

CFD Modeling and Simulation of a Hydrotreatment Reactor Countercurrent Using Jatropha Curcas L. Vegetable Oil

Pablo Vizguerra Morales (✉ p.vizguerramoraes@ugto.mx)

Instituto Politécnico Nacional

Fabian S. Mederos Nieto

Instituto Politécnico Nacional

Article

Keywords: CFD, Hydrotreatment, Jatropha Curcas L., countercurrent

Posted Date: May 29th, 2023

DOI: <https://doi.org/10.21203/rs.3.rs-2953198/v1>

License:   This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Additional Declarations: No competing interests reported.

CFD MODELING AND SIMULATION OF A HYDROTREATMENT REACTOR COUNTERCURRENT USING JATROPHA CURCAS L. VEGETABLE OIL

Pablo Vizguerra Morales^{1}, Fabián S. Mederos Nieto¹.*

¹Centro Mexicano para la Producción más Limpia (CMPL), Instituto Politécnico Nacional Posgrado, Av. Acueducto s/n, Col. La Laguna Ticomán, 07340 Ciudad de México, México. p.vizguerramoraes@ugto.mx

* Corresponding author

Abstract

In this work, a drained bed reactor (TBR) was analyzed for the hydrotreatment process, using a commercial catalyst CoMo/ γ -Al₂O₃, vegetable oil from Jatropha Curcas L. was used as raw material. The mode of operation of the reactor was considered in countercurrent. The operating conditions that were considered for the CFD simulation were temperature 320–380 °C, pressure 8 MPa, LHSV 0.8–8.0 h⁻¹. The reactor model considers a single hydrocracking reaction of triglycerides to renewable fuels. The CFD simulation was carried out in Ansys Fluent 16.0 in transient state and in 3 dimensions, considering the turbulence model $k - \epsilon$ standard, Eulerian multiphase model for 3 phases and the porous medium model, obtaining results very similar to the experimental ones, a good approximation with the experimental results which can be applied to the industrial scale was shown.

Keyword: CFD, Hydrotreatment, Jatropha Curcas L., countercurrent

Introduction

In recent years, the demand for energy is increasing worldwide, In Mexico City this phenomenon has been observed., and it is expected that in the coming years it will increase due to the growth of the population and the industry. The main source of energy generation to meet current needs is fossil fuels, this causes the emission of polluting gases, especially CO₂, SO₂, and particulate matter, leading to environmental problems such as climate change and global warming. Therefore, it is important to reduce the environmental impact and generate alternative sources of fuel to meet the demand.

Therefore, the use of other types of renewable energy such as wind, solar and biofuels is important. Biofuels are an alternative source of energy due to their sustainability and low CO₂ emissions. Biofuels are derived from biological carbon sequestration and are obtained primarily from biomass feedstocks. Some characteristics of biomass is that they have low or zero concentrations of sulfur, nitrogen, and ash; therefore, the emissions are also free of NO_x, CO₂ y SO_x. Biofuels are an option for the sustainable development of the country through varying the energy matrix, in addition to serving as a tool to mitigate climate change. These biofuels are called advanced renewable biofuels or next generation sustainable fuels. This classification depends on the type of raw material, conversion technology, formed product, carbon source and formed product¹.

Biodiesel and bioethanol are called first generation biofuels originating from biomass and second generation biofuels originating from lignocellulosic biomass. One problem with biofuels is biomass degradation.

Third generation biofuels are derived from microalgae and cyanobacteria. The bio-oil obtained from the pyrolysis of lignocellulosic biomass has a high-water content, low pH, high viscosity, low calorific value, and is highly corrosive. The produced bio-oil made of 300 different organic compounds, mostly consists of (20-30% by weight) water, (15-30% by weight) lignin fragments, (10-20% by weight), (5-10% by weight) carbohydrates, aldehydes, (10-15% by weight) carboxylic acids, (2-5% by weight) phenols, (1-4% by weight) furfurals, (2-5% by weight) alcohols and ketones (1-5% by weight)⁵. To improve the deterioration of the properties of biomass oil by pyrolysis, an optimization process is required before its application. There are various techniques to convert bio-oils into fuels; Catalytic hydrodeoxygenation^{2,3} zeolite upgrading^{4,5} catalytic cracking⁶, supercritical technology^{7,8} and emulsification⁹.

HDO hydrodeoxygenation activities for the improvement of biooils have more than 50 years. The first to work on the bio-oil upgrading process using HDO was Furimsky. Furimsky explained chemistry and the difficulties in determining chemical kinetics; speed constants, problems due to the presence of oxygen, the importance of improving fuels derived from biomass. This caused an evolution for research towards techniques related to the improvement of bio-oils, Oyama¹⁰ conclude that the HDO process is similar to hydrodenitrogenation (HDN), but 10 times more efficient than the technique using vanadium nitride catalysts. Gutiérrez reported that HDO from biooil needs high pressures of 7-20 MPa to convert some of the low reactivity compounds into O-free products.

Another study on catalytic chemistry, chemical kinetics¹¹, and various mechanisms of HDO reactions suggesting models of oxygenates with the review of Furimsky, Senol¹², Mahfud¹³ and Gutierrez¹⁴ explained the process for the removal of oxygen from biofuel using HDO at high pressure in the presence of cobalt-molybdenum or nickel-molybdenum catalysts¹⁵. Mahfud presented the reaction stoichiometry of the bioacetite HDO process and concluded that it is more efficient in terms of carbon and saturation of aromatic bonds and rings, resulting in the production of liquid fuels such as gasoline and diesel.

Wildschut performed various HDO tests in an autoclave using glucose and cellobiose for the sugar fraction of the pyrolysis oil¹⁶. Their results were that during HDO and using a ruthenium-on-carbon (Ru/C) catalyst, it leads to the formation of tar/solids (humins), and polyols and gas products.

Another study found that there is no benzene formation in the product in the HDO reaction of phenol over Ru/C catalyst. The HDO process removes oxygen at high pressure with a zeolite catalyst in the form of CO, CO₂, and H₂O¹⁷.

Others experiments used acetic acid and furfural to represent pyrolysis products of hemicellulose and cellulose¹⁴, in the absence of a catalyst, reported the formation of a solid polymeric furfural at 250 °C. Using Ru/C as catalyst and acetic acid as feed, they observed very small conversions at low temperatures (<200 °C) and large gas production at high temperatures (>250 °C), their results show a reduction in oxygen content from 41.3% to 27.0 wt%.

Other investigation focused the improvement of bio-oil catalysts to obtain motor fuels, he suggested two paths: hydrodeoxygenation and zeolite cracking, it was reported that the HDO process occurs in a temperature range of 310-350 °C and pressures of 10 -140 bars ¹⁷.

