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MODELING AND SIMULATION OF THE BIODIESEL PRODUCTION IN A PILOT CONTINUOUS REACTOR

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Abstract. The finite elements method (FEM) is a numerical method especially useful for solve coupled engineering problems where the analytical solution is not possible due its high complex. In this paper, the liquid-phase biodiesel production in a pilot continuous reactor at the Pilot Plant of Reaction, Chemical Engineering Dept. (UNCPBA) was studied. The objectives were: a) develop a program based on FEM to simulate the transfer of momentum and heat in a pilot tubular reactor, b) couple the kinetic reaction of catalytic transesterification of a non-conventional oil with an alcohol into the general program, with the aim to optimize the process, c) to use the computational tool Aspen-HYSYS® to simulate the process of biodiesel production and estimate useful data for the FEM model, d) to validate the numerical model with experimental data. This work presents the study and simulation of the catalytic reaction of transesterification of palm oil with methanol employing an alkaline catalysts to obtain methyl esters (biodiesel) and glycerol under different conditions (oil/methanol feed rates, reaction temperatures, catalyst concentrations) at the pilot plant reaction (PPR). The properties of the streams of reactants and products were obtained from the NRTL fluid package of Aspen-HYSYS®. The reaction was defined as kinetics of first order for both oil and methanol. The kinetics constant for the forward reaction was expressed in Arrhenius form equation. The activation energy was determined from literature (Cheng et al., *J Oil Palm Res*, 16(2):19-29, 2004) and resulted 60737 J/mol with a frequency factor of 9.153×10^9 $m^3/(mol\text{-}s)$ for the condition of maximum velocity of biodiesel production (using 0.125 mol NaOH/oil kg at 60ºC with oil:methanol feed rate of 1:10). Solving the mass balance of an isothermal plug flow reactor under these conditions, it was estimated that the pilot reactor (assumed ideal) could reach 99% conversion in 5 minutes. For modeling the process of biodiesel production in the PPR, the mass balance, energy and momentum were planed, along with other equations, conforming a system of coupled differential equations. For its resolution, a CFD model previously developed to describe the flow patterns in the mixer-reactor system through the Navier-Stokes module for incompressible fluids in stationary stage of COMSOL Multiphysics® 3.5a was used. This model was coupled with the mass Convection and Diffusion, and the Heat Transfer by Convection and Conduction modules to the CFD model, including the reaction kinetics of transesterification of tripalmitin and esterification of palmitic acid. A 2D domain was considered which was discretized with Lagrange quadrangular elements. First, the transfer of momentum problem was solved; for that, fluid properties (density, viscosity) were defined based on Aspen-HYSYS®. The initial conditions of null velocity and pressure were imposed. The boundary conditions were: fixed normal fluid velocity at the reactor inlet, no slip at lateral walls, and null pressure at the reactor outlet. The Direct (UNFPACK) solver was used. Convergence of solution was obtained for different feed conditions (velocity, Reynolds number, temperature), allowing to determine the velocity and pressure profiles which were stored for later solve the Convection and Diffusion, and Heat Transfer modules with the fluid moving inside the reactor. The reaction velocities of transesterification and esterification were defined such as global expressions and the diffusivities of the species were assumed identical. As results from the resolution of the whole coupled MEF model, conversions at the outlet reactor were corresponding with experimental data.

1 INTRODUCTION

The rapid growth of global energy demand is met primarily by fossil fuel nonrenewable. This makes it necessary to find clean energy sources to effectively replace fossil fuels and to mitigate the negative effects caused by them. Biodiesel obtained from vegetable and animal fats appears as a good alternative to petroleum fuel (Demirbas, 2009). Biodiesel may be produced from the transesterification reaction of fatty acids of vegetable origin with short chain alcohols catalyzed by bases such as NaOH or sodium methylate.

The transesterification reaction is a reversible reaction of an oil composed of triglycerides with an alcohol to form fatty acid alkyl esters and glycerol. Reaction stoichiometrically requires a 3:1 molar ratio of alcohol to oil with an excess of alcohol (West et al. 2008).

The alcohols used should be of low molecular weight being one of the most used ethanol for its low cost (Zapata et al. 2007; Demirbas, 2009). However, greater conversions into biodiesel can be reached using methanol.

Although the transesterification reaction can be catalyzed by acids or bases, alkaline catalysis is the technique most frequently used for the production of biodiesel. This path has lower reaction times and catalyst cost than those posed by acid catalysis. However, alkaline catalysis has the disadvantage of its high sensitivity to both water and a fatty acid (FFA) present in the oils.

