MODELING AND SIMULATION OF SOYBEAN OIL TRANSESTERIFICATION REACTION USING CFD AND EXPERIMENTAL DATA

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Abstract *The use of fuels from petroleum rises annually which results in the increase of the atmospheric pollution. The biofuel exists as an alternative to diesel. The goal of this work is to simulate the reaction of transesterification of soybean oil with methanol in presence of sodium hydroxide to produce biofuel using different impellers, using experimental data to estimate the kinetics of the reaction which was consider first order. The reaction was conducted with baffles, agitation velocity of 450 rpm, 1:7 oil/alcohol molar ratio, 0.5% oil mass of catalyst, 30ºC and 60 minutes. The impellers evaluated were Rushton turbine and Oblique blade impeller. The computational fluid dynamics (CFD) approach provides a deep and detailed study. This technique is developed mainly in computational packages like Ansys. Since the reaction is very dependent of the quality of the mixing of the oil and the alcohol, it was necessary to use a turbulence model and we used k-ε, which is currently the one with best industry validation. The mass fractions obtained by the simulation were very close to those found experimentally so the simulation was very satisfactory.*

Keywords: *Computational fluid dynamics, soybean oil transesterification reaction, experimental data validation, reacting mixture.*

INTRODUCTION

Petroleum and its derivatives still are the major source of energy consumed in the world. The possible scarcity of fossil fuels brings the necessity of the development of energy coming from renewable sources. To substitute the diesel oil in engines of ignition by compression, the vegetable oils are an alternative, but the vegetable oil has a high viscosity and when applied directly in the engine it can cause damage and has an incomplete combustion. Looking for minimizing the viscosity of the vegetable oils, the modifications of oils and fat to produce alternative fuels is more and more studied. The most used way for this transformation is the transesterification with methanol or ethanol to produce biofuel (Tretin, 2010).

Biodiesel has good potential as an alternative fuel to diesel. The number of cetane, energy content and viscosity are similar to those of petroleum diesel. The transesterification reaction occurs with triglyceride and short chain alcohol, using acid or hydroxide as the catalyst, to produce esters and glycerol (Darnoko, Cheryan, 2000).

Among the oilseeds already investigated, it is worth mentioning the soybean that does not present technical limitations and has a cultivation area to support a biodiesel program for the formation of blends with conventional diesel (Ma, Hanna, 1999).

Computational Fluid Dynamics (CFD) helps to estimate local behavior within the mixing tank. CFD is the denomination conferred to the group of mathematical, numerical and computational techniques used to obtain, visualize and interpret computational solutions for the conservation equations of physical quantities of interest at a given flow (Fontes, Guimaraes, 2005).

In this work the reactionary process of soybean methyl biodiesel production will be studied, aiming at new reactor designs. The study aims to verify the behavior of the fluid in the tank when using different reactors.

1 BIODIESEL

Biodiesel is an attractive alternative fuel due to its physico-chemical characteristics that closely resemble conventional petroleum diesel, allowing it to be used with minimal or nonexistent modifications in diesel engines. The use of biodiesel as fuel has a market that grows faster and faster. This is due to the contribution of biodiesel to the environment, which reduces levels of environmental pollution, especially in large urban centers (Ismail et al., 2013).

Vegetable oils can be used as fuel, but their direct use in engines is problematic. Due to the high viscosity and low volatility, they do not burn completely and form deposits in the engine fuel injectors (Ferella et al., 2010).

Transesterification is the most widely used way to produce biodiesel. Transesterification is the conversion of triglycerides to esters of fatty acids and glycerol by reaction with low molecular weight alcohol such as methanol and ethanol in the presence of catalyst (Atadashi et al., 2013).

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Soy is the most used raw material in Brazil for the production of biodiesel, followed by bovine fat. Soy is produced in large scale because it is a plant of great crop in Brazil, but the soybean grain has an oil content between 18%-20%, which compared to other oilseeds, such as castor oil, palm oil and sunflower oil that have 30%-45% oil content, is a low productivity. However, soybean cultivation requires less initial investment and its return is more immediate (Dall'agnol, 2007).

The transesterification reaction undergoes the effects of the variations caused by the type of alcohol, by the necessary proportions of alcohol, by different catalysts, by the amount of catalyst, by the stirring of the mixture, by the temperature and by the duration of the reaction (Stamenkovic et al. 2007).

Agitated tanks are widely used in most industries, such as: chemical, petrochemical, biotech, pharmaceutical, metallurgical and so on. Mechanical rotating motion supply with minimal energy consumption is important in a wide variety of processes in the chemical and process industry because the cost associated with energy input contributes significantly to the plant's total cost of operation (Alfaro-ayala et al. , 2015).

Under turbulent flow conditions, the efficiency of the mixing is easily increased by the use of the rectangular plates called baffles (Hashimoto, Natami, Inoue, 2011).

The impellers are initially classified according to the movement they impart to the agitating fluid. There is axial flow where the liquid travels a path parallel to the axis of the agitator and radial flow, wherein the fluid moves perpendicular to the axis of the agitator. As for form, they can be propeller type, blades and turbine (Cubas, 2004).

In a reactor with impeller type propeller and oblique blade impeller the movement of the fluid is classified as axial. Turbine impellers and non-oblique blades impart radial flow (Michelan, 2006).

