Computational Fluid Dynamics for Microreactors Used in Catalytic Oxidation of Propane

S. Odiba[1], M. Olea[1], S. Hodgson[1], A. Adgar[1]

[1]Teesside University, School of Science and Engineering, Middlesbrough, United Kingdom

Abstract

Recent advances in microfabrication technology have been adapted in the field of chemical engineering to produce microreactor devices with higher efficiency than those in conventional systems. This is mainly due to their large surface area to volume ratio and excellent heat and mass transfer properties. The optimal design for a specific application can be explored based on simulation results obtained by using the CFD Module of COMSOL Multiphysics®. This research deals with the design of suitable microreactors for the catalytic oxidation of volatile organic compounds (VOCs), using propane as a model molecule. The microreactor considered consists of eleven parallel channels, in which an Au/Cr/γ-Al2O3-catalyzed combustion reaction takes place. Each channel is 0.5 mm in diameter and 100 mm long. The first design step was the selection of the most suitable microreactor geometry. This was based on cold flow (without reaction) and the simulation results were obtained by using the above software. Four different geometries had been proposed and simulated in 2D to evaluate the fluid behavior in the microchannels. The design of a microreactor relies on having uniform flow distribution in all parallel microchannels for optimum yield and product selectivity. The so-called A2 geometry gave the optimum flow distribution from laminar to transitional regime (the lowest relative standard deviation).

The second step involved the simulation of the selected microreactor for propane oxidation. Geometry A2 was modified in a 3D model to further investigate the catalytic oxidation of the model VOCs. The catalytic reaction takes place at the surface of the microchannel wall.

The catalytic microreactor was simulated for temperatures between 563 K and 663 K and inlet flow velocities between 0.05 and 1 m/s. As expected, the propane conversion increased quickly with increasing temperature for a fixed inlet flow velocity. For a fixed temperature, the propane conversion increased as the inlet flow velocity decreased. As the target conversion was set to 99.99%, a number of isothermal microreactors with A2 geometry were connected in series and the conversion profile in each of them was determined. Their number decreased as the temperature increased and the inlet flow velocities decreased (as such, the residence time within each reactor increased).

Figures used in the abstract

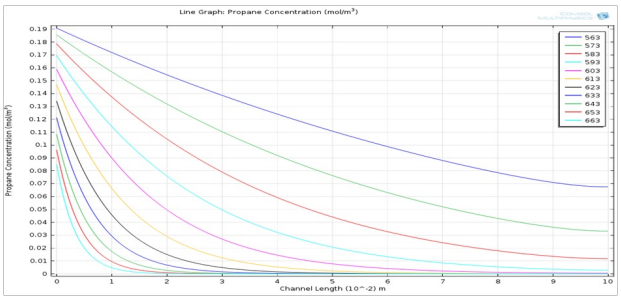

Figure 1: Propane concentration gradient along a channel at a velocity of 0.01m/s.

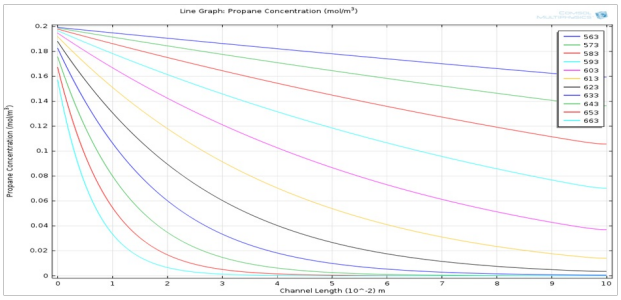

Figure 2: Propane concentration gradient along a channel at a velocity of 0.05m/s.

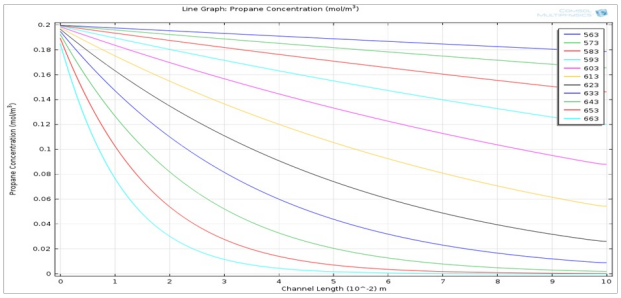

Figure 3: Propane concentration gradient along a channel at a velocity of 0.1m/s.

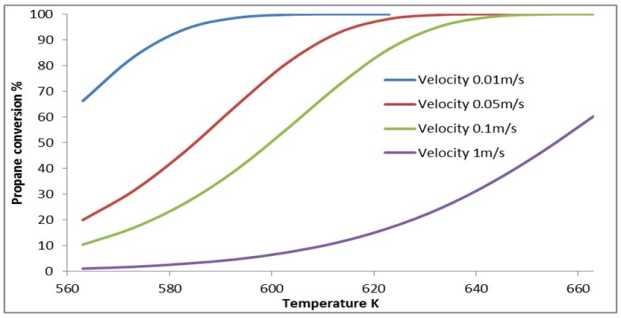

Figure 4: Propane exit conversion against temperature at velocity of 0.01, 0.05, 0.1, and 1 m/s.