Computational Fluid Dynamic Study of Fixed Bed Reactor of Hydrotreating of Vegetable Oil

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Introduction: Hydrotreatment process allows removing of oxygen from triglycerides of vegetable oils to produce mixtures whose boiling points are similar to those of fossil diesel. To gain insight on such a process, models and simulations of the hydrotreatment reactors are carried, also to predict and improve the behavior of the reaction systems. A key factor to be understood is the hydrodynamics of reactor in order to optimize the yield of desirable products. In this contribution the preliminary design of a fixed bed hydrotreatment reactor of vegetable oils is presented.

The following reactor parameters and operation conditions were used: Reactor diameter: 0.7937 cm, height: 26.67 cm, volume: 10 ml, Tmax: 600 ° C, pressure: 5 MPa, LHSV: 1.5 H^{-1}.The physicochemical properties of commercial NiMo / Al_2O_3 were employed to represent the porous zone or reactor.

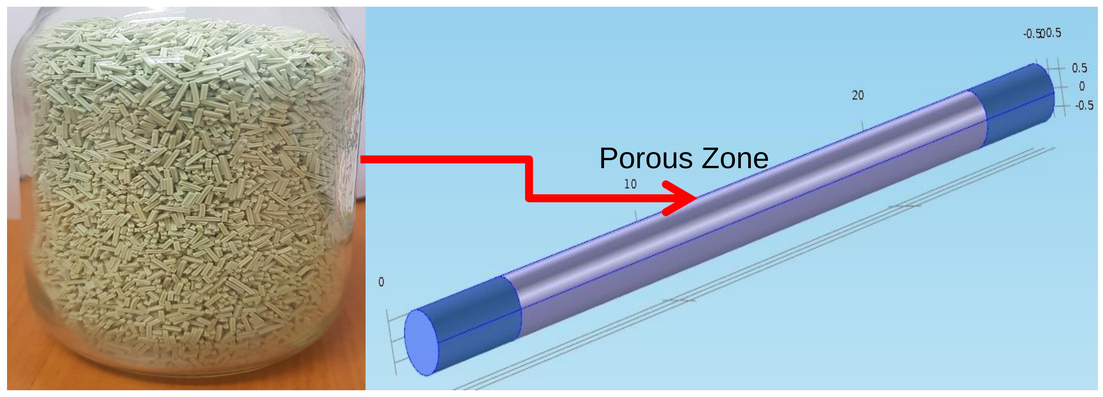

Figure 1. Porous zone

Model: In order to analyze the chemical reactor, in a first approximation a Species Transport in Porous Media was used. This physical model involves the equations of Diffusion and the Navier- Stokes equations. The Navier – Stokes equations is an expression of the conservation of momentum, meanwhile the diffusion is analyzed with the Tortuosity model for the porous zone and the species concentration. The mathematical model is described in eq. (1).

It is assumed a uniform velocity profile that implies that the expression of the Darcy Law can be used. To make the determination of the permeability from the porous zone the equations of Carman- Kozeny are involved, and in the adsorption section the Langmuir model was employed.

$$P_{1,i}\frac{\partial_{ci}}{\partial t} + P_{2,j} + \nabla \cdot \Gamma_i + u \cdot \nabla c_i = R_i + S_i \qquad (1)$$

The properties used for the porous material are reported in Table 1:

Table 1. Properties of the porous zone

Property	Value	Units
Density	3957.86	Kg/m^3
Permeability	0.6	m^2
Relative Permeability	0.8	1
Porosity	0.7	1