Many works are found in the literature on kinetics of transesterification of vegetable oils in batch mode. Mathematical models are proposed to evaluate the effect of some variables such as the type of alcohol, molar ratio oil: alcohol, amount of catalyst, type of catalyst and temperature, kinetic order of reaction, reaction rate and activation energy. A second-order model for the three reversible reactions is a satisfactory mechanism in most studies. The kinetic model results in a set of ordinary differential equations with complex solutions, numerical simulation being important to help solve these systems and to evaluate the best reaction conditions (Tretin, 2010).

2 COMPUTATIONAL FLUID DYNAMICS

Computational fluid dynamics has evolved as an efficient and effective tool for obtaining detailed information about the flow of complex fluids using less time and resources. This technique can be used to retrieve detailed information about velocity and concentration programs in the mixing tanks. Although CFD cannot entirely replace experimental measurements, it can substantially reduce the number of experimental measurements and costs involved (Mishra, Ein-mozaffari, 2017).

In CFD modeling, equations describing the laws of mass conservation or continuity (Equation 1), linear momentum or Navier-Stokes (Equation 2) and energy are discretized. If

an infinitesimal volume is considered, it may be noted that, over time, it moves in space and additionally also distorts itself by changing its shape (Santos, 2016).

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial U_i}{\partial x_i} = 0 \tag{1}$$

$$\rho \frac{\partial (\rho, U_i, U_j)}{\partial x_j} = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\right)\right] + \rho . g_i + F \tag{2}$$

And the variables and parameters involved are:

ρ is density of the continuous phase;

t is the time;

U is the velocity;

x is the cartesian coordinate;

μ is the dynamic viscosity;

g is the acceleration of gravity and

F is the function of combination.

The mixture of fluids with different physical properties can be expressed by preserving mass of each species. The numerical solution of these equations can predict how different fluids are mixed. The conservation of species *i*, in terms of its mass fraction m_i, is given by Equation 3 (Castro, 2011):

$$\frac{\partial (m_i)}{\partial t} + \frac{\partial (\rho U_i m_i)}{\partial x_i} = \frac{\partial J_{i,i}}{\partial x_i} + R_i + S_i \tag{3}$$

where:

$J_{i,i}$ is the component *i* of the diffusive flux of the species i on the mixture;

R_i is the rate in which the species *i* is consumed or produced;

S_i is the general font term for species *i*.

When two or more species are involved, the sum of the mass fractions has to be 1 (Equation 4), so for n species, we only need n-1 to be predicted, so:

$$\sum_{i=1}^{n} m_i = 1 \tag{4}$$

The Ansys computational package encompasses several software for computational fluid dynamics analysis. Generally, modeling and simulation in Ansys involves the following steps to reach the results: creation of the geometry, generation of the mesh, definition of the physics of the model, resolution of the problem and visualization of the results.

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The geometry consists of the representation developed in a CAD (Computer Aided Design) of the physical system and its boundary conditions (wall, input, output, objects, etc.). Ansys offers a variety of geometry development software, such as ICEM CFD, Design Modeler and Blade Modeler.

The mesh consists of the discretization elements of the problem for the numerical solution of the system of differential equations. Ansys offers software such as ICEM CFD, Meshing and Fluent Meshing for this step. To solve the problems in CFD, the finite volume method is used most often (Maliska, 2004).

The solution of the problem is done by configuring the boundary conditions, domains and entering the initial conditions, as well as models of multiphase, multicomponent, turbulence, combustion, buoyancy and etc. After this the solver is in charge of solving the discretized equations and generating the result. In Ansys, there are, for example, CFX (CFX-Pre for configuration and CFX-solver for solution) and Fluent.

The post-processor, CFD-Post, is the component used to analyze, visualize and present the results interactively. Postprocessing includes anything from getting point values to complex animated sequences.

3 METHODOLOGY

3.1 Production of biodiesel

To determine the kinetics of the reaction, two reactions were made to vary the experimental conditions for the production of ethyl and methyl soybean. For soybean methyl biodiesel the studied variable was impeller type. The fixed parameters were: temperature (30 ºC); molar ratio oil / alcohol (1/7); reaction time (60 min), agitation speed (450 rpm), amount of catalyst (0.5% of oil mass) and presence of chicane. The impellers used were oblique blade (reaction M1) and turbine type (reaction M2). Figure 1 below shows the impellers used in the experiments.

Figure 1. Rushton turbine to the left and oblique blade impeller to the right

The biodiesel under study was obtained from the commercial soybean oil through the transesterification reaction. The reagents used were: commercial soybean oil (800 g), absolute

methyl alcohol P.A. (205,3 g) and sodium hydroxide P.A. (4 g) as catalyst. The reaction was carried out in a jacketed bench reactor coupled to a mechanical stirrer (Model ET-14000) and a thermostatic bath (Model TE-184).

Initially the catalyst is dissolved in the alcohol until a homogeneous mixture is obtained and the oil is placed in the reactor to reach the reaction temperature. Then the catalyst and alcohol mixture is added to the reactor and stirring is switched on. This moment is the beginning of the reaction.

Biodiesel production and yield analysis were performed as described in 4.2, but during the experimental run samples were taken at the following times: 1 min, 2 min, 3 min, 5 min, 7 min, 10 min, 15 min, 20 min, 30 min, 40 min, 50 min and 60 min.

