The multiphase three-phase model," *Chemical Engineering Science*, vol. 43, no. 9, pp. 2477-2486, 1988.