In this paper, the liquid-phase biodiesel production in a pilot continuous reactor at the Pilot Plant of Reaction, Chemical Engineering Dept. (UNCPBA) was studied in order to develop a numerical full model of momentum-mass-heat transfer to predict conversions at the outlet reactor, based on the finite elements method (FEM), a technique especially useful for solve coupled engineering problems where the analytical solution is not possible due its high complex.

The objectives of the present work were: a) to develop a program based on FEM to simulate the transfer of momentum and heat in a pilot tubular reactor, b) to couple the kinetic reaction of catalytic transesterification of a non-conventional oil with an alcohol into the general program, with the aim to optimize the process, c) to use the computational tool Aspen-HYSYS to simulate the process of biodiesel production and estimate useful data for the FEM model, d) to validate the numerical model with experimental data.

2 APPROACH AND DISCUSSION

2.1 PPR Description

The pilot plant reaction (PPR) of the Chemical Engineering Dept. (UNCPBA) comprises a jacketed stainless steel continuous tubular reactor, fed from the bottom by two electric pumps with variable flow in the range 0-50 L/h, which driving reactants through a pipe passing through a mixer (mixer) to the reactor. Major detail can be found in Bahl et al. (2012).

2.2 Experimental data of reaction kinetic

Experimental data of the kinetics production of palm oil methyl esters by transesterification of crude palm oil (CPO) with methanol using alkaline catalysts in a batch reactor under different conditions (catalyst: sodium methoxide and sodium hydroxide; catalyst concentration: 0.125, 0.1875 and 0.250 mol/oil kg; reaction temperature: 50, 60 and 70ºC; ratio of oil to methanol: 1:6, 1:8, and 1:10) were taken from literature (Cheng et al. 2004;

Zapata et al. 2007).

Cheng et al. (2004) demonstrated that both catalysts (sodium methoxide and sodium hydroxide) provide good catalytic activity for the transesterification of CPO, and that fast formation of the methyl esters of palm oil is obtained when the reaction is performed at 60°C with a molar ratio of methanol to oil of 01:10 and catalyst concentration of 0.125 mol NaOH/kg oil. In virtue of this, these experimental conditions were preferably preselected for the following development of the PPR model simulation; however, other conditions of reaction were subsequently explored.

Based on electronic curves captured from the original pdf-type archive of Cheng et al. (2004), pairs of experimentally measured values of time of reaction (t) and conversion of CPO into methyl esters (x_{TG}) were obtained from using the software Paint of Microsoft Windows® version 6.1 (2009). To illustrate, Figure 1 presents the experimental points (green symbols) for the preselected reaction condition.