2.5 mL of dilute sulfuric acid was placed in 12 vials and the 10 mL aliquots of the reaction mixture were added at each instant to be added to the flasks with the acid. Then centrifugation was performed using the Petro Teste Model 6-15H centrifuge, and the bottom of the separation was separated. The pH of the biodiesel was determined; if the pH was not between 6 and 7, the biodiesel was washed with distilled water in half the amount of acid used in the previous wash until the pH remained within that range. After the washes, magnesium sulfate, drying agent, was added to remove moisture. The drying agent was then removed from the biodiesel by simple filtration.

Yield determination was via gas chromatography using the SHIMADZU GC-Plus model chromatograph with flame ionization detector and a 2.2 m column with injector temperature of 250 °C, detector temperature 340 °C, temperature of column of 50 °C, column pressure of 6 kPa. The entrainment gases used were hydrogen, nitrogen and synthetic air.

The internal standard added to the samples was glycerol trioctanoate (tricaprilin), at a concentration of 0.8 g / 10 mL of hexane. The biodiesel samples had a mass of approximately 0.15 g and were diluted in 1 mL of the standard solution (tricaprylin and hexane), and 1 μL of the sample was injected into the chromatograph. The injections were made in duplicate.

The yield in esters was calculated according to Equation 5:

$$Yield(\%) = \frac{m_{tricaprilina} \times As \times f \times 100}{A_{tricapilina} \times m_s} \tag{5}$$

where:
$m_{tricaprilina}$ is the mass of the intern standard;
As is the sum of the areas of the peaks related to the esters contained in the sample;
f is the response factor;
$A_{tricapilina}$ is the area of the peak related to the intern standard;
m_s is the mass of the sample.

3.2 Modeling

In order to construct the geometry, the tank, the Rushton turbine, oblique blade impeller and the baffles used in the experimental part were used. The dimensions for each impeller were taken with the aid of the pachymeter and are set out in Table 1.

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Table 1. Dimensions of the oblique blade impeller and Rushton turbine

Component	Property	Oblique blade	Rushton
Blade	Number	4	6
	Length	17 mm	17.4 mm
	Width	10 mm	10.6 mm
	Inclination	45º	0º
Cube	Height	19 mm	21 mm
	Diameter	19.2 mm	18.7 mm
Ring	Diameter	-	28 mm

Figures 2 and 3 show, respectively, the tank with the oblique blade impeller and baffles and the tank with Rushton turbine and baffles.

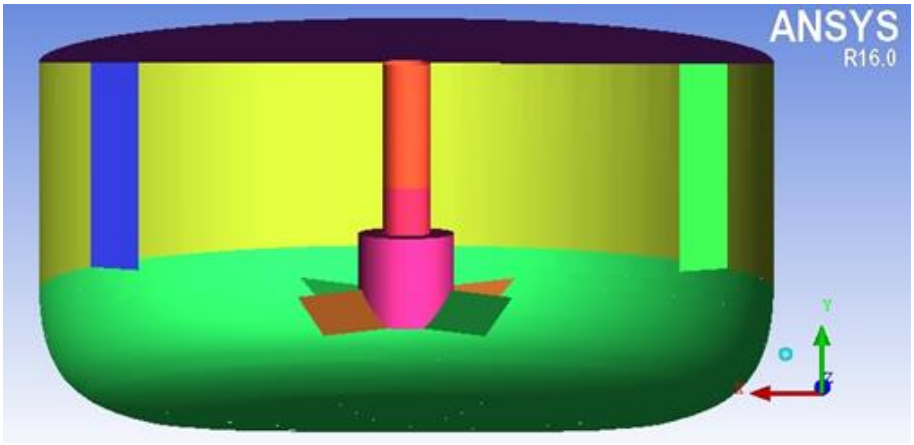

Figure 2. Tank with the oblique blade impeller and baffles

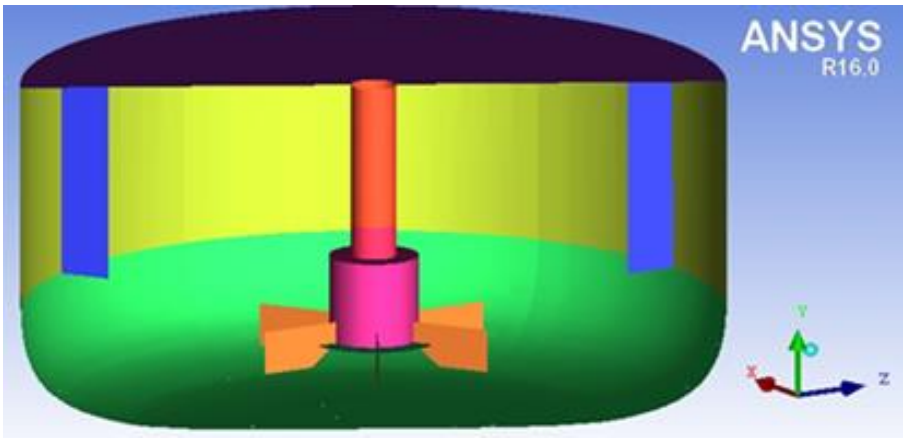

Figure 3. Tank with the Rushton turbine and baffles

The tank length measurements were taken with the aid of the pachymeter and are shown in Table 2. In the geometry only the useful volume of the reactor (filled by the reagents) was considered.