Bridgwater did a job on fast pyrolysis of biomass and how biorefineries can be improved for biofuel production. Yaseen is working on the HDO process of fast pyrolysis bio-oils with various feedstocks that use carbon as a catalyst support, conclude that the biooil worked with the Pt/C catalyst in efficiency of hydrogen consumption, deoxygenation¹⁹.

In the last 50 years, more research has been done on the HDO process using biomass of various materials and its operating conditions and efficiency have been analyzed by various researchers.

Regarding the simulation of the HDO process, we have Gallakota perform CFD simulations on the effect of different catalysts (Pt/Al₂O₃, Ni–Mo/Al₂O₃, Co–Mo/Al₂O₃) for the HDO process of biooils.

Another study focused on CFD modeling of mass transfer and the effects of interparticle diffusion in the supercritical hydrogenation of sunflower oil²¹, Mendoza's work was on the CFD analysis of the heat coefficient during the hydrotreating process of palm oil ²². Muharram worked on the modeling of a hydrotreating reactor to produce green diesel using non-edible vegetable oils by applying the CFD tool ²³.

Another job focused on the prediction of the effects of reactor performance in the HDT process, analyzing the input velocity and the length of the reactor to produce renewable diesel ²⁴. Muharam also worked on the phenomenological model of a sludge bubble column reactor for the production of green diesel to measure performance ²⁵. Another study focused on the CFD simulation of a fixed-bed reactor for the biooil catalytic hydrodeoxygenation process using Pt/Al₂O₃ as a catalyst ²⁶.

Therefore, this study aims to numerically investigate the hydrodynamics and mass transfer of the hydrotreatment process of *Jatropha Curcas* L. oil in the presence of a commercial Co–Mo/γ-Al₂O₃ catalyst in wide ranges of temperature and pressure using the CFD tool (Ansys Fluent), in a countercurrent trickle-bed reactor.

This work has the following objective:

1. Find the mathematical model of hydrodynamics and mass transport in the countercurrent hydrotreating reactor using Fluent 16 to validate with the experimental data.

2. Simulate with Fluent the kinetics of a reaction and the mass transfer in the reactor.

The study reactor is a dynamic trickling bed reactor (TBR) where the hydrotreating process is carried out, using a commercial $\text{CoMo}/\gamma\text{-Al}_2\text{O}_3$ catalyst, as feed raw material *Jatropha Curcas* L vegetable oil was used, the reactor is shown in figure 1.

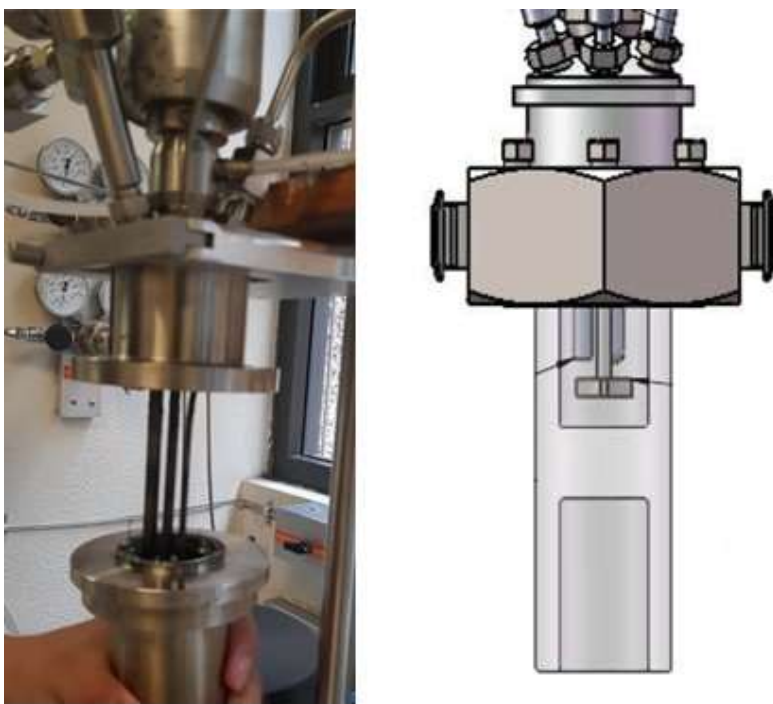


Figure 1. TBR reactor in countercurrent that was studied.

The dimensions and operating conditions of the reactor are shown in table 1.

Table 1. Operating conditions

Reactor	
Scale	Micro
Mode	Countercurrent
Type	Isothermal
Operation variables	
Pressure (bar)	80
Temperature (°C)	320 - 380

H ₂ / Oil volume ratio (NL/L)	1000 - 1500
Gas phase	
Volumetric flow NL/h	-
Mass flow (Kg/s)	4.8 x10 ⁻⁶
Composition (%mol)	100
Liquid phase	
Volumetric flow NL/h	-
Mass flow (Kg/s)	1.1 x10 ⁻⁶
Composition (% mol)	10
Solid phase	
Particle shape	Trilobe Extrudate
Catalyst mass (g)	2
Catalyst volume (cm ₃)	2.4
Inert volume (cm ₃)	2.4
Bed volume (cm ₃)	3.7165
Bed length (cm)	2.8
Equivalent particle diameter (cm)	0.052
reactor dimensions	
Diameter (cm)	1.3
Total length (cm)	30

The following equations are involved in solving the problem posed by the physical phenomenon to be modelled: Reynolds Navier-Stokes average equation (RANS), turbulence model ($k - \varepsilon$) standard, equations of state and coupled methods; FLUENT 16TM uses the finite volume method as a numerical method to solve the governing equations and those mentioned above ¹⁹.

The partial differential equations that describe the phenomenon of mass transport are the following:

The equation of conservation of mass or continuity

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_x}{\partial x} + \frac{\partial \rho u_y}{\partial y} + \frac{\partial \rho u_z}{\partial z} = 0 \quad (1)$$

The momentum conservation equations or the amount of movement theorem

Component X

$$u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} = \nu \left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right) \quad (2)$$

Component Y

$$u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} = -\frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right) + \rho g_y \quad (3)$$

Component Z

$$u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} = \nu \left(\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right) \quad (4)$$

Standard turbulence model ($k - \varepsilon$)

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M \quad (5)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = & \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_1 \frac{\varepsilon}{k} (G_k + C_3 G_b) \\ & - C_2 \rho \frac{\varepsilon^2}{k} \end{aligned} \quad (6)$$

$$\mu_t = \rho C \frac{k^2}{\varepsilon} \quad (7)$$

The above equations are considered in Cartesian coordinates, C_1 , C_2 , C_3 , σ_k , y σ_ε are closure coefficients for the standard turbulence model ($\kappa - \varepsilon$) equations 5 and 6. The values of these coefficients are: 1.44, 1.92, 0.09, 1.0 y 1.3, respectively.