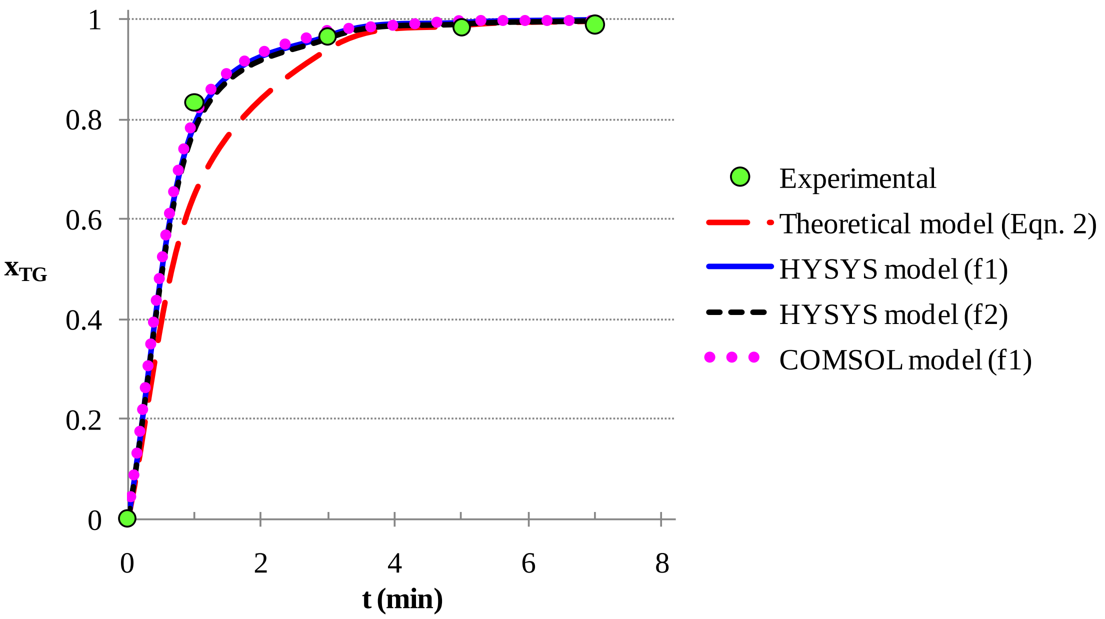

Figure 1. Temporal profile of conversion into methyl esters for the transesterification reaction of CPO with methanol using molar ratio of oil to methanol at 1:10, reaction temperature of 60ºC, catalyst concentration 0.125 kg NaOH/kg oil.

2.3 Reaction modeling

The reversible reaction of transesterification of CPO at constant density can be described by an expression of second order showed in Eq. (1), and also in its integrated form in Eq. (2) proposed by Cheng et al. (2004), when the great excess of methanol used in order to force the equilibrium to the right side of the reaction.

$$\text{triglycerides}\,[\mathrm{TG}] + 3\,\text{methanol}\,[\mathrm{ML}] \rightarrow 3\,\text{methylesters} + \text{glycerol}$$

$$r = -\frac{d[\mathrm{TG}]}{dt} = k[\mathrm{TG}][\mathrm{ML}] \tag{1}$$

$$t=\frac{1}{k[TG]_o\left([ML]_o/[TG]_o-3\right)}\ln\left\{\frac{[ML]_o/[TG]_o-3x_{TG}}{[ML]_o/[TG]_o\left(1-x_{TG}\right)}\right\} \tag{2}$$

where: r = reaction rate of transesterification; [TG] = oil concentration; [ML] = methanol concentration; t = time; $[TG]_o$ = initial oil concentration; $[ML]_o$ = initial methanol concentration; k = kinetic parameter; x_{TG} = conversion of triglycerides.

The kinetic parameter (k) obtained by Cheng et al. (2004) at different experimental conditions was used to construct the predictor curve of x_{TG} *vs*. t as is drawn in Figure 1 like dotted red line. Comparing the observed data and the predicted values of x_{TG} by mean of regression of minimum squares, the correlation coefficient (R^2) resulted of about 0.96, showing good quality of this theoretical kinetic model.

From data values of k tabulated by Cheng et al. (2004) at different temperatures and fixed catalyst concentration and oil:methanol feed rate of 0.125 kg NaOH/kg oil and 1:10, respectively, the activation energy (Ea) was determined and resulted 60737 J/mol with a frequency factor (ko) of 9.153×10^9 m^3/(mol-s) for the condition of maximum velocity of biodiesel production. Zapata et al. (2007) reported closely values Ea and ko (60701 J/mol and 9.1534×10^6 L/(mol-s), respectively) also taken from for the transesterification reaction under the preselected experimental conditions.

Moreover, palm oil can frequently content a level of free fat acids of about 3.8% p/p (expressed in palmitic acid) which reacting with methanol to produce methyl palmitate and water. This reaction of esterification can be described by the following rate expression of first order (Eq. 3) proposed by Zapata et al. (2007).

$$\text{palmitic acid}\,[PA]+\text{methanol}\,[ML]\rightarrow \text{methylpalmitate}+\text{water}$$

$$r'=-\frac{d[PA]}{dt}=k'[PA] \tag{3}$$

where: r´ = reaction rate of esterification; [PA] = palmitic acid concentration; k´ = kinetic parameter.

The activation energy and the frequency factor for the esterification reaction corresponded to 13300 J/mol and 1.27 s^{-1}, respectively (Zapata et al. 2007).

The mentioned kinetic models for the transesterificacion and esterification reactions and the corresponding kinetic parameters were used for design of the continuous ideal pilot plant (PPR) of palm oil methyl esters production in the Aspen HYSYS® interface, that was then used as tool to develop the full FEM-model of the PPR in COMSOL Multiphyisics®.

2.4 ASPEN HYSYS® modeling

Components and reactions

For the characterization of CPO in the Aspen HYSYS® interface, the majority component in the oil (tripalmitin) was considered, including –or not– the presence of 3.8% of FAA (Zapata et al. 2007). That is, two oil formulations were used: 100% tripalmitin (f1) and 96.2%

tripalmitin-3.8% palmitic acid (f2).