Table 2. Tank measurements

Property	Length (m)
Diameter	0.147
Height	0.078
Diameter of the shaft	0.0095
Width of the baffle	0.011

Two domains were used for tank geometry - one rotating domain (impeller) and one stationary domain for the remainder of the tank. To reduce computational effort, the geometries were made so as to represent a longitudinal section of the tank. In the case of the oblique blade impeller, which has 4 blades, in the presence of baffle, 6 baffles, an angle section equal to 180 ° was used. For the Rushton turbine, which has 6 blades, the angle was 60 °. Geometry and mesh were created in Ansys ICEM software 16.0.

To find a reasonable maximum element size, 1/20 of the tank height (approximately 10 cm), *i.e.* about 0.005 m, was considered. However, it is understandable that in regions such as the thin impeller blade, this element size is not suitable, so a smaller maximum size was used on smaller surfaces as a form of refinement. Then, 1/10 of the blade width (10 mm), or 0.001 m, was taken, which was applied to the blade, hub, stem and ring surfaces (in the case of the turbine). This surface refinement is propagated decreasingly by the surface mesh of other parts and by the volumetric mesh.

Hybrid meshes were used through the Tetra / Mixed method in ICEM. This method allows the generation of layers of prisms on the surfaces and cores of hexahedra. The mesh contains elements of maximum size equal to 0.005 (0.001 in smaller parts), 5 layers of prism in the surfaces and hexahedron core (hexacore), Table 3. The quality percentage less than 0.3 was less than 3% for the two meshes, which proves that the quality is satisfactory. The mesh

M2 does not have hexahedra because using this element generated several elements of poor quality. This may be associated with the fact that the height of the tank is smaller than the others (since we use the liquid level to generate the geometry), leaving less space between the blades and the wall so that automatically generated hexahedrons, which are not very versatile, could not be generated with good quality. The non-use of the hexahedron core should only influence the computational time and not the result obtained.

Table 3. Number of elements in the meshes

Mesh	Nº tetra	Nº hexa	Nº prysm	Nº pira	Nº nodes	%quality<0,3
M1	78181	1561	46135	3470	42519	1.880
M2	44629	0	15707	1030	17804	2.653

The simulations were conducted in Ansys CFX software. Considering that the simulations were performed in a transient state, the connection between domains Transient Rotor / Stator in the CFX-Pre was used.

The reference pressure used was 1 atm. The systems were considered monophasic, so a multicomponent reactive homogeneous mixture of variable composition was used, therefore the complete flotation model was used.

The RFR model was used and in relation to turbulence, the turbulence model k-ε was used. The reaction model used was the Combined EDM / Finite Rate Chemistry Model because it is more versatile and because it is understood that both the reaction rate and the agitation are important for the process.

To represent the initial condition, in which the oil and alcohol are separate phases with alcohol on top, a height-dependent step function was used. For boundary condition, the top of the tank was considered at atmospheric pressure, since the tank was not sealed.

Since it generally presents faster results, the simulations were done using local parallelization in 4 cores.

4 RESULTS

4.1 Kinetics

To obtain the kinetic data of the reaction of the soybean oil with methanol to produce methyl biodiesel of soybean, the yields in biodiesel were calculated in different times for each one of the reactions. Then, the mass fractions of soybean oil (x_o), methyl alcohol (x_a), methyl biodiesel (x_b) and glycerol (x_g) were calculated.

Table 4. Yields of the reactions with methanol

		M1	M2
Impeller		Oblique blade	Rushton turbine
Yield	0 min	0.0%	0.0%
	1 min	3.8%	5.2%
	2 min	9.6%	13.6%
	3 min	17.4%	22.2%
	5 min	32.3%	42.3%
	7 min	48.7%	59.7%
	10 min	69.6%	74.3%
	15 min	82.6%	88.0%
	20 min	87.8%	92.0%
	30 min	93.2%	95.7%
	40 min	94.0%	97.0%
	50 min	94.3%	97.4%
	60 min	94.5%	97.6%

The Tables 5 and 6 contain the data of the mass fractions for the reactions of transesterification with methanol.

Table 5. Data of the mass fractions for reaction M1

Time (min)	Oil (x_o)	Methanol (x_a)	Biodiesel (x_b)	Glycerol (x_g)
0	79.58%	20.42%	0.00%	0.00%
1	76.56%	20.09%	3.03%	0.32%
2	71.94%	19.58%	7.67%	0.81%
3	65.74%	18.90%	13.90%	1.46%
5	53.89%	17.60%	25.80%	2.71%

7	40.83%	16.17%	38.91%	4.09%
10	24.19%	14.34%	55.63%	5.84%
15	13.84%	13.20%	66.03%	6.93%
20	9.69%	12.75%	70.19%	7.37%
30	5.39%	12.27%	74.51%	7.83%
40	4.75%	12.20%	75.15%	7.89%
50	4.51%	12.18%	75.39%	7.92%
60	4.35%	12.16%	75.55%	7.94%

Table 6. Data of the mass fractions for reaction M2

Time (min)	Oil (x_o)	Methanol (x_a)	Biodiesel (x_b)	Glycerol (x_g)
0	79.58%	20.42%	0.00%	0.00%
1	75.44%	19.97%	4.15%	0.44%
2	68.76%	19.23%	10.86%	1.14%
3	61.92%	18.48%	17.73%	1.86%
5	45.93%	16.73%	33.80%	3.55%
7	32.07%	15.20%	47.71%	5.01%
10	20.45%	13.93%	59.39%	6.24%
15	9.53%	12.73%	70.35%	7.39%
20	6.35%	12.38%	73.55%	7.73%
30	3.40%	12.06%	76.51%	8.04%
40	2.36%	11.94%	77.55%	8.15%
50	2.04%	11.91%	77.87%	8.18%
60	1.88%	11.89%	78.03%	8.20%