The energy conservation equation is given by the following expression:

$$\frac{\partial}{\partial t}(\rho E) = -\nabla \cdot (\vec{v}(\rho E)) - (\nabla \cdot q) + \rho(v \cdot g) - (\nabla \cdot p v) - (\nabla \cdot [\tau \cdot v]) + S_h \quad (8)$$

Porous media models for single-phase and multiphase flows use a porous surface velocity formula as the default value. Fluent calculates surface phase or mix rates based on volumetric flow rate. The porous surface velocity formulation generally provides good representations of pressure loss in the porous region. Porous media are modeled by adding a momentum source term to the standard fluid flow equations. The source term is made up of two parts: a viscous loss term (Darcy, the first term on the right hand side of Equation 9) and an inertial loss term (the second term on the right hand side of Equation 9).

$$S_i = - \left(\sum_{j=1}^3 D_{ij} \mu v_i + \sum_{j=1}^3 C_{ij} \frac{1}{2} \rho |v| v_j \right) \quad (9)$$

Where S_i is the source term for the i -th momentum equation (x, y, z), $|v|$ is the velocity magnitude, D and C are prescribed matrices. This momentum contributes to the pressure gradient in the porous cell, creating a pressure drop that is proportional to the velocity of the fluid. (or velocity squared) in the cell.

Multiphase flow

For multiphase flows, Fluent solves the equations for 2 types of scalars, for each phase and for the mixture. For an arbitrary scalar k in phase – 1, denoted by ϕ_l^k .

Fluent solves the transport equation in the volume occupied by the phase – 1 y is equation 10;

$$\frac{\partial \alpha_l \rho_l \phi_l^k}{\partial t} + \nabla \cdot (\alpha_l \rho_l \vec{u}_l \phi_l^k - \alpha_l \Gamma_l^k \phi_l^k) = S_l^k \quad k = 1, \dots, N \quad (10)$$

Where; α_l is the volume fraction; ρ_l is the physical density; u_l is the phase velocity -1, Γ_l^k is the diffusion coefficient; S_l^k is the source term which we need to specify.

Eulerian model

For the Eulerian model, a series of n momentum and heat continuity equations are solved for each phase, coupling the phases with pressure and exchange coefficients between phases. This coupling depends on the type of phases involved; for granular flows the properties are obtained from the kinetic theory. This model also makes use of the concept of volumetric phase fractions α_q , satisfying the continuity and momentum equations for each individual phase. The derivation of these equations can be done by averaging the set of

local instantaneous balances for each phase or by using the mixing theory treatment. The general phase conservation equation q is;

$$\frac{\partial}{\partial t}(\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q) = \sum_{q=1}^n (m_{pq} - m_{qp}) + S_q \quad (11)$$

The moment balance for the phase q;

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_q \rho_q \vec{v}_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q \vec{v}_q) = & -\alpha_q \nabla p + \nabla \cdot \vec{\tau}_q + \alpha_q \rho_q \vec{g} + \\ & + \sum_{p=1}^n (R_{pq} \vec{v}_q - m_{pq} \vec{v}_q + m_{qp} \vec{v}_q) + (\vec{F}_q + \vec{F}_{lift,q} + \vec{F}_{vm,q}) \end{aligned} \quad (12)$$

The countercurrent dynamic trickled bed reactor (TBR) that was simulated in CFD, is shown in figure 2. The models, as shown in this work, can be used by the CFD tool to predict the operating behavior of the unit under different reaction conditions and designs to find the best scheme to control the effects of high temperature rise²⁹. Global forward kinetics of HDC, including Jatropha oil oligomerization, where the components produced within the HDC reaction were classified: reactive (TG), light (nC5 - C8), medium (nC9-C14), heavy (nC15 - C18) and oligomerized (>nC18)²⁷.

The four groups of reaction products light (LP), medium (MP), heavy (HP) and oligomerized products (OP) are shown in the kinetic model A7 (Fig.3).

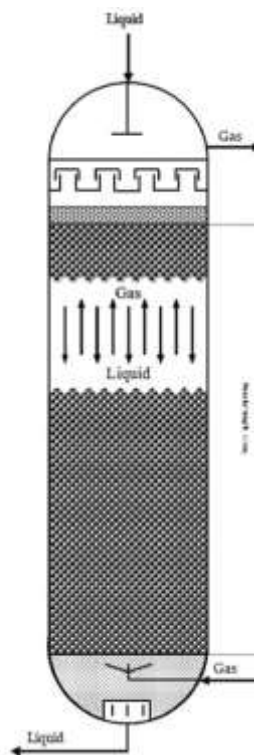


Figure 2. Countercurrent trickled bed reactor (TBR)

The HDT reactions of the TGs were simulated using the five-group model shown in Fig. 3, including Jatrophia oil (C16–C18 triglyceride molecules), naphtha range (C5–C8), kerosene range (C9–C14), diesel range (C15–C18), and polymerized hydrocarbons (> C18) ²⁸.

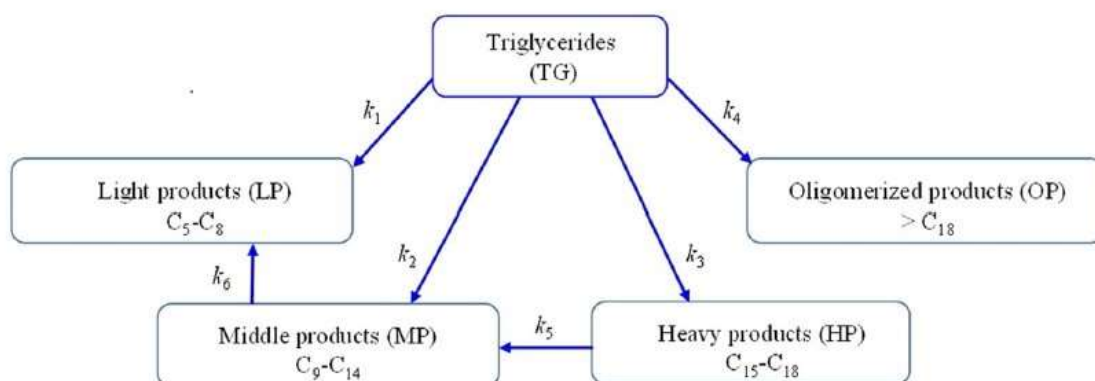


Figure 3. Kinetic model for the hydroconversion of triglycerides.

