



Three-dimensional reaction-convection-diffusion analysis with temperature influence for biodiesel synthesis in micro-reactors



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ABSTRACT

A three-dimensional nonlinear reaction-convection-diffusion model is proposed to analyze mass transfer with temperature effects, within micro-reactors of rectangular cross-section, towards the simulation of the transesterification process in biodiesel synthesis. The coupled nonlinear partial differential equations that govern the concentration of the species involved in the synthesis, is obtained from the general three-dimensional species balance equations for an isothermal and steady state system with constant physical properties. A kinetic model is considered to describe the variation of the species due to the transesterification process, assuming second order homogeneous and reversible chemical reactions. The velocity profile is analytically derived from the Navier-Stokes equations, considering fully developed stratified laminar flow of two immiscible Newtonian fluids in a rectangular cross section micro-reactor, with a plane interface between them and without field forces, and obtained by the Classical Integral Transform Technique (CITT). The nonlinear mass transport equations are then solved by the hybrid numerical-analytical approach known as the Generalized Integral Transform Technique (GITT). In the present GITT solution, two alternative eigenvalue problems are proposed, accounting or not accounting for the space variable velocity profile influence in the eigenfunction expansion basis, in order to investigate the differences in the convergence behavior of the solutions obtained through the two different auxiliary problems. The results for the concentration profiles of the biodiesel and triglyceride species are critically compared with literature data for the limiting case of parallel plates, showing a good agreement among them. The analysis also indicates that improved convergence rates are achievable through the eigenvalue problem with variable coefficients. The effects of governing parameters such as residence time, micro-reactor dimensions, and especially temperature, are investigated. It is then inspected the relative gains in triglycerides conversion rates at higher temperatures and residence times and lower micro-reactor hydraulic diameter.

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1. Introduction

Sustainable development premises have been pushing efforts, worldwide, in developing or at least improving energy generation systems and components. In this context, biofuels such as biodiesel have been progressively considered and adopted as an alternative fuel, mainly due to its feedstock flexibility and biodegradable

characteristics [1]. Biodiesel is a renewable energy source that can fully or partially substitute the conventional diesel due to their similar properties, but presenting low emissions of carbon, sulfur, particulate matter, and unburned hydrocarbons [2].

The process most widely employed for the production of biodiesel 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 or batch reactors. According to the literature [3–7], the main factors that influence the transesterification reaction are the residence time, the reaction temperature, the type and concentration of the catalyst, the feedstock, the solubility of the

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Nomenclature		X, Y, Z dimensionless spatial variables
O, S	transformed system coefficients	<i>Greek symbols</i>
C	dimensionless concentration	$\beta, \gamma, \nu, \lambda$ eigenvalues
C^*	dimensional concentration, $\text{mol}\cdot\text{m}^{-3}$	$\Phi, \Omega, \phi, \varphi, \Gamma, \Psi$ eigenfunctions
D	diffusion coefficient, $\text{m}^2\cdot\text{s}^{-1}$	δ Kronecker delta
D_h	hydraulic diameter, m	μ dynamic viscosity, Pa.s
E	activation energy, $\text{J}\cdot\text{mol}^{-1}$	ρ density, $\text{kg}\cdot\text{m}^{-3}$
G	dimensionless reaction kinetics term	τ residence time, s
H	micro-reactor height, m	<i>Subscripts and superscripts</i>
k	kinetic constant, $\text{m}^3\cdot\text{mol}^{-1}\cdot\text{s}^{-1}$	A alcohol
L	micro-reactor length, m	Ah homogeneous potential for alcohol species
<i>Norm</i>	normalization integral	Av average concentration
MT	truncation order of algebraic system	B biodiesel
NT	number of terms in eigenfunction expansion	DG diglyceride
P	pressure, Pa	GL glycerol
Pe	Péclet number	i, j, k, l, m, n order of eigenvalues and eigenfunctions
Q	volumetric flow rate, $\text{m}^3\cdot\text{s}^{-1}$	M methanol
R	ideal gas constant, $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	MG monoglyceride
T	temperature, K	r referred to the species involved in the transesterification reaction
u	velocity component in the longitudinal direction, $\text{m}\cdot\text{s}^{-1}$	<i>vel</i> referred to the velocity profile
U	dimensionless velocity component in the longitudinal direction	TG triglyceride
W	width of rectangular micro-reactor, m	\sim normalized eigenfunction
x_e	hydrodynamic entry length, m	$-$ desired potential at the transformed domain
x, y, z	spatial variables	Ae_q equilibrium concentration of alcohol at interface

species reactants, the kind of alcohol and the molar ratio between triglyceride and alcohol. Due to the immiscible nature of the reactants, a considerable stirring mechanical work is required, together with high temperature levels, to favor the reaction process, which imply in unavoidable large energy input and long residence times, in the order of a few hours [8].

As an alternative to overcome the energetic cost and the large residence times, new technologies have recently emerged to enhance the synthesis of biodiesel, such as through micro-reactors, which are typical micro-devices that have been developed within the very important and recent research area called Microfluidics.

The use of micro-reactors for continuous processes with chemical reaction has received great attention due to the high flexibility and agility in obtaining results and the possibility of carrying out reactions in exceptional conditions in comparison with the traditional ones. In addition to the possibility of integration with other micro-devices, the micro-reactors allow the development of liquid-liquid, liquid-gas, catalyzed or non-catalyzed reactions under electric or magnetic field effects, with manifold introduction of reactants and with micro-channel geometries that can intensify the mixture [9–11].

The employment of micro-reactors for the reaction process, like transesterification reaction, in light of the reduced dimensions, ensured high surface area to volume ratio and shorter diffusion paths for the reactive system, which results in enhanced mass and heat transfer and faster reactions, consequently with lower energy and materials consumption [12–16]. As the two main reactants of the transesterification, triglycerides and alcohol, are immiscible fluids, a liquid-liquid two-phase flow develops in such micro-reactors, as the immiscible fluids are brought into contact and subjected to the same pressure gradient, with the associated properties and characteristics of the system such as interfacial tension, flow rates, viscous forces and wetting behavior of the

channel walls [17]. According with Guan et al. [18,19] and Xie et al. [2], the two flow regimen that are commonly observed in micro-reactors during the transesterification reaction are the stratified flow, in which one phase flows on top or by the side of another, and droplet/plug flow, in which drops or plugs of one fluid are dispersed in the continuous phase represented by the other fluid [17].

Fairly recent works in the literature present promising results for the conversion of biodiesel in micro-reactors under different reactive conditions and different reactants and catalysts [12,13,20]. Integrated systems are also presented, suggesting the possibility of combining micro-reactors with conventional reactors [21], or even with other micro-systems [11,22], aiming at increasing the yields of biodiesel production with significant reduction on operating time. The idea of micro-chemical plant [11,23,24], or of various micro-systems integrated for a chemical reaction process, allows overcoming a very important disadvantage of micro-reactor, which are the low volumetric flow rates of products. Billo et al. [22], for example, presented an important paper about the design and operation of a plant for the production of biodiesel, containing various micro-reactors in a parallel association. To better understand the transesterification process in micro-reactors, for decisions in design tasks, the development of representative mathematical models to describe the physico-chemical phenomena is mandatory. Although there are well-defined transesterification reaction models for the conventional reactors [4,25,26], generally such kinetic models are not suitable to describe the observed behavior at the micro-scale [27]. Therefore, it is necessary and very important to develop, first, mathematical models for mass transfer problems in micro-reactors and, second, computational tools and methodologies that provide solutions at low computational cost, to be used in both inverse problem analysis, for properties identification, and optimization analysis, for system design.

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