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For the reactions with methanol, the best kinetics fit was the first order. The reaction velocity constant is calculated based in the decrease in the mass fraction of oil. The Equation 5.3.1.1 used for the first order fit was:

$$x_o = x_{oi}.e^{-k.t} \tag{6}$$

where:
x_o is the mass fraction of oil;
x_{oi} is the initial mass fraction of oil;
t is the time;
k is the kinetics constant.

The Table 7 presents the values of k for the reactions, the value of R^2 and RMSE. The value of k varies for the different reaction conditions. The correlation coefficient R^2 was equal or higher than 0.98 for all reactions, proving the strong relation between data and the fit. The root mean square error (RMSE) was smaller than 0.05 for all reaction, which is a relatively small error.

Table 7. Results of the kinetics fit for methanol

Reaction	Order	K	R^2	RMSE
M1	1	0.096	0.98	0.04342
M2	1	0.118	0.99	0.03525

4.2 Modeling

The Table 8 represents the results of the needed characterizations for the simulation of the reactions in Ansys.

Table 8. Properties of the biodiesel, oil and alcohol

	Viscosity (Pa.s)	Density (kg/m3)
Methyl biodiesel	0.004568	874.6
Soybean oil	0.040605	910.4
Methyl alcohol + catalyst	0.000719	803.5

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The Figures 4 and 5 show a comparison between the experimental and CFX results for the reactions M1 and M2, respectively. It is possible to observe that the data are very proximate, so the simulation represented the experimental data very well.

