



Investigation of convection and diffusion during biodiesel production in packed membrane reactor using 3D simulation



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ABSTRACT

The 3D simulation of convection and diffusion phenomena within a ceramic membrane during transesterification reaction was the aim of this study. The ceramic membrane was a tubular micro porous $\text{TiO}_2/\text{Al}_2\text{O}_3$ packed with the heterogeneous catalyst. The Navier–Stokes, Brinkman and Stephan–Maxwell equations were applied for investigation of fluid flow reaction and mass transfer within the system. The value of the convection was generally between 10^4 and 10^7 times higher than diffusion. It depends on concentration component, the diffusion coefficient and components velocity. A good agreement was found with the maximum deviation of 8% from experimental data.

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1. Introduction

Biodiesel (fatty acid methyl ester) is considered as a clean-burning fuel which is produced from renewable sources [1]. It has excellent lubricating properties and does not contain any aromatic hydrocarbons, metals, sulphur or crude oil residues. Thus, it is a good alternative for petroleum based diesel because it reduces volatile organic compounds emissions (VOC) and greenhouse gases (GHG). It is much safer than mineral diesel because of its higher flash point. Furthermore, it has a high capacity of self-ignition because of its high cetane number [2]. Transesterification is the most common process for fatty acid methyl ester (FAME) production. It includes three chain reactions. In each step, one molecule of alcohol reacts with one molecule of glyceride (tri, di or mono) and produces one molecule of alkyl ester. Diglyceride (DG) and mono-glyceride (MG) are intermediate products which converted to glycerol and alkyl ester during the reaction [3]. These chain reactions assist by enzymatic, homogeneous or heterogeneous catalysts [4]. Catalyst free transesterification is another technique. However it requires a high temperature ($>350^\circ\text{C}$) and pressure (20 MPa) [5].

The enzymatic catalysts give a high conversion rate and are selective. Besides, their productions can be separated easily. But,

those which show unstable activities and require long reaction time, also are not economical yet [6]. Homogeneous (acidic or alkaline) catalyzed processes also suffer from some weaknesses such as high cost of purification and wastewater generation for final removal of the catalyst. In acidic homogeneous transesterification, increase in the reaction time, temperature and the corrosive nature of the catalyst are the other problems. More sensitivity to the purity of the reactant is also reported in case of alkaline catalyzed reaction. Heterogeneous catalyst can overcome some of the mentioned problems, because it can be easily removed by filtration and it is non-corrosive. The only problem is the spread of the catalyst which is due to providing an enough space for active site for production. For this purpose several techniques have been applied to increase the constitution of the three-phase system (triglycerides, alcohol and solid catalyst). The most preferred techniques are those which support the catalysts on non-reaction materials, or use them in porous media [7]. Using membrane is the newest technology which has been applied for both production and purification of FAME. This method can concentrate on process streams, recover valuable products and improve the conversion rate of the reaction. The selectivity of the membrane is the other advantage of this method which depends on its pore sizes. Also, their special physical and chemical consistency makes their function reproducible in all over of their life time [8]. Therefore, membrane bioreactors can be suitable alternatives to produce biodiesel due to its ability to overcome some limitations during production and purification. The high-quality biodiesel production of FAME via this technique (more than 99%) has been also reported

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Nomenclature

Symbols

CV	control volume (m ³)
<i>c</i>	component concentration (mol/m ³)
<i>D_{ij}</i>	Fick diffusivity (m ² /s)
<i>D_i^T</i>	thermal diffusion coefficient (kg/m s)
<i>div</i>	divergence
<i>E</i>	rate-of-strain tensor
<i>F</i>	acting force (N)
<i>K</i>	kinetic rate constant (dm ³ /mol min)
<i>M</i>	molecular mass (g/mol)
<i>n</i>	normal vector
<i>t</i>	time (s)
<i>T</i>	temperature (°C)
<i>T</i>	deviatoric stress tensor
<i>u</i>	velocity vector (m/s)
<i>V</i>	volume (m ³)
<i>w</i>	weight, various
<i>p</i>	pressure (Pa)
<i>x_j</i>	molar fraction of species (<i>j</i>)
<i>R_i</i>	reaction rate (kg/m ³ s)
<i>Q_{br}</i>	mass sink source (kg/m ³ s)

