Transport-Kinetic Interactions for SO2 Oxidation to SO3 in Particulate and Monolith Catalysts

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Abstract

Introduction: Development of next-generation chemical processes that have zero emissions is a key environmental objective for sustainable development. The manufacture of H_2SO_4 by the air oxidation of SO_2 to SO_3 is an important technology where an opportunity exists for new catalyst development and process innovation by reducing emissions of unconverted SO_2 in process reactor tail gases owing to the sheer number and scale of typical plants [1]. Emissions control technologies using new catalyst technology, improved reactor designs, and process strategies have notable potential.

The primary objective of this study is three-fold: (1) to review current H_2SO_4 catalysts utilized in the oxidation of SO_2 to SO_3; (2) to evaluate monoliths as potential candidates as SO_2 oxidation catalysts; and (3) to develop a modeling framework based upon COMSOL Multiphysics® software to compare reactor designs for both particulate and monolith catalysts under typical multi-pass convertor operation.

Methods: COMSOL Multiphysics® is used to model transport-kinetic interactions in both particulate and monolithic catalyst geometries. This builds upon our previous work on modeling of transport-kinetic interactions in particulate catalysts having various complex shapes [2].

A new model that describes transport-kinetic interactions in both particulate and monolith catalysts is described that is valid for process conditions encountered in multi-pass convertor operation. The reaction kinetic model is based upon the work of Collina et al. [3] since it accounts for the dependence of the SO_2 oxidation rate on the partial pressures of SO_2, O_2, and SO_3. COMSOL Reaction Engineering Lab is used to evaluate adiabatic reactor performance under ideal reactor conditions. An advanced COMSOL Multiphysics model that accounts for non-ideal gas and thermal energy interphase and intraphase transport effects in both catalyst forms is described.

Results and Discussion: The concentration profiles shown in Figure 1 are from a case study of catalytic abatement of a volatile organic compound (VOC) to describe monolith reactor performance for contaminant removal from waste gas. A similar approach will be followed to develop monolith catalyst model for SO_2 oxidation reaction.

Additional results that compare the performance of particulate versus monolithic catalyst shapes using typical process conditions will be presented and discussed, thereby showing the incentive for development of monolithic catalyst with higher activity and reduced emissions.

Conclusions: COMSOL Multiphysics provides a convenient platform for quantifying detailed transport-kinetic interactions in commercial catalyst particles having complex shapes. The model-predicted results provide a realistic basis for comparison to experimental data.

Reference

1. British Sulphur Consultants, Sulphuric Acid : Global Supply and Demand in the Next Decade, Topsøe Catalysis Forum – Denmark, August 23rd to 24th 2007.

2. Nagaraj, A., & Mills, P. L. “Analysis of Heat, Mass Transport, and Momentum Transport Effects in Complex Catalyst Shapes for Gas-phase Heterogeneous Reactions Using COMSOL Multiphysics”. Paper Presented at the COMSOL Conference 2008 Boston, MA.

3. Collina, A., Corbetta. D. and Cappelli, A. "Use of Computers in the Design of Chemical Plants," 97th Event of the European Federation of Chemical Engineering, Firenze (1970).

Figures used in the abstract

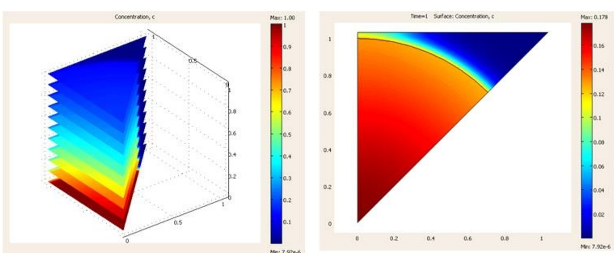

Figure 1: Figure 1. (a) Concentration profile along the length of the reactor. (b) Concentration profile at the outlet.