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Mass transfer simulation of biodiesel synthesis in microreactors

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ABSTRACT

A coupled nonlinear mathematical model for the mass transfer of the species involved in the transesterification reaction between soybean oil and methanol in a parallel plates geometry microreactor is presented. The set of partial differential equations that governs the concentration profile of these species were obtained from the general mass balance equation for the case of isothermal flow and steady state with constant physical properties. The velocity profile was obtained from the Navier-Stokes equations assuming fully developed stratified laminar flow for two immiscible Newtonian fluids, with a plane interface between them, based on experimental observation of this flow pattern. The second order kinetic equations for the species were developed assuming homogeneous and reversible chemical reactions and these equations were written as source terms in the main equations. The mathematical model was solved using the hybrid method known as Generalized Integral Transform Technique (GITT). The simulation results were critically compared with those obtained by using the COMSOL multiphysics platform, showing a good agreement between the hybrid and fully numerical simulations. The effects of governing parameters such as residence time, temperature and microreactor dimensions were investigated. It was observed that higher triglycerides conversion rates occurred at higher temperatures and residence times and lower microreactor depths.

1. Introduction

Most of the consumed energy in the world comes from nonrenewable fossil fuels. However, these resources are limited and their use results in harmful environmental effects such as global warming and, consequently, climate change. Hence, in order to reduce further damage to the environment, the development of alternative energy sources are of major interest. Recently, increased attention has been given to biofuels such as biodiesel, which has been increasingly adopted as an alternative fuel due to its feedstock flexibility and biodegradable characteristics (Anastopoulos et al., 2009).

Biodiesel is a renewable energy source that can fully or partially substitute petro-diesel due to their similar properties. The main process in biodiesel production is the transesterification of vegetable oils or animal fats with an alcohol, usually methanol or ethanol, in the presence of a catalyst within stirred tank reactors. Even though the process is well established, some limitations remain, such as considerably large energy input and long residence times of the order of a few hours (Charoenwat and Dennis, 2009). Hence, new technologies have recently emerged to overcome the problems of energetic cost and residence time, such as the synthesis of biodiesel in microfluidic devices or microreactors.

Microfluidics, in recent years, has emerged as a very important area of research, and the use of specialized microfluidic devices such as microreactors has received considerable attention in the literature. In microfluidic devices the viscous forces are in general dominant over

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Nomenclature

C	Concentration
D	Diffusion coefficient
D_h	Hydraulic diameter
E	Activation energy
F	Dimensionless concentration
G	Dimensionless reaction kinetics term
H	Microreactor height
k	Kinetic constant
L	Microreactor length
MT, NT	Number of terms in eigenfunctions expansion
$Norm$	Normalization integral
O	Transformed system coefficient
P	Pressure
Pe	Péclet number
Q	Volumetric flow rate
R	Ideal gas constant
T	Temperature
u	Velocity component in the longitudinal direction
W	Microreactor width
x, y	Spatial variables
X, Y	Dimensionless spatial variables

Greek symbols

β, γ, υ	Eigenvalues
Γ, Φ, Ψ, Ω	Eigenfunctions
μ	Eigenvalue or dynamic viscosity
ρ	Specific mass
τ	Residence time

Subscripts and superscripts

A	Alcohol
Ah	Homogeneous potential for alcohol species
Av	Average potential
B	Biodiesel
DG	Diglyceride
GL	Glycerol
i, j, k, l, m, n	Order of eigenvalues and eigenfunctions
M	Methanol
MG	Monoglyceride
s	Referred to the species involved in the transesterification reaction
TG	Triglyceride
$\sim$	Normalized eigenfunction
—	Integral transform
*	Equilibrium concentration at interface

inertial forces, ensuring low Reynolds numbers (<100) and consequently a laminar flow regime. Microreactors have several advantages over traditional reactors such as lower energy and material consumption, improved mass and heat transfer, and faster reactions and transport phenomena (Martinez et al., 2012). Such advantages of using microreactors are due to the reduced dimensions that result in a high surface area to volume ratio and shorter diffusion paths, thus enhanced mass and heat transfer (Martinez et al., 2012). Different types of flow regimen can occur under these conditions when two immiscible fluids are brought into contact, which depend on properties and characteristics of the system such as interfacial tension, flow rates, viscous forces and wetting behavior of the channel walls. Two commonly observed flow regimen in microsystems are stratified flow, in which one phase flows on top or side-by-side with another, and drop/plug flow, in which drops or plugs of one fluid are dispersed in the continuous phase of another fluid (Malengier et al., 2011). Because of the unique flow and mass transfer phenomena, which occur on the micro-level and can be precisely controlled, the implementation of microreactors can often lead to process intensification in many common chemical processes, such as biodiesel synthesis.

A comparison of the performance of soybean oil conversion in the transesterification reaction with methanol catalyzed by sodium hydroxide in both microreactors (Al-Dhubabian, 2005) and batch reactors (Noureddini and Zhu, 1997), for different residence times, is illustrated in Table 1. Although the experiments were conducted at different values of alcohol-oil molar ratio and catalyst concentrations, soybean oil conversion rates obtained in the microreactors, even at room temperature and small residence times, were shown to be more significant than those achieved through the batch reactor at much higher temperatures and residence times. However, it is very important to note that to make a more just and careful comparison about the biodiesel production in both types of reactors it is suggested to work with the same molar ratio values alcohol oil, reactants, catalyst concentration and temperature.