Due the lack of the component tripalmitin in the Aspen HYSYS® Library, this component was generated as “Hypothetical component” using the “Hypo Manager”, defining its physical properties density, molecular weight, UNIFAC molecular formulae and structure, boiling point, critical properties (Chemeo, 2013; Caballero Moreno, 2012; Avellaneda Vargas, 2010).

The properties of the reactants streams (methanol with dissolved NaOH, tripalmitin with/or not palmitic acid) and products (methyl palmitate, glycerol, water, remaining methanol, remaining tripalmitin, remaining palmitic acid, dissolved NaOH) were obtained from the NRTL fluid package of Aspen HYSYS®, estimating binary coefficients with UNIFAC method for liquid-liquid equilibrium and Peng-Robinson for vapor.

The reaction of transesterification was defined as “Kinetics”, irreversible of first order for both tripalmitin and methanol (Eq. 2), expressing the kinetics constant for the forward reaction expressed in Arrhenius form equation. While, where appropriate, the esterification reaction was defined as “Kinetics”, irreversible of first order referred to the palmitic acid (Eq. 3).

Equipment design

For the continuous biodiesel (methyl palmitate) production, an ideal “plug-flow" type reactor was selected from the “Object Palette” of Aspen HYSYS®, by analogy of behavior with the ideal stirred batch reactor with constant density (Levenspiel, 1998, 2004; Fogler, 2005) employed in the kinetic study of Cheng et al. (2004). This procedure is based on the concept of existing equivalence between the time of reaction in a ideal stirred batch reactor and the spatial time in a ideal plug flow reactor, when density of the reacting mix maintains constant (Levenspiel, 1998, 2004).

Dimensions of the reactor (diameter and length) were defined equal the corresponding to the PPR tubular reactor. Two mixers were installed at the reactor inlet to provide the reactants streams with the prefixed molar relation (1:10) and catalysts concentration (0.125 mol NaOH/kg oil) using the “Set” tool of Aspen HYSYS® (Figure 2). Negligible pressure loss in the equipments were considered.

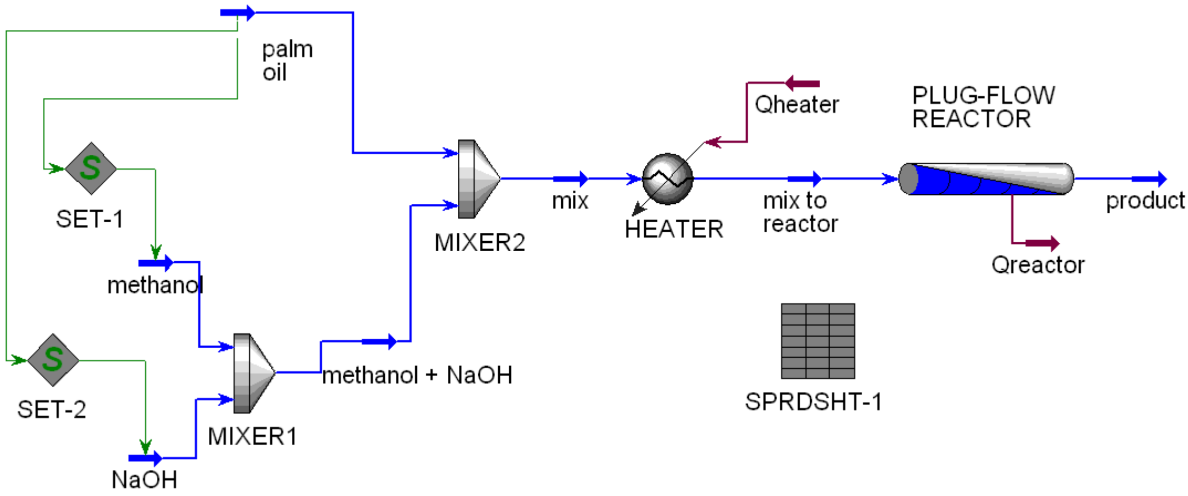

Figure 2. Aspen HYSYS® Flowsheet of the PPR tubular reactor pilot plant for the transesterification reaction of CPO with methanol using molar ratio of oil to methanol at 1:10, reaction temperature of 60ºC, catalyst concentration 0.125 kg NaOH/kg oil.