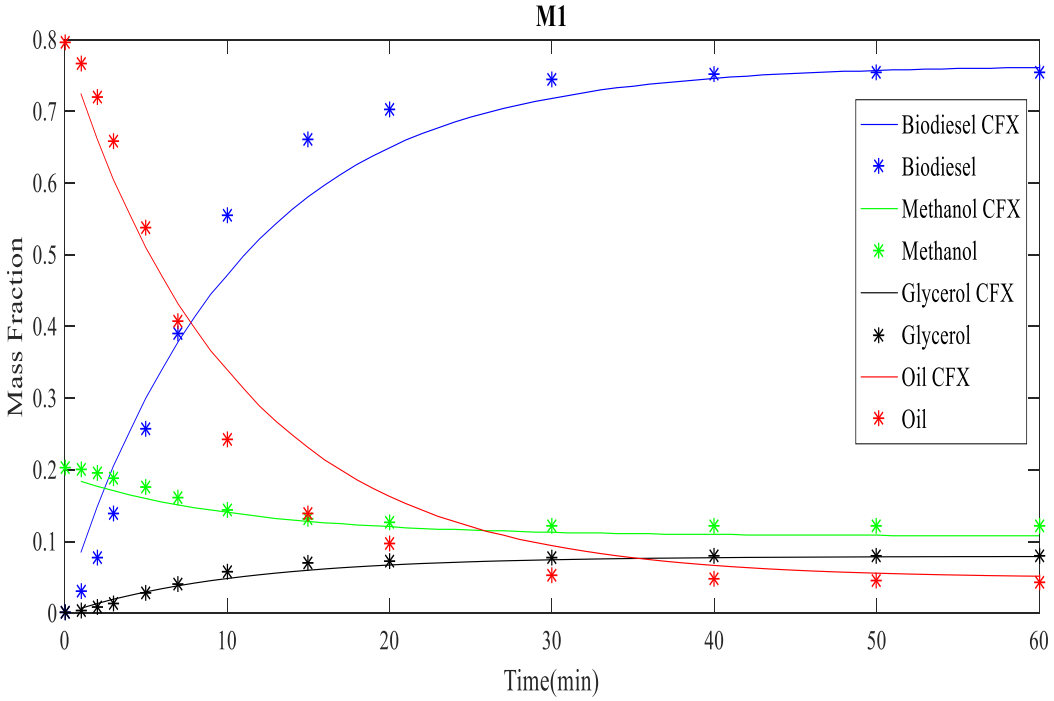

Figure 4. Comparison of the experimental and CFX mass fractions for reaction M1

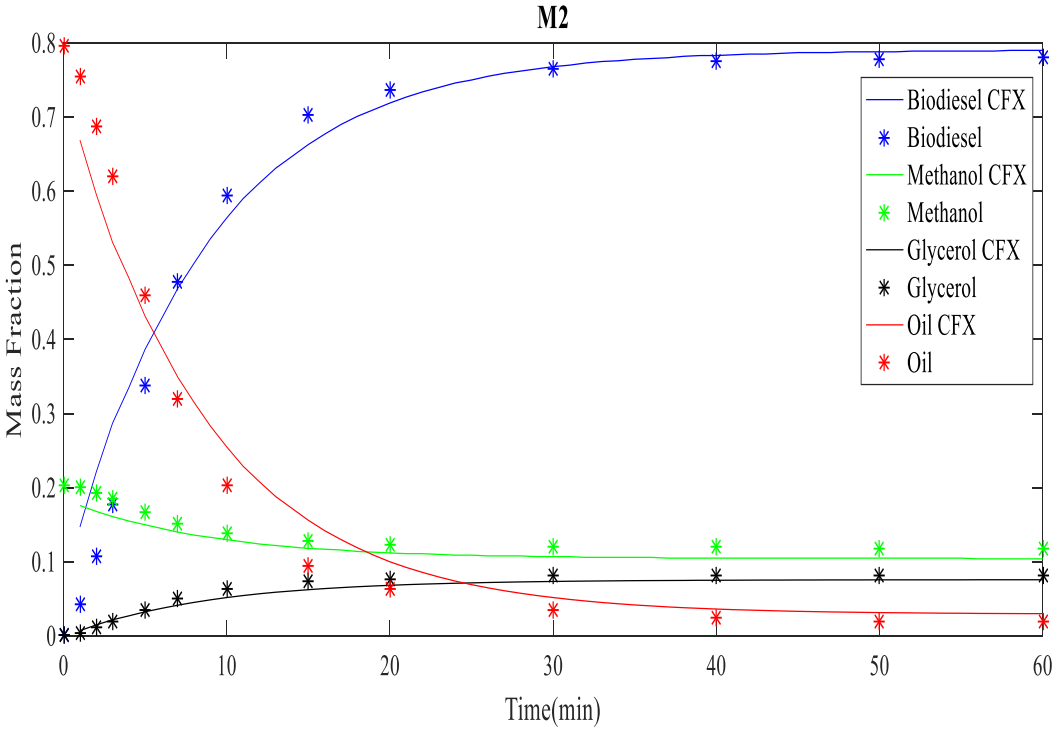

Figure 5. Comparison of the experimental and CFX mass fractions for reaction M2

The Figure 6 shows the graph for pressure of the reaction M1 at 60 minutes, which has an oblique blade impeller and the Figure 7 shows the graph for pressure for the reaction M2 at 60 minutes, which differs from reaction M1 only in the impeller type, which is Rushton turbine for M2. The tank with Rushton turbine shows a higher pressure when compared with the one with oblique blade impeller. For reaction M1, a higher pressure is observed in the inferior part of the tank near the wall and the baffles region, which is the region where the blade moves the fluid. The smallest pressure for M1 is under the shaft. On the other hand, the reaction M2 has mostly a constant pressure in the whole tank.