;

The reaction rates were represented by first order kinetic equations;

$$\begin{aligned}
r_{TG}^L &= (k_1 + k_2 + k_3 + k_4)(C_{SLTG}^S) \\
r_{LP}^L &= -k_1(C_{SLTG}^S) - k_6(C_{SLMP}^S) \\
r_{MP}^L &= -k_2(C_{SLTG}^S) - k_5(C_{SLHP}^S) + k_6(C_{SLMP}^S) \\
r_{HP}^L &= -k_3(C_{SLTG}^S) + k_5(C_{SLHP}^S) \\
r_{OP}^L &= -k_4(C_{SLTG}^S)
\end{aligned} \tag{13}$$

For the simulation in Fluent, only the reaction was taken;

$$r_{TG}^L = (k_1 + k_2 + k_3 + k_4)(C_{SLTG}^S) \tag{14}$$

Materials and Method

The study of the hydrodynamics and mass transfer was carried out with CFD tools in Fluent 16.0, which will give us the profile of the products obtained. A computer with 8 GB RAM memory and an AMD A 8 processor was used. The essential parameters to carry out a study of this type were to obtain an adequate mesh that represents our study area, propose ANSYS models to represent our process, turbulent model, porous model and multiphase model.

Simulation in CFD

Preprocessing

1) Reactor meshing was performed in ANSYS ICEM software and boundary conditions were also entered into the mesh. The mesh was made with a hexahedral structure with a size of 101369 cells (Figure 4) and the boundary conditions are shown in Figure 5.

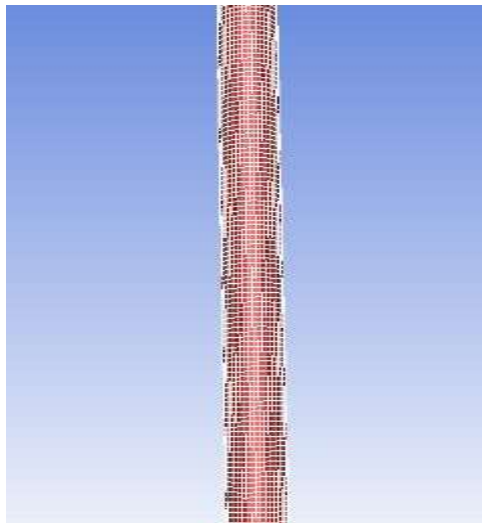


Figure 4. Mesh generated for the reactor.

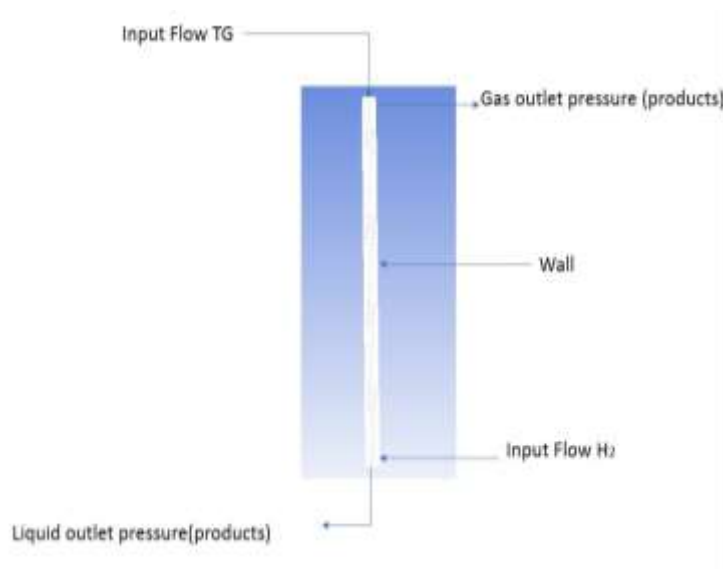


Figure 5. The boundary conditions in the mesh.

A mesh quality study was also carried out with three different mesh sizes with a hexahedral structure with three sizes, 506845, 50685 and 101369 cells, taking the 101369 cell mesh for the study to reduce computational work.

Processing

2) The simulation in Fluent 16.0 was performed in 3 dimensions and in transient and steady state, using the viscous model of $k - \epsilon$ standard, the Eulerian multiphase model was used, for the gas, liquid and solid phases, and the Porous Medium model was also used.

3) The kinetic parameters of the simulated chemical reaction are shown in table 2.

Table 2. Kinetic parameters for Jatropha oil for HDC reactions

			kj (h ⁻¹)			$\Delta H^L_{R,j}$ (kJ mol ⁻¹)
Reacción (j)	$k_{o,j}$ (h ⁻¹)	Ea (kJ mol ⁻¹)	320 °C	360 °C	380°C	
Triglicéridos (TG)	489128.248	52.1712	17.5798	24.2887	32.9001	-1014

3) The boundary conditions used for the simulation in Fluent are shown in Table 3.

Table 3. Boundary conditions for simulation in CFD

Zones	Boundary condition	Data	Pressure (Pa)	Temperature (°K)	Species (mole fraction)
Oil inlet (TG)	Mass flow (kg/s)	4.80E-06	100	330	0.0006
inlet H ₂	Mass flow (kg/s)	1.10E-06	200	325	1
Gas product outlet	Outlet pressure (Pa)	0	0	750	-

Liquid product outlet	Outlet pressure (Pa)	0	0	750	-
Wall	Wall	Estacionaria	0	800	-

4) The convergence criteria were 0.001 for all the equations, for 600 seconds of simulation.

Post Processing

5) The profiles and contours of temperature and pressure of the reactors will be obtained, as well as those of speed within the same, product profiles will be obtained and as well as those of triglyceride conversion profiles at a temperature of 380 °C, the mathematical model will be validated in Fluent with the experimental data carried out in an operating reactor.

Results and discussion

Simulation and conversion analysis of the Ansys Fluent reaction of the countercurrent micro-reactor was carried out using Jatropa oil and hydrogen as raw material. You can see in figure 6 the countercurrent reactor that was simulated where the Jatropa vegetable oil enters from the top and there is also an exit of volatile products, and in the lower part the hydrogen enters and the liquid products are obtained.

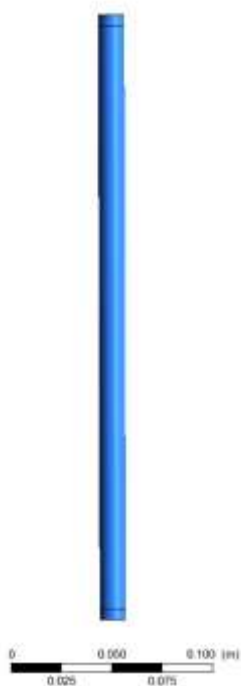


Figure 6. Countercurrent drained bed reactor.

Figure 7 shows the temperature contour on the walls of the reactor varying from 750 to 800 ° K and varies according to time and at the end of the simulation 600 seconds it reaches that temperature, in the first 100 seconds it reaches 600°K and as time progresses it reaches a temperature of 751.3°K.

