COMSOL Computational Fluid Dynamics for Microreactors Used in Volatile Organic Compounds Catalytic Elimination

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Abstract

Volatile organic compounds (VOCs) are organic chemicals that will evaporate easily into the air at room temperature and contribute majorly to the formation of photochemical ozone. They are emitted as gases from certain solids and liquids in to the atmosphere and affect indoor and outdoor air quality. They includes acetone, benzene, ethylene glycol, formaldehyde, methylene chloride, perchloroethylene, toluene, xylene, 1,3-butadiene, butane, pentane, propane, ethanol, etc. Source of VOCs emission include paints, industrial processes, transportation activities, household products such as cleaning agents, aerosols, fuel and cosmetics. Catalytic oxidation is one of the most promising elimination techniques for VOCs as a result of it flexibility and energy saving. The catalytic materials enhance the chemical reactions that convert VOCs (through oxidation) into carbon dioxide and water. Removal of volatile organic compounds at room temperature has always been a challenge to researchers. Developing a catalyst which could completely oxidize the VOCs at very low temperature in order to avoid catalyst deactivation and promote energy saving has been the key focus among researchers in the recent years. Moreover, as the oxidation reaction is highly exothermic, the use of catalytic microreactors instead of packed bed reactors was considered. Microreactors are microfabricated catalytic chemical reactors with at least one linear dimension in the micrometer range. Usually, they consist of narrow channels and exhibit large surface area-to-volume ratios which leads to high heat and mass transfer properties. The gas flow through the microreactors is laminar. Modern development in microfabrication has given the possibility of low cost replication of microreactor structures for industrial scale processes (number up). Computational fluid dynamics modeling is one of the modern approaches used to design proper geometry of a microreactor to ensure uniform velocity distribution in all the parallel microchannels for optimum yield and product selectivity. A two dimensional CFD simulation was performed and the influence of the following parameters was assessed: shape of manifolds, length of the parallel microchannels (reaction section), width of the parallel microchannels and the magnitude of the inlet velocity. The simulation results presented in figures below shows uniformity with rectangular parallel microchannel 100 mm long, 0.2 mm wide, and a manifold area of 23 mm^2.

Reference

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Figures used in the abstract

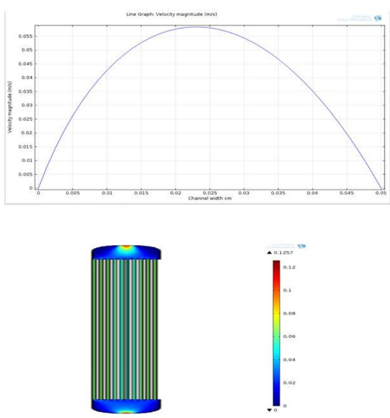

Fig. 1. Velocity profile for laminar flow

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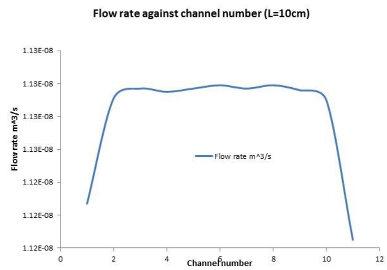

Figure 2: Influence of shape parameters on flow distribution.