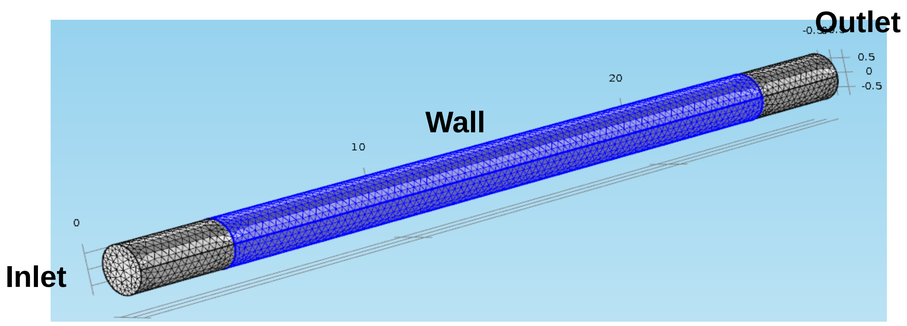

Figure 2. Mesh distribution and boundary conditions of the reactor

The simulation was carried out in this first approach by taking into account the presence of chemical reactions and without chemical transformations, in order to analyze the concentration profiles of the materials involved during the operation of the reactor. Therefore the equations used in the reaction steps are described in eq. (2)

$$R_{c1} = -k * c1 * c2 \qquad (2)$$
$$R_{c2} = -k * c1 * c2$$
$$R_{c3} = k * c1 * c2$$

Mathematical approach

The computational geometry employed for the simulation assumes, as a general domain, a cylindrical region that considers a gas and liquid inlet velocity (0.01m/s) and boundary conditions of outlet pressure, Figure 2, in the fully developed gas flow. In the wall, it was considered a non-slip border condition, both, for the liquid phase and for the gas phase.

Results: A packed-bed reactor is illustrated in Figures 3 and 4. The central region in the cylinders represent the catalytic bed porous zone.

The mass and heat transport in a solid and fluids involve both diffusive and convective mechanisms, the latter couples the scalar concentration and temperature fields to the vector velocity field. Also, the nonlinearity in the convective momentum transport terms leads to the regime of flow, which is inherently convective but is usually modeled as an enhancement of mass, heat and momentum diffusivity (Figure 5 and 6). The simulations were done making variations with and without chemical reactions. In the last case the concentrations and the linear velocity convective flux magnitude gives additional information on how the chemical reactions affect the flux and provides more details to keep working on the trickle flow regime.