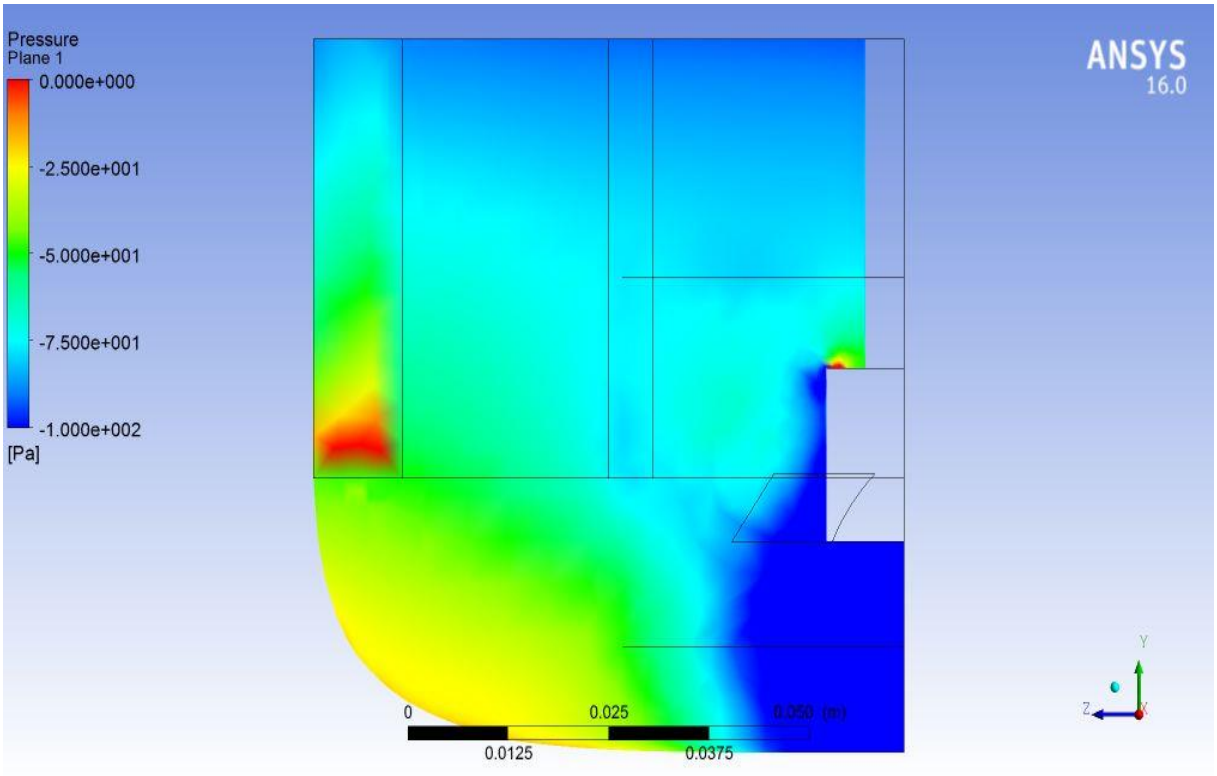

Figure 6. Pressure distribution for reaction M1

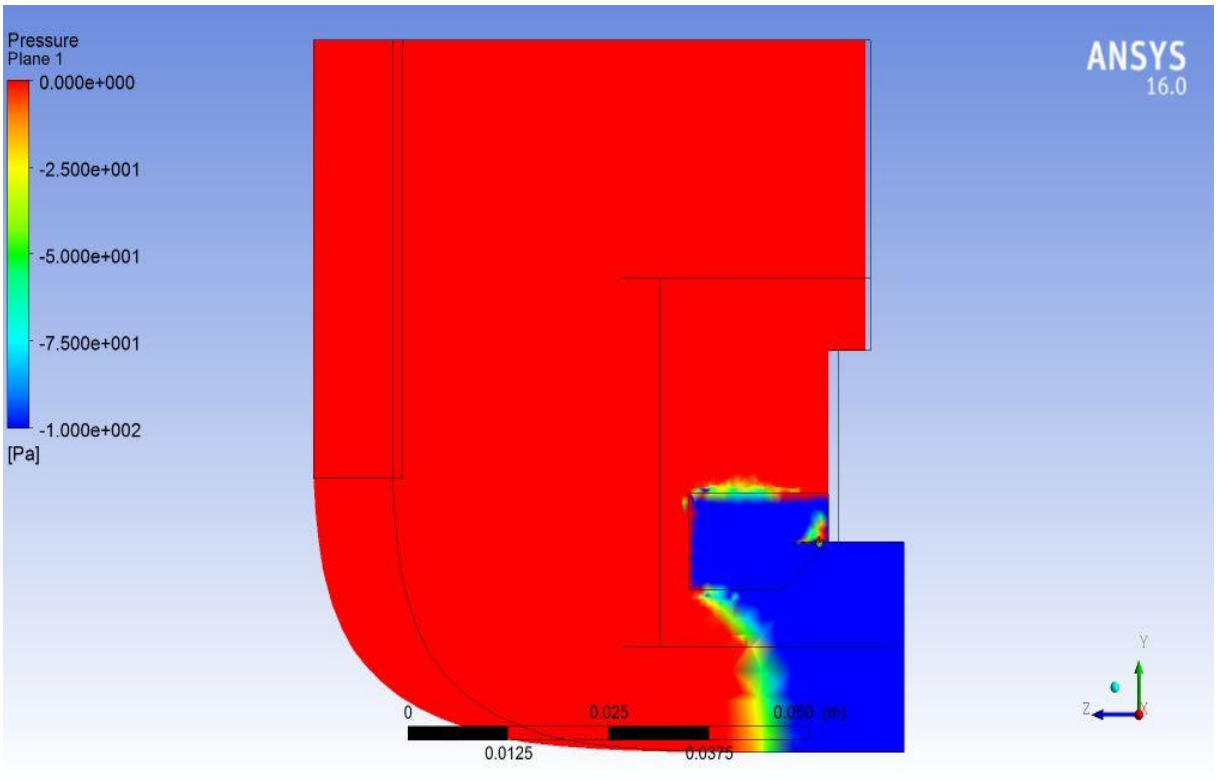

Figure 7. Pressure distribution for reaction M2

The Figures 8 and 9 show the velocity distribution for the 60th minute of the reactions M1 and M2, respectively. We can also see the direction of the fluid in the tank. For the reaction with the oblique blade impeller, M1, the flow is axial. In the case of the reaction with the Rushton turbine, M2, there is a radial flow.