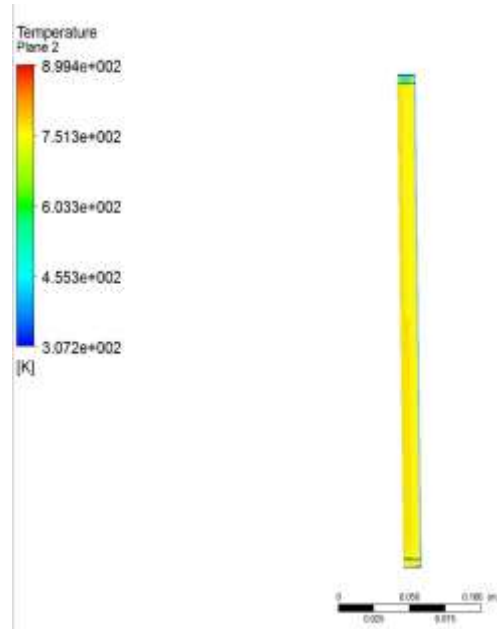


Figure 7. Total temperature contour at 600 seconds of simulation.

Figure 8 shows the contour of the mass fraction of triglycerides (Jatropha oil) after 600 seconds of reaction, where it is observed that most of the oil has been consumed and only an amount remains between 5 and 10 cm from the reactor inlet with a mass fraction of 0.0009972.

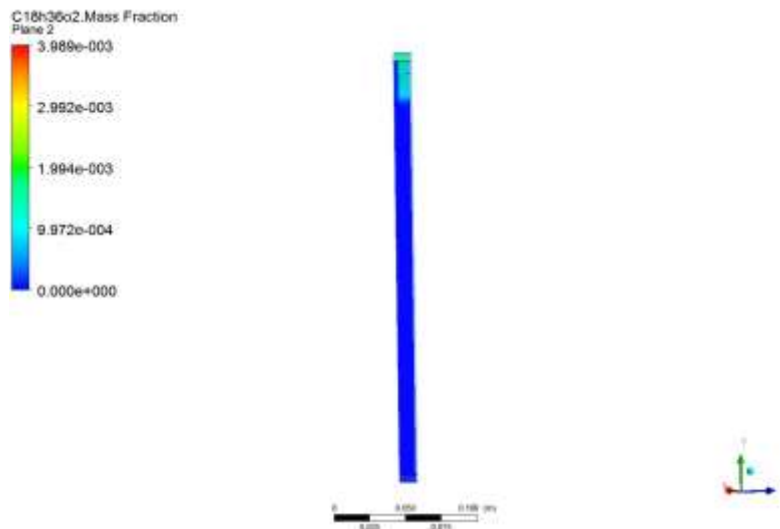


Figure 8. Mass fraction contour of TG (Jatropha oil) at 600 seconds of simulation.

Figure 9 shows the contour of the water reaction product after 600 seconds of simulation where there is a higher concentration in the central part of the reactor approximately 15 cm and at the bottom of the reactor, which is the outlet for products with a mass fraction of 0.015.

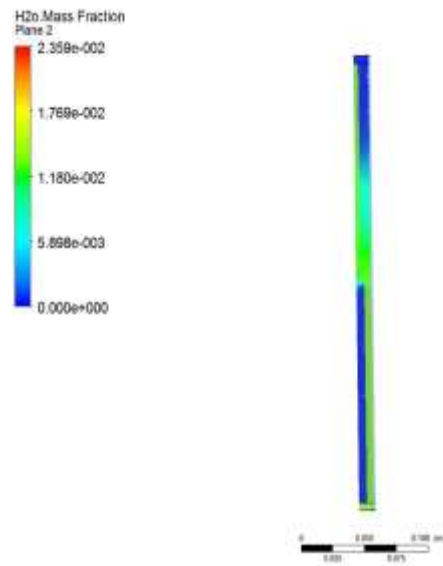


Figure 9. Mass fraction contour of H₂O at 600 seconds of simulation.

Figure 10 shows the contour of the mass fraction of the product (C₁₇H₃₆) after 600 seconds of simulation between 10 and 15 cm, taking the top of the reactor as the axis, we have mass fractions of 0.003871 and 0.0161, at the outlet of the reactor there is a mass fraction of 0.01548.

Figure 11 shows the contour of the mass fraction of the product (CO) after 600 seconds of simulation between 10 and 15 cm, taking the top of the reactor as the axis, having mass fractions of 0.009509, at the outlet of the reactor there is a mass fraction of 0.0091.

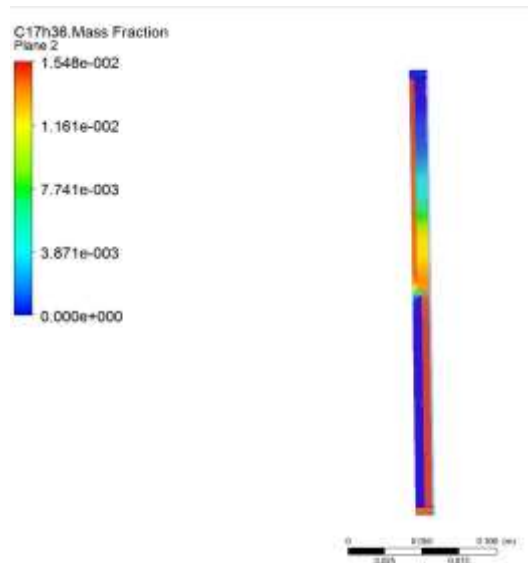


Figure 10. Product mass fraction contour ($C_{17}H_{36}$) at 600 seconds of simulation.

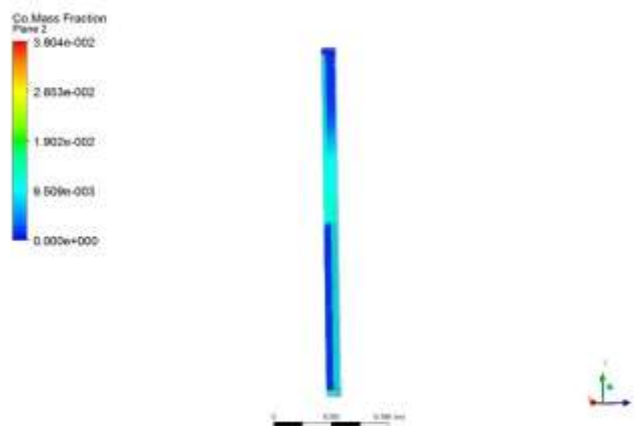


Figure 11. Product mass fraction contour (CO) at 600 seconds of simulation.

It is important to compare the results of the cocurrent microscale reactor used to obtain the experimental data that was operated within an almost ideal behavior, of the simulation in Matlab of the Mederos and this simulation work in CFD with Fluent. Figure 12 shows the comparison of the simulation in Fluent, considering a turbulent model $k - \epsilon$ standard, the moment equation in transient state, in 3 dimensions, the energy equation with the highest source by convection and the Eulerian multiphase model and the porous medium model were considered, the chemical reaction shown above using the Arrhenius model was also considered.

With a simulation of 600 seconds, temperature conditions of 380 °C, pressure of 8 MPa. Similar behaviors were observed between the experimental part, Matlab and Fluent, only that the simulation in CFD, it is observed in the simulation that after 50 seconds the reaction begins to start this due to the fact that there is contact between the two reagents.