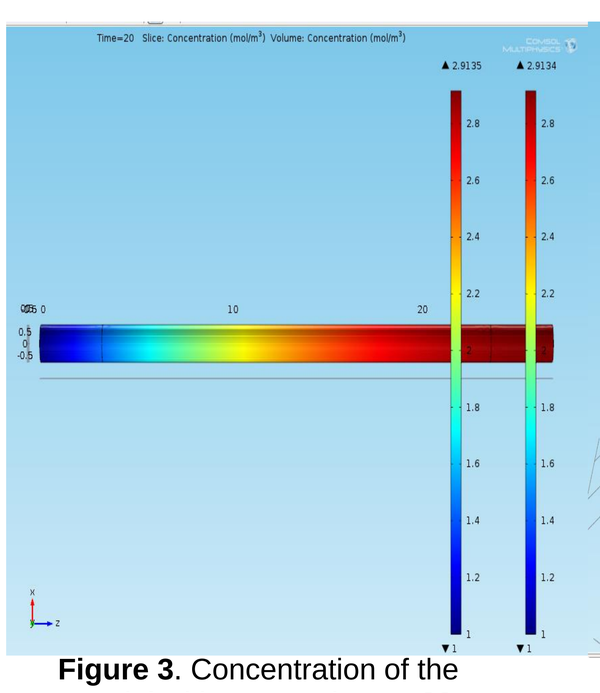

Figure 3. Concentration of the material without reactions t=20 s

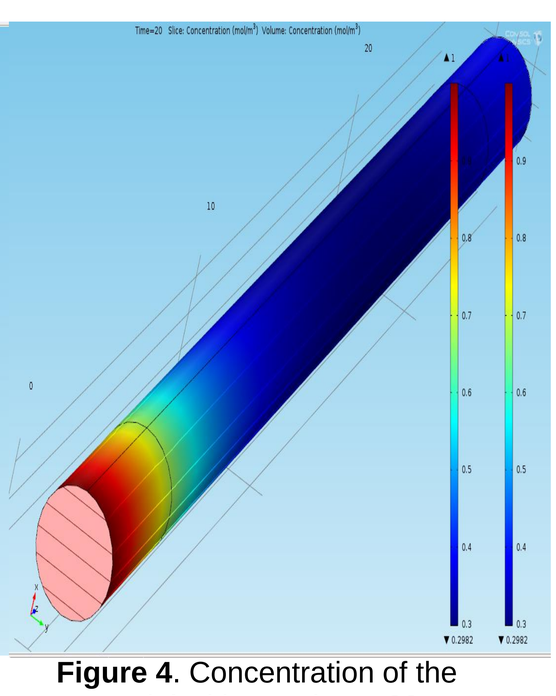

Figure 4. Concentration of the material with reaction t=20 s

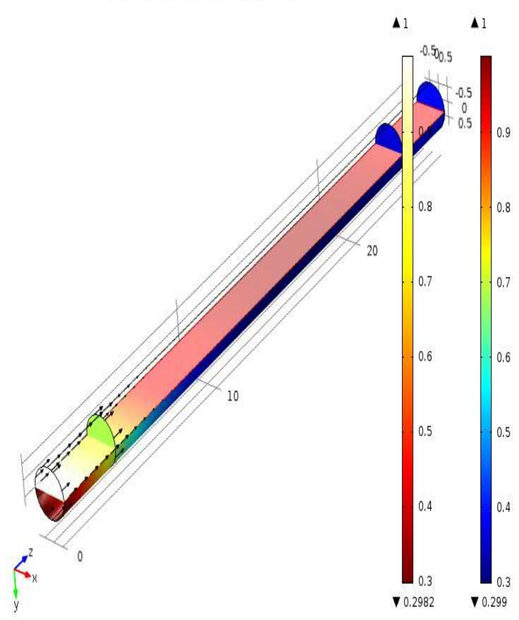

Figure 5. Average linear velocity convective flux magnitude without reactions t=20 s

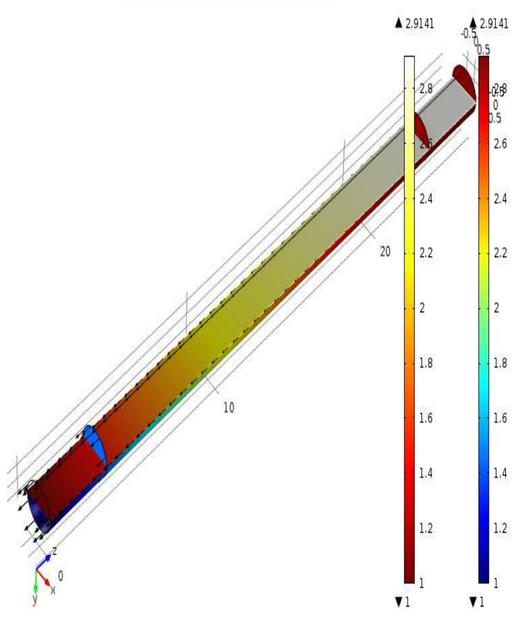

Figure 6. Average linear velocity convective flux magnitude in presence of chemical reactions t=20 s

Conclusions:

A first approach of the modeling of the porous media zone was carried out to model an hydrotreatment process in catalytic packed-bed reactor. The model is used to describe the concentration profiles of reagents and products. This model is associated with the condition of local mass equilibrium. The expressions for effective diffusivity, dispersion, total dispersion and the Darcy's law permeability tensors were used. Solution of the set of final equations allowed calculate the variations of concentration of the chemical species along the packed-bed reactor. The last information is essential for the design of packed-bed reactors and in this way improve the efficiency of reactors to future production of cleaner biofuels.

Acknowledgements

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