Solving the mass and energy balances of the plug flow reactor at isothermal operation, the conversion of TG into ME was estimated as a function of volumetric flow, and hence the spatial time. Figure 1 shows (in blue solid line) the predictor curve of triglycerides (100% tripalmitin) conversion into biodiesel (methyl palmitate) obtained by Aspen HYSYS®, demonstrating the agree of this model with the experimental data in the whole range (R^2=0.9975 for the preselected reaction condition). When a level of FAA of 3.8% palmitic acid in the composition of the CPO was considered, similar results of triglycerides conversions were obtained (dashed black line in Figure 1). These behavior evidences that both models with different oil characterization are equally capable to reproduce the experimental curve, with a regression coefficient of 0.9999 between them.

In virtue of this, the following analysis were made considering only the more simple CPO characterization corresponding to 100% triplamitin.

The continuous plug-flow model developed in Aspen HYSYS® interface was used as tool to predict properties and conditions of the involved streams of reagent and products. These information resulted very useful for the following numerical modeling of the palm oil methyl esters production at the pilot reactor, based on the method of the finite elements (FEM) performed in COMSOL Multiphysics® version 3.5a (COMSOL, 2008).

2.5 FEM modeling by COMSOL MULTIPHYSICS®

To modeling the process of biodiesel production from the non-conventional oil (palm oil) with methanol in the PPR, the balance of mass, energy and momentum has to be raised, along with other equations, conforming a system of coupled differential equations.

For its resolution, a CFD model (Bahl et al. 2012) previously developed for describe the flow patterns in the mixer-reactor system of the PPR through the Navier-Stokes Module for incompressible fluids in stationary stage of COMSOL Multiphysics® 3.5a was used.

Later, this CFD model was coupled with the Convection and Diffusion, and the Heat Transfer by Convection and Conduction modules, including the reaction kinetics.

The CFD model was constructed considering a 2D domain which was discretized with Lagrange quadrangular elements. First, the transfer of momentum problem in stationary state was solved to obtain the velocity field and pressure profiles at different values of volumetric fluid flow in the range 0-100 L/h. For that, the fluid properties (density and viscosity) were defined as the corresponding to the effluent reactor of the model Aspen HYSYS®.

Initial conditions of null velocity and pressure at t=t0 were used. The boundary conditions were: fixed normal fluid velocity at reactor inlet, no slip at lateral walls, and null pressure at reactor outlet. The Direct (UNFPACK) solver was used with tolerance of 0.01. Convergence of solution was obtained for different feed conditions (flow velocity, Reynolds number, temperature), allowing to determine the velocity and pressure profiles in the domain.

As example, Figure 3 presents the profiles of the velocity field in two cross-sections located, one, immediately at the outlet of the mixer, and the other, next to the outlet of the reactor. The characteristic parabolic shape of these curves denote the laminar behavior of the flux in these transversal sections of the reaction system. Similar profiles were obtained for the other evaluated conditions.