The conversion of triglycerides or their consumption in the reaction is faster in CFD simulations than in Matlab, in 0.5 m in the simulation in Fluent it reaches 0.0004 of contraction, the simulation in Matlab of 0.00045 and the experimental data of 0.0005, follows this behavior up to the distance of 2.5 m where the molar concentration of TG in the simulations of 0.0001 and in the Matlab simulation is 0.0002, at the end of 600 seconds and at the outlet of the reactor the three reach the molar concentration of 0.0001.

In figure 13 the partial pressure profile is shown and the comparison of the pressure in the two simulations tend to behave in the same way, the simulation in Matlab has a total pressure that varies from 8.06 MPa to 8.08 MPa. For the simulation in Fluent varies between 7.99 MPa to 8 MPa.

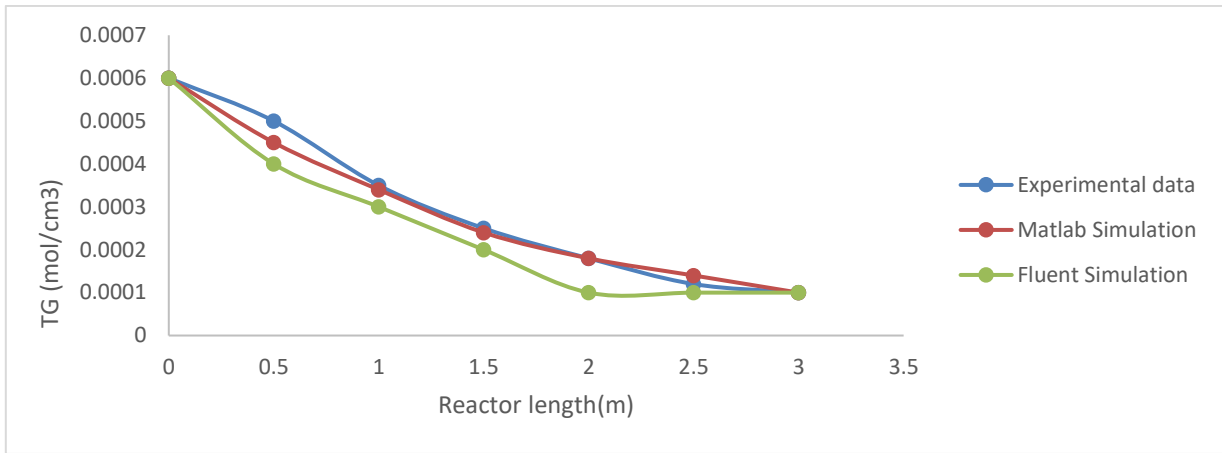


Figure 12. Molar concentration profile of TG (C₁₇H₃₆O₂) at 600 seconds of simulation compared with the experimental data and the simulation in Matlab, and simulation in Fluent (CFD)

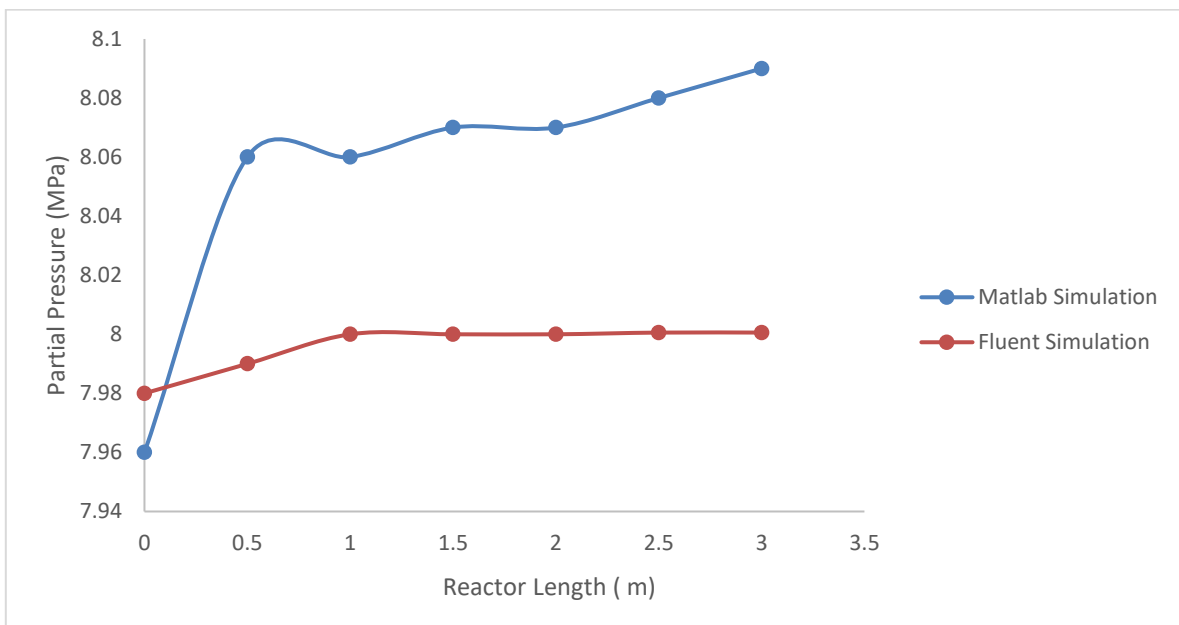


Figure 13. Pressure profile at 600 seconds of simulation compared to those of the simulation in Matlab and the simulation in Fluent.

Figure 14 shows the hydrogen profile and the comparison between the two simulations tend to behave in the same way, the simulation in Matlab has a total pressure that varies in concentration between 0.0007 and 0.00075 molar concentration. For simulation in CFD varies between 0.0001 to 0.0007.

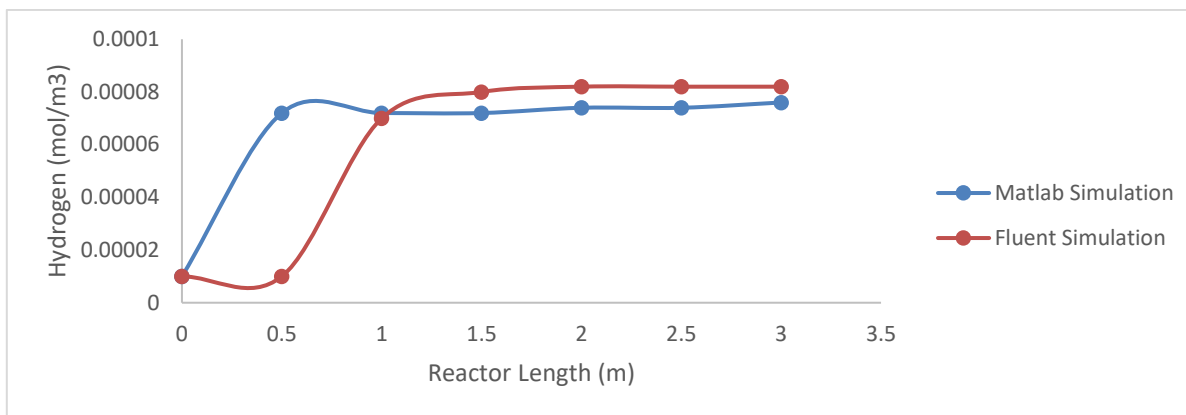


Figure 14. Profile of molar concentration of H_2 at 600 seconds of simulation compared with the data of the simulation in Matlab and the simulation in Fluent