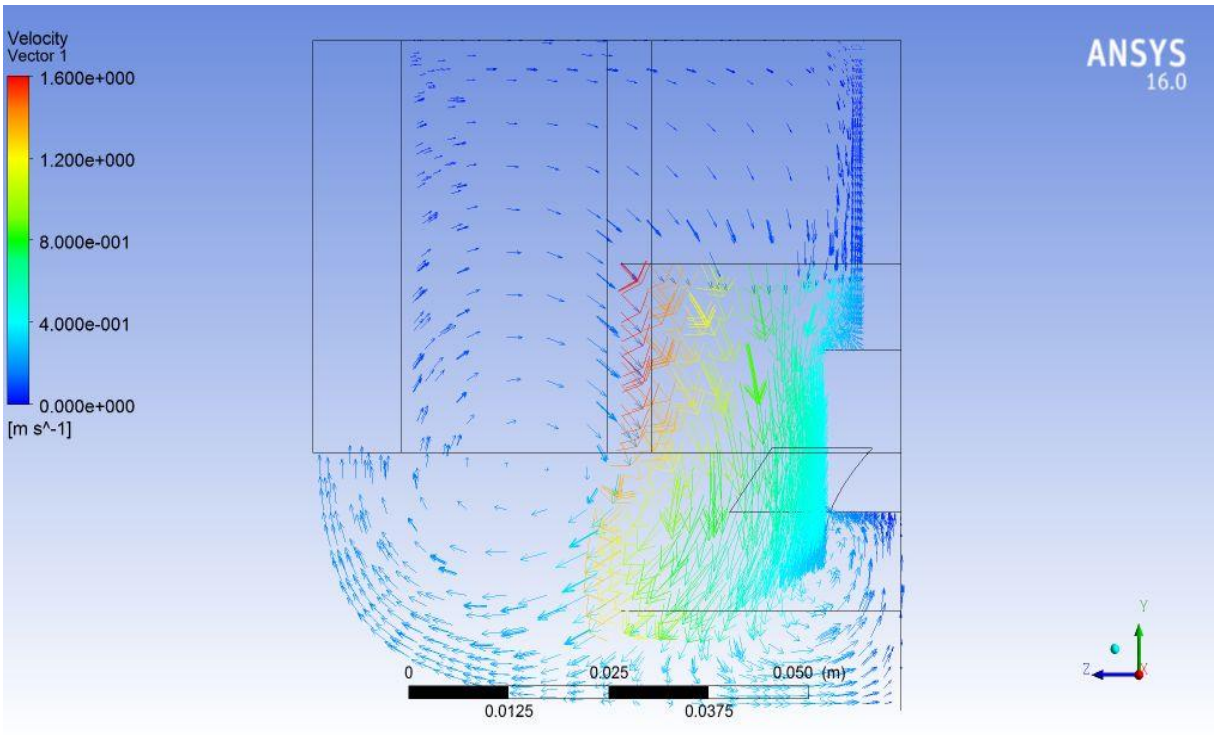

Figure 8. Velocity vectors field for the reaction M1

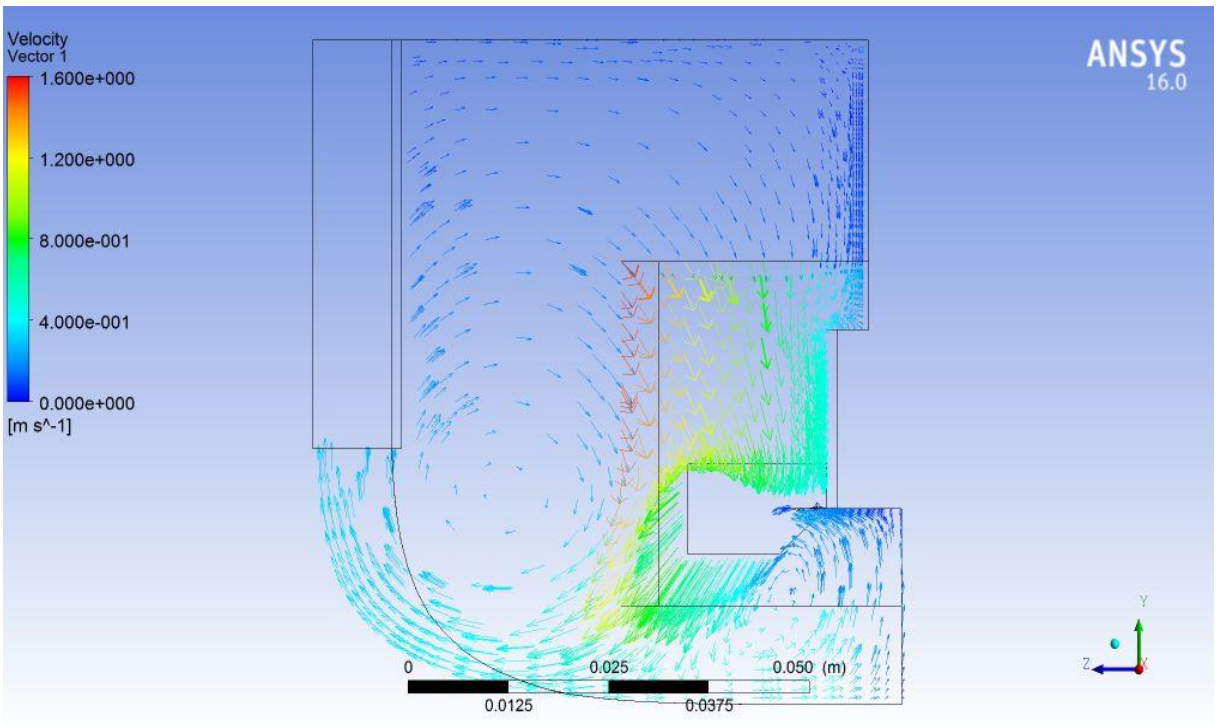

Figure 9. Velocity vectors field for the reaction M2

The Table 9 presents a comparative between the final yield obtained experimentally and the yield obtained in the simulation. The results were very proximate, but the simulated was always inferior to the experimental.

Table 9. Comparison of the experimental and simulated yields

Reaction	Experimental yield	Simulated yield
M1	94.5%	93.6%
M2	97.6%	96.3%

5 CONCLUSION

The kinetics for the reactions with methanol was found for different conditions. The kinetics was considered first order for methanol. The value of for the reactions was superior to 0.98, showing that the kinetic fit was satisfying.

The CFD tool offers several kinds of analysis and studies of a certain process. The necessary time to develop the models is compensated with a large amount of results obtained, from velocity vectors field and pressure gradients to kinetic data.

The experimental condition simulated represented very well the initial condition of the experiments. It was possible to observe the distribution of pressure in the tank. For the reaction with the oblique blade impeller, the highest pressure was verified in the inferior part of the tank, next to the wall. Although, in the tank with the Rushton turbine, the pressure was much more uniform in the whole tank.

When analyzing the velocity fields, it was possible to verify the direction of the fluid in both impellers, axial flux in the oblique blade impeller and radial flux in the Rushton turbine.

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