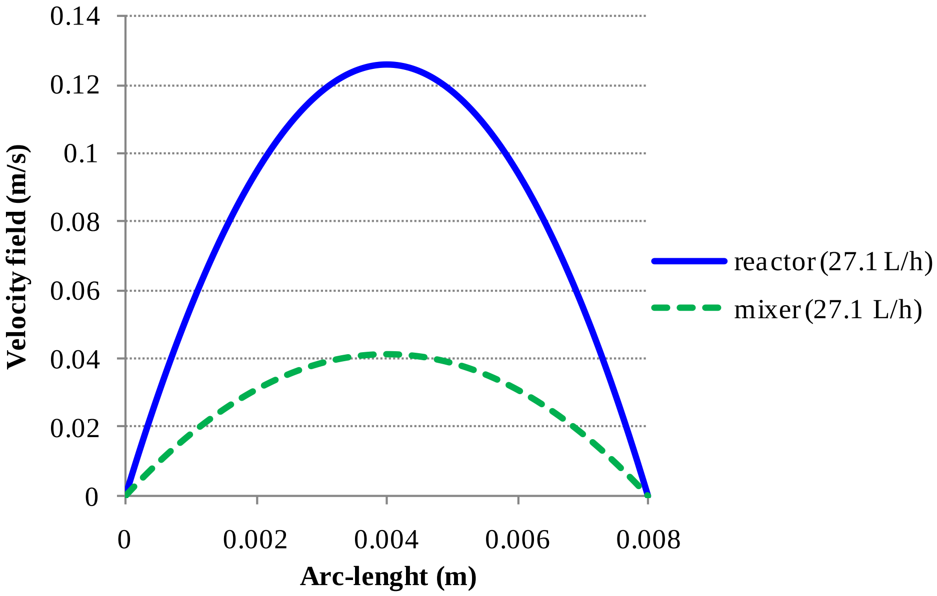

Figure 3. Velocity field profiles in the cross-sections located at the mixer and reactor outputs, for an imposed volumetric flow of 27.1 L/h (7.53×10^{-6} m^3/s), using molar ratio of oil to methanol at 1:10, reaction temperature of 60ºC, catalyst concentration 0.125 kg NaOH/kg oil.

These results of the resolution of the Navier-Stokes Module were storage for the subsequent resolution of the Convection and Diffusion, and Heat Transfer Modules with the reacting fluid moving inside the reactor.

The reaction of transesterification was assembled to the CFD model using the Modules of Convection and Diffusion, and Heat Transfer for the reacting fluid moving inside the reactor in stationary state.

The Module Convection and Diffusion was employed to determine the concentration distribution of the involved species and the conversion of the TG at every reaction condition.

To this end, necessary data as the coefficient of diffusion, the reaction rate and fluid velocity should be introduced.

Due to the difficulty in predicting the molecular diffusion coefficient (D) in a multi-component system, and considering that a back mixing of turbulence may also exist inside reactor, so it is necessary to incorporate diffusivity swirl (Cunill et al. 2010). It was led to replacing the molecular diffusion coefficient by an effective diffusion coefficient (Def). In literature, there are many correlations for estimating the dispersion module (Def/uL) using as variables the dispersion intensity (Def/ud) and system properties; dispersion module can be then calculated multiplying the intensity of scattering by the geometry factor (d/L) (Cunill et al. 2010). Among these correlations, the following Eq. (4) provides the relationship between the dispersion intensity and the product of the Numbers of Reynolds and Schmidt (Re×Sc = u d/D) for laminar flow in tubes (for L>>3d, L>>30d, L>>300d):

$$\mathrm{Def} = \mathrm{D} + \left(\frac{u^2 d^2}{192\,\mathrm{D}}\right) \tag{4}$$

where: u = fluid velocity; d = diameter reactor; L = length reactor.

In the previous study of the residence time distribution in the PPR for different volumetric flows (Bahl et al. 2012), the effective diffusion coefficient and the dispersion module (Def/uL) –dimensionless group that characterizing the spread in the whole vessel– have been determined. In that work, from the analysis of the residence time distribution determined experimentally by the stimulus-response method using a tracer injected with a echelon-type signal, the Peclet Number (equal to the reciprocal of the module of axial dispersion) resulted higher than 100 in the whole range of volumetric fluid flow, evidencing that the fluid dynamic behavior of the reaction plant can perfectly close with “plug flow”.

This behavior has been illustrated in Figure 4 through normalized response curves for different fluid flows predicted from experimental data; the green dotted line corresponds to the same experimental conditions of the velocity profiles displayed in Figure 3.