Figure 15 shows the variation of liquid products ($C_{17}H_{36}$) along the reactor at 600 seconds of simulation in Fluent, In the upper part of the reactor there is almost no molar concentration of products, but at 1.5 cm there is a molar concentration of 0.1 and at the outlet of 0.45

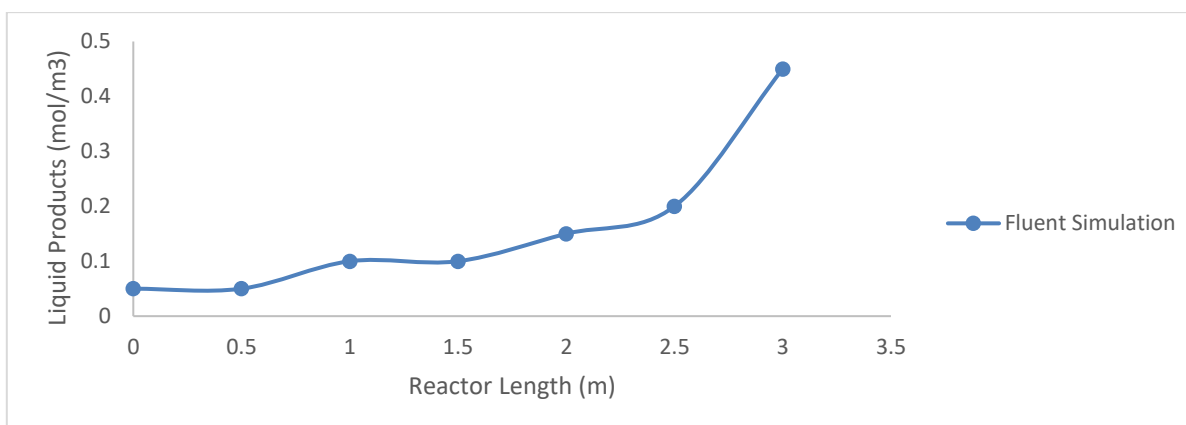


Figure 15. Profile of molar concentration of products at 600 seconds of simulation in Fluent.

Figure 16 shows the total temperature profile throughout the reactor at 600 seconds of simulation in Fluent, in the upper part of the reactor there is a temperature of 330 °K and throughout the reactor it remains almost constant with values from 700 to 720 °K until the reactor outlet.

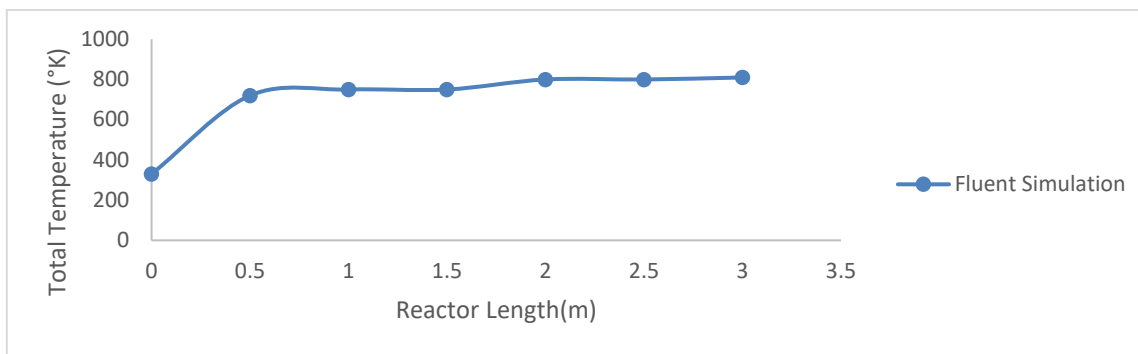


Figure 16. Total temperature profile at 600 seconds of simulation in Fluent.

Conclusions

It is concluded that using a trickled bed reactor (TBR) for the hydrotreatment process for vegetable oil of *Jatropha Curcas L.* in this case it gives us good results, the hydrocracking of this vegetable oil for a countercurrent microreactor was successfully simulated in Ansys Fluent.

The simulation conditions in Fluent that were considered were; temperature 320–380 °C, pressure 8 MPa. The reactor model considers a single hydrocracking reaction of triglycerides to renewable fuels. The CFD simulation was carried out in Ansys Fluent 16.0 in transitory state and in 3 dimensions, considering the turbulence model $k - \epsilon$ standard, the Eulerian multiphase model for 3 phases and the porous medium model, obtaining results very similar to the experimental ones and to the simulation in Matlab, a good approximation was shown with the Fluent tool comparing them with the experimental results which can be applied to the industrial scale.

Data availability

Data sets generated and/or analyzed during the current study are available from the corresponding author upon reasonable request.

References

1. Anjani R. K. Gollakota, Malladi D. Subramanyam, CFD simulations on the effect of catalysts on the hydrodeoxygenation of bio-oil, Royal Society of Chemistry, 5, 41855. DOI: [10.1039/C5RA02626A](https://doi.org/10.1039/C5RA02626A) (2015)
2. E. Furimsky, Appl. Catal., A, 199, 147. [https://doi.org/10.1016/S0926-860X\(99\)00555-4](https://doi.org/10.1016/S0926-860X(99)00555-4) (2000)
3. E. Furimsky, Catal. Rev.: Sci. Eng. 25, 421. <https://doi.org/10.1080/01614948308078052> (1983)
4. J. D. Adjaye and N. N. Bakhshi, Biomass and Bioenerg, 8, 265–277. [https://doi.org/10.1016/0961-9534\(95\)00019-4](https://doi.org/10.1016/0961-9534(95)00019-4) (1995)

