The Effects of Micromixing on Heterogeneous Catalysis in Microbioreactor Channels

Stephanie Wilson and Dr. Frank Jones

The University of Tennessee at Chattanooga

EXTENDED ABSTRACT

The results of a numerical study of the fundamental interactions of engineering design and micromixing on conversion in packed microchannels are presented. Previously, channel-based microreactors made of molded silicon plastic were designed, fabricated, and experimentally tested. These reactors have enzymes immobilized on the channel walls by various methods. They also contain molded packing particles to add reactive surface area and to redistribute the fluid. An intuitive packing arrangement was used in experimental studies and modeled successfully by computer simulation. A computer simulation study has been conducted in order to understand how changes in packing arrangement and number of packing particles affect micromixing and conversion efficiency. The behavior in empty and pack channels is compared. The experimental reactors have been simulated using CFD-ACE+ multiphysics software. The focus of this study is to vary the placement and number of packing particles to more efficiently meet conversion goals while taking into account micro fabrication and operational constraints. Microfluidic fundamentals such as Reynolds number (Re), shear stress, and pressure drop are also explored due to variations in design features. The micro scale dimensions of the channel cross section (125 by 500 micrometers) cause all flows to be laminar. Behavior in the range $0.1 < Re < 100$ is examined.

Objectives

To improve fundamental understanding of micromixing and increase conversion efficiency of microbioreactors through the design of packing configurations.

Theory

The Computational Fluid Dynamics software produced by ESI (Huntsville, AL) is used to model the packed microchannels. All inside surfaces of the microchannels, including the packing, are programmed as reactive surfaces. The reaction taking place is $H_2O_2 \xrightarrow{\text{catalase}} H_2O + \frac{1}{2} O_2$. CFD-ACE+ solves the following equations using finite-volume analysis: Navier Stokes Equation (momentum continuity), Conservation of Mass, Michaelis-Menten Kinetics, and Species Conservation.

Results

Significant increases in conversion are found due to coated packing over the range $0.1 < Re < 100$. These increases are always greater than the increase in reactive surface area. Conversion has been increased by as much as 150%. Changes in the positions of the particles improved conversion as much as 35%. Pressure drop increases with packing population and fluid velocity. Pressure drops and shear stresses may be problematic for heavily packed channels at Re=10.