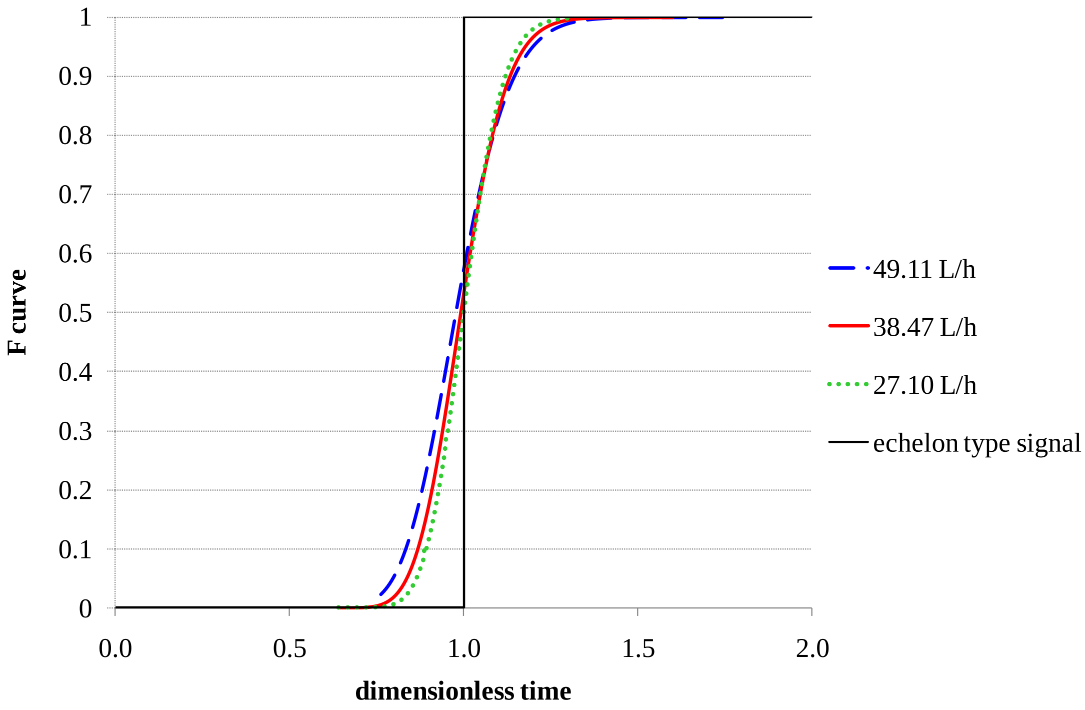

Figure 4. Normalized response curves for different fluid flows predicted for the CFD model (Bahl et al. 2012) developed from experimental data obtained by the stimulus-response method using a tracer injected with a echelon-type signal.

From the obtained values of the dispersion module, the corresponding values of dispersion intensity (Def/ud) were correlated with the product (Re×Sc) (Eq. 4) in order to obtain the molecular diffusivity D for the reacting mix.

Figure 5 shows the agreement of the Eq. (4) to drawn the experimental data (points) (R^2=0.99). The resulting D=2.21085×10^{-7} m^2/s was considered equal for the whole joint of the reaction species in the further analysis performed in COMSOL Multiphysics®.

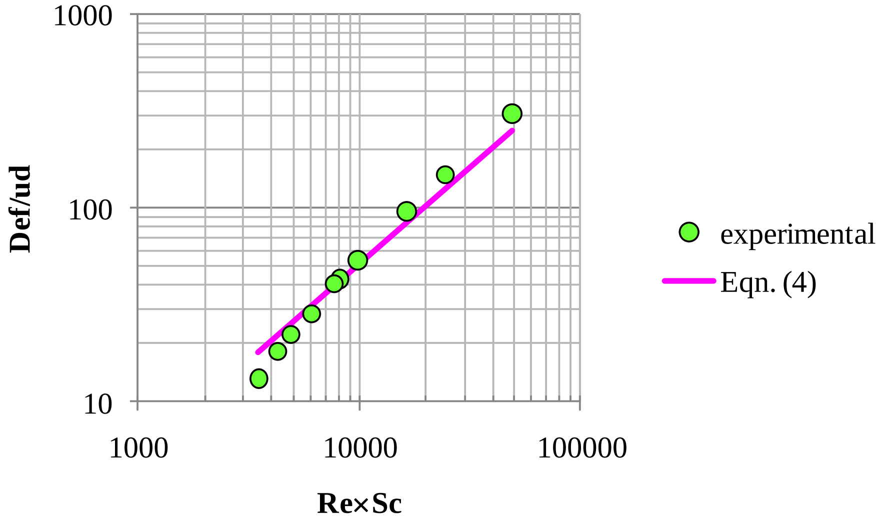

Figure 5. Experimental (points) dispersion intensity obtained by the CFD model (Bahl et al. 2012) in function of the adimensional product Re×Sc compared with the prediction of Eq.(4).

Respect to the reaction rate of transesterification (Eq. 1), it was described into "Global expressions" as well as the kinetic constant k which was defined by mean of the Arrhenius equation in terms of the absolute temperature.

The components of the fluid velocity were referred to the stored values resulting from the resolution of the Navier-Stokes Module.

For the resolution of mass transfer equation be mean of the Diffusion and Convection module, each initial concentration of TG was imposed as initial condition. The boundary conditions were: fixed initial concentration of TG at reactor inlet for each case, insulation at lateral walls, and convective flux at the reactor outlet.

Moreover, to solve the thermal problem for the reacting fluid moving inside the reactor, the Heat Transfer Module was included. Necessary thermal properties such as standard heat of reaction, thermal conductivity and heat capacity of the reaction mix were taken from Aspen HYSYS®. The heat of reaction was defined into the "Global Expressions" in function of both local temperature and conversion of TG.