5. A. Oasmaa, D. Meier and A. Bridgwater, *Fast Pyrolysis of Biomass: A Handbook*, vol. 1CPL Press, Newbury, UK. (2002)
6. K. L. Hew, A. M. Tamidi, S. Yusup, K. T. Lee and M. M. Ahmad, *Bioresour. Technol.*, 2010, 101, 8855–8858. <https://doi.org/10.1016/j.biortech.2010.05.036> (2010)
7. Z. Tang, L. Qiang, Z. Ying and G. Qingxiang, *Ind. Eng. Chem. Res.*, 48, 6923–6929. <https://doi.org/10.1021/ie900108d> (2009)
8. Y. Zhang, W. Li, S. Zhang, Q. Xu and Y. Yan, *Chem. Eng. Technol.*, (2012), 35, 302–308, <https://doi.org/10.1002/ceat.201100301> (2012)
9. A. V. Bridgwater, *Biomass Bioenergy*, 38, 68–94, <https://doi.org/10.1016/j.biombioe.2011.01.048> (2012)
10. S. T. Oyama, *The Chemistry of Transition Metal Carbides and Nitrides* Blackie Academic and Professional, Springer, Glasgow, [https://DOI: 10.1007/978-94-009-1565-7_1](https://doi.org/10.1007/978-94-009-1565-7_1) (1996)
11. R. Maggi and B. Delmon, *Stud. Surf. Sci. Catal.*, 106, 99. [https://doi.org/10.1016/S0167-2991\(97\)80009-2](https://doi.org/10.1016/S0167-2991(97)80009-2) (1997)
12. O. Senol, PhD thesis, Helsinki University of Technology, (2007). <http://lib.tkk.fi/Diss/2007/isbn9789512290369/> (2007)
13. F. H. Mahfud, PhD thesis, (2007), University of Gronigen. <https://research.rug.nl/en/publications/exploratory-studies-on-fast-pyrolysis-oil-upgrading> (2007)
14. A. Gutierrez, M. E. Domine and Y. Solantausta, *Coprocessing of upgraded bio-liquids in standard refinery units-fundamentals*, 15th European Biomass Conference and Exhibition, Berlin, 7–11. <https://cris.vtt.fi/en/publications/co-processing-of-upgraded-bio-liquids-in-standard-refinery-units-> (2007)
15. D. C. Elliott and T. R. Hart, *Energy Fuels*, 23, 631–637. <https://doi.org/10.1021/ef8007773> (2009)
16. J. Wildschut, I. M. Cabrerre and H. J. Heeres, *Ind. Eng. Chem. Res.*, 48, 10324–10334. <https://doi.org/10.1039/B923170F> (2009)
17. P. M. Mortensen, J. D. Grunwaldt, P. A. Jensen, K. G. Knudsen and A. D. Jensen, *Appl. Catal., A*, 407, 1–19. <https://doi.org/10.1016/j.apcata.2011.08.046> (2011)
18. Y. Wang, Y. Fang, T. He, H. Hu and J. Wu, (2011) *Catal. Commun.*, 12, 1201–1225. <https://doi.org/10.1016/j.catcom.2011.04.010> (2011)
19. E. Yaseen, C. A. Mullen, A. L. M. T. Pighinelli and A. A. Boateng, (2014), *Fuel Process. Technol.*, 123, 11–18. <https://doi.org/10.1016/j.fuproc.2014.01.039>

20. FLUENT Inc., FLUENT User's Guide, 2016.
<http://www.pmt.usp.br/academic/martoran/notasmodelosgrad/ANSYS%20Fluent%20Users%20Guide.pdf>
(2016)
21. A. Guardo, M. Casanovas, CFD modeling on external mass transfer and intra-particle diffusional effects on the supercritical hydrogenation of sunflower oil, *Chemical Engineering Science* 62, 5054 – 5061.
<https://doi.org/10.1016/j.ces.2007.01.08> (2007)
22. César Camilo Mendoza, Juan Felipe Vélez, CFD analysis of the heat transfer coefficient during hydrotreatment of Palm Oil, V Simposio Internacional de Biofábricas. <https://investigaciones-pure.udem.edu.co/es/publications/simposio-v-simposio-internacional-de-biof%C3%A1bricas> (2015)
23. Yuswan Muharam, Osman Abhimata Nugraha, Modelling of a Hydrotreating Reactor to Produce Renewable Diesel from Non-Edible Vegetable Oils, *CHEMICAL ENGINEERING TRANSACTIONS*, VOL. 56. <https://doi.org/10.3303/CET1756261> (2017)
24. Muharam, Yuswan; Nugraha, Osman Abhimata, Prediction of the Effects of the Inlet Velocity and the Reactor Length on the Performance of a Trickle-Bed Reactor for Renewable Diesel Production, *Advanced Science Letters*, Volume 23, Number 6, pp. 5609-5614, <https://doi.org/10.1166/asl.2017.8781> (2017)
25. Y Muharam *et al*, Phenomenological model for the prediction of the performance of a slurry bubble column reactor for green diesel production, *J. Phys.: Conf. Ser.* 1349 012057, DOI 10.1088/1742-6596/1349/1/012057 (2019)
26. Malladi D. Subramanyam, Anjani R. K. Gollakota, CFD simulations of catalytic hydrodeoxygenation of bio-oil using Pt/Al₂O₃ in a fixed bed reactor, *Royal Society Chemistry*, 5, 90354. <https://doi.org/10.1039/C5RA14985A> (2015)
27. Anand M, Sinha AK, Temperature-dependent reaction pathways for the anomalous hydrocracking of triglycerides in the presence of sulfided Co–Mo–catalyst. *Bioresour Technol* 126(1):148–155. <https://doi.org/10.1016/j.biortech.2012.08.105> (2012)
28. Sinha AK, Anand M, Rana BS, Kumar R, Farooqui SA, Sibi MG, Kumar R, Joshi RK Development of hydroprocessing route to transportation fuels from non-edible plant-oils. *Catal Surv Asia* 17(1):1–13. <https://doi.org/10.1007/s10563-012-9148-x> (2013)
29. Mederos Nieto F, Elizalde Martínez I., Trejo Zárraga F.(2020), Dynamic modeling and simulation of three-phase reactors for hydrocracking of vegetable oils, *Reaction Kinetics, Mechanisms and Catalysis*, 131:613–644. <https://doi.org/10.1007/s11144-020-01896-4> (2020)

Acknowledgments

Acknowledgement to Dr. Fabián Salvador Mederos Nieto for his support in the research work, and his research project SIP - IPN 20231028.

Author Information

Pablo Vizguerra Morales

Current address: Centro Mexicano de producción más limpia, IPN

Authors and Affiliations

Centro Mexicano para la Producción más Limpia (CMPL), Instituto Politécnico Nacional Posgrado, Av. Acueducto s/n, Col. La Laguna Ticomán, 07340 Ciudad de México, México.

Pablo Vizguerra Morales, Fabián S. Mederos Nieto.

Author contributions

PVM and FMN contributed to the conception and design, data analysis and writing of the manuscript and contributed to the processing of the CFD simulation of the hydrotreating process. PVM and FMN contributed to the experimental design and simulation. All authors contributed to the drafting of parts of the manuscript and approved the final content of the manuscript.

Corresponding Author

p.vizguerramoraless@ugto.mx

Ethics Statements

Conflict of interests:

The authors declare that there are no conflicts of interest.