Greek symbols

ρ	density of the mixture (kg/m ³)
μ	molecular viscosity (Ns/m ²)
<i>S_φ</i>	source-sink term
ε	fractional hold up of each component
ε_p	porosity
κ	permeability (m ²)
β_f	Forchheimer coefficient (kg/m ⁴), for considering of the drag of the fluid on the porous matrix (kg/m ⁴)
ω_i	mass fraction of species <i>i</i>
Γ	appropriate coefficient for variable ε (here is the diffusion constant)
<i>S_φ</i>	source-sink term per unit volume
∂	gradient

Subscripts

MeOH	methanol
TG	triglyceride
DG	diglyceride
MG	monoglyceride
G	glyceride
FAME	fatty acid methyl ester
RBD	refined, bleached and deodorized

by some authors [2,9–11]. But, to better comprehend the design, control and optimization of the process we require the knowledge of membrane phenomena such as convection and diffusion.

The relative complexity of fluid flow in membrane systems or thin channels surrounded by permeable walls highlights the necessity of understanding the underlying problems.

The study of convection and diffusion in such systems is accompanied by some challenges. These two mechanisms are affected by fluid flow rates, membrane surface area, temperature and the membrane thickness.

Generally, there are two main models which make it possible to understand the mathematics and physics of the membrane

phenomenon. The first model is based on the concept of capillarity. It is a solubilization–diffusion model which is developed by Kadem and Katchalsky [12]. The second one is the model of polarization that results in a progressive accumulation of species (molecules, particles, etc.) stopped on the surface of the membrane [13]. The complexity of these models decreases by CFD simulations. These numerical simulations help us to minimize the number of experiments and better comprehend the processes in a shorter time. However, the numerical simulation of fluid flow and transport in membrane systems is a challenging problem; because these are composed of porous materials and contain fractures and cavities on multiple scales. On micro scale, which fluid flows at low Reynold's numbers through pore throats and individual pores, incompressible Navier–Stokes equation is applicable for description of situation. But on macro scale, flow should be described by set of effective petro physical parameters such as porosity and permeability. These parameters describe the average ability of the membrane to store or transport fluids. Then the flow should be modeled using Darcy's law along with the Navier–Stokes and mass conservation. In Stokes–Darcy approach, Darcy's law is applicable for porous material and the Stokes equation for the voids. The boundaries between the porous and void volumes can be described by the Beavers–Joseph–Saffman method [14]. Stokes–Brinkman is another approach which gives a seamless transition between the Darcy and Stokes equations. In this model, a new term is added to the Stokes equations that accounts for viscous transport in momentum balance. Solving either Stokes–Brinkman or Darcy–Stokes equations in 3D systems because of its computational cost is not applicable even in a high-performance supercomputer. Therefore, well parallelizable iterative solvers are usually employed. In this technique, the number of iterations converges to a satisfactory solution with the least error which depends on the condition number of the matrix system.

In this study, we focused on the simulation of a tubular ceramic (TiO₂/Al₂O₃) membrane which was used for biodiesel production. The ceramic membrane was packed with potassium hydroxide supported on activated carbon as the heterogeneous catalytic bed. A set of 3D model using finite element method (FEM) was considered for time dependent simulation of the mentioned system. The transport equations were described by Navier–Stokes for fluid flow, Brinkman equations for porous media and Stephan–Maxwell equations for conversion rate of reaction and convection–diffusion mechanisms. Besides, the PARDISO algorithm was applied to combine and solve the equations. This algorithm is a direct sparse solver which supports parallel processing. The numerical discretization and analysis schemes were then validated with experimental results of velocity distribution and reaction yield.

2. Experimental setup

The experimental data has been taken from the work of Baroutian et al, and it is summarized briefly for easier understanding of readers [15]. Fig. 1 shows the schematic diagram of experimental setup of biodiesel production. The membrane reactor consisted of a shell and a tube with one feed inlet and two outlets. One outlet is the end of the catalytic bed and the other is the ceramic membrane body. Commercial ceramic membrane (Atech Innovations GmbH, Germany) was used as both catalytic bed and separator. This system was covered by another shell which only used for gathering the production. The membrane was a porous media of TiO₂/Al₂O₃ with the pore sizes of 0.05 μm and the filtration surface of 0.0201 m². The length and the diameters of the inner and outer of the membrane were 40 cm, 1.60 cm and 2.54 cm, respectively. Both ends of the ceramic tube were enameled in order to keep the inside separate from the outside

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