The Direct (UNFPACK) solver was used with tolerance of 0.01. Convergence of solution was obtained for different feed conditions (flow velocity, Reynolds number, temperature), allowing to determine the velocity and pressure profiles in the domain.

First, the coupled thermal-mass problem was solved for isothermal conditions used by Cheng et al. (2004) in order to validate the predictions of the COMSOL model. As results from the resolution of the whole coupled MEF model, conversions at the outlet reactor were corresponding with experimental data, as is shown in Figure 1 in pink dotted line for the preselected condition (molar ratio of oil to methanol at 1:10, reaction temperature of 60ºC, catalyst concentration 0.125 kg NaOH/kg oil).

The versatility of the COMSOL model was probed contrasting its predictions with experimental data at other conditions, demonstrating that the model is poweful to describe the measured data of CPO isothermal transesterifacion (Figure 6).

Additionally, the developed FEM-model was used to estimate the behavior of the reaction system under non isothermal conditions. Figure 6 shows the predicted profiles of conversion of TG for adiabatic conditions. It can be noted that the process could be optimized at adiabatic conditions due that more higher conversions could be reached involved lesser reaction times, principally in the initial phase of the process.

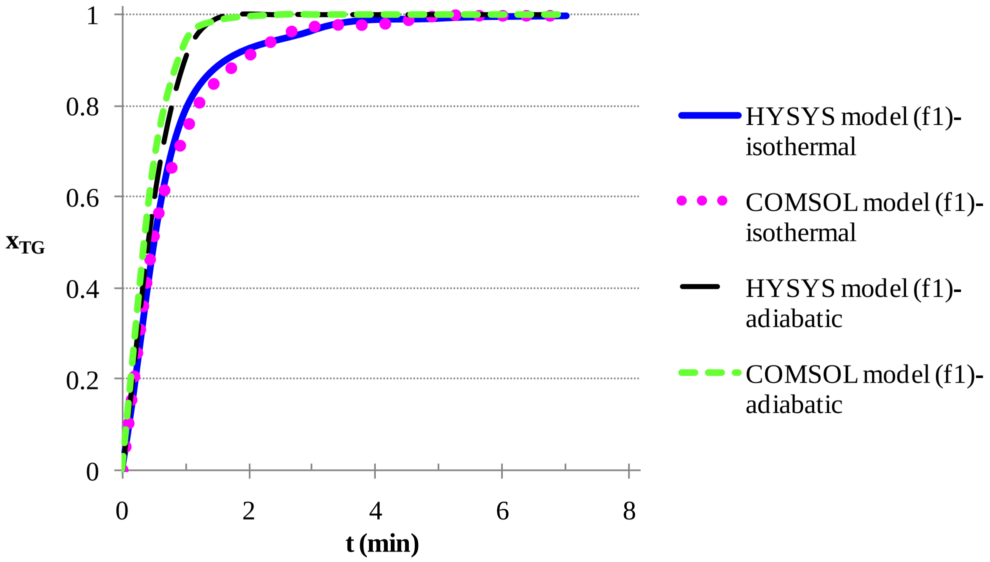

Figure 6. Comparison of the at isothermal and adiabatic temporal profiles of conversion into methyl esters for the transesterification reaction of CPO with methanol using molar ratio of oil to methanol at 1:10, reaction temperature of 60ºC, catalyst concentration 0.125 kg NaOH/kg oil.

3 CONCLUSIONS

The liquid-phase biodiesel production in a pilot continuous reactor at the Pilot Plant of Reaction (PPR), Chemical Engineering Dept. (UNCPBA) has been studied and simulated. A full model based on FEM was developed to simulate the transfer of momentum, heat and mass in the PPR coupling the kinetic reaction of catalytic transesterification of the palm oil with methanol into the general program.

A model of the plug-flow reactor to simulate the process of biodiesel production was performed in the Aspen-HYSYS® environment and validated with experimental data from literature, and then used to estimate useful data for the FEM model developed in COMSOL Multiphysics®.

Predictions of the FEM model were wholly congruent with HYSYS model and consequently with experimental data. As results from the resolution of the full COMSOL model, profiles of flow velocity, pressure, temperature, concentration of reacting species, and conversion of tryglicerides -among others- were obtained. Additionally, other operative conditions were explored in order to optimize the performance of the process.

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