Experimental and Computational Investigation of the Combustion of Glycerol-Heavy Fuel Oil Emulsions

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Heavy fuel-oil-based emulsions show a great promise to become a viable alternative for heating facilities, especially for the proved decrease in pollutant emissions, which derives from the shortage of the flame and carbonaceous residue. Glycerol-heavy fuel oil emulsions are an important choice in handling both bio- and petro-residuals in an integrated management, obtaining energy with lower environmental impact. The main aim of this paper is to prove the feasibility of such combustion material, with the aid of both domestic heating unit and computational simulation of spray combustion model. In order to simulate the reactive flow inside the boiler, the finite-volume based commercial code FLUENT was used, testing the combustion relying on the mixture fraction, $k-\varepsilon$ turbulence and probability density function (PDF). The computational results enable a comparison between the heavy fuel oil and its glycerol-emulsified forms, which is in accordance with the experimental result obtained from the equipment used, recording a decrease in pollutant gas (SO$_2$, NO$_x$) in comparison with heavy fuel oil.

Keywords: emulsion, spray combustion, heavy fuel oil, glycerol

Recent economical and environmental constraints faced new problems arising from increasing amounts of by-products, such as glycerol from the biodiesel production and heavy fuel oil from petroleum processing. As the physical and chemical properties of these by-products depend on the preparation method, new possibilities for using them are needed, including the attractive option of energy production [1].

Direct use as fuels for various facilities of each of those by-products, glycerol and heavy fuel oil respectively, faced the difficulty of conventional atomization of such dense and viscous liquids on one hand, and the toxic gases released, on the other hand, represented by the acrolein in the case of glycerol and sulfuric oxides in the case of heavy fuel oil. Producing fuel emulsion by mixing these materials solves these aspects.

Few studies concern the use of glycerol and heavy fuel oil together in emulsions [1-3], as most work leads towards water emulsions [4].

Due to different polarities, glycerol and heavy fuel oil are slightly miscible, highly viscous and dense needing the addition of an emulsifier [3]. For spray combustion, the geometry of the emulsion droplet represents an important characteristic, which depends on the volume fraction of the disperse phase, and of the dispersion phenomenon [4,5].

A challenging task is to perform the numerical simulation of both heavy fuel oil and glycerol-heavy fuel oil emulsion combustion, due to the difficulties represented by gas-phase combustion (the need to model turbulence, combustion and radiation heat transfer), as well as the complex atomization, spray combustion, soot formation and also the fuel composition [4,5]. Therefore, few numerical studies of the combustion of heavy fuel oil and its emulsions have been published [4,5].

The modern commercial codes allow the simulation of complex geometries and phenomena using several reliable models, which, despite their limitations, offer a satisfactory perspective on both equipment and processes. The present paper presents the FLUENT simulation of the combustion of heavy fuel oil and glycerol-heavy fuel oil emulsions in a domestic boiler, which is in accordance with the experimental test carried out in the real equipment.

**Experimental part**

**Materials and methods**

**Emulsion preparation**

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Heavy fuel oil</th>
<th>5% Glycerol emulsified in heavy fuel oil</th>
<th>50% Glycerol emulsified in heavy fuel oil</th>
<th>95% Glycerol emulsified in heavy fuel oil</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density at 20°C, kg/m³</td>
<td>960.4</td>
<td>975</td>
<td>1180</td>
<td>1235</td>
</tr>
<tr>
<td>Dynamic viscosity, Pa·s</td>
<td>7.63</td>
<td>7.40</td>
<td>3.820</td>
<td>1.230</td>
</tr>
<tr>
<td>Flash point, °C</td>
<td>177</td>
<td>180</td>
<td>186</td>
<td>188</td>
</tr>
<tr>
<td>Freezing point, °C</td>
<td>-6</td>
<td>-7</td>
<td>-11</td>
<td>-14</td>
</tr>
<tr>
<td>Lower calorific value, kcal/kg</td>
<td>8160</td>
<td>8000</td>
<td>7439</td>
<td>4501</td>
</tr>
<tr>
<td>Total sulfur, %</td>
<td>1.501</td>
<td>1.425</td>
<td>0.752</td>
<td>0.072</td>
</tr>
<tr>
<td>Mereaptanie sulfur, mg R-SH/kg fuel</td>
<td>16.1</td>
<td>15.2</td>
<td>8.1</td>
<td>0.82</td>
</tr>
<tr>
<td>Asphaltenes, %</td>
<td>2.5</td>
<td>2.374</td>
<td>1.23</td>
<td>0.122</td>
</tr>
</tbody>
</table>

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Table 1

FUELS PROPERTIES
heavy fuel oil (557°C+ residue from Rompetrol), by 4 h, 1300-1500 RPM mechanical stirring at 70°C and atmospheric pressure.

**Combustion Experiment**

Combustion test was performed with a horizontal steel gas tabular boiler from Thermostahl, of three of burned gases with counter-pressure in the boiler furnace, suitable for both liquid and gas combustion. The main body of the boiler is manufactured from hot rolling inapprehensive steel sheets St 37-2. The cylindrical combustion chamber is 0.6 m in inside diameter and 1 m in length.

Figure 1 shows the arrangement of the boiler. The burner consists of a central atomizer, supplied by an electronically controlled pump which loads the fuel from a variable tank. In this experiment, a 30 kg storage tank was used.

![Fig. 1. Scheme of the domestic boiler](image)

**Table 2**

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal power, Mcal/h</td>
<td>50</td>
</tr>
<tr>
<td>Maximum working pressure, bar</td>
<td>4</td>
</tr>
<tr>
<td>Pressure drop, mm H2O</td>
<td>2...4</td>
</tr>
</tbody>
</table>

The boiler is based on the counter-pressure created by the returnable flame in the combustion chamber and by the transmission of heat with radiation. This returnable flame represents the evolution of three strokes boilers, achieved by the increase of the diameter of the fire box and the blocking of its outlet in the interior part of the boiler. The flame enters the combustion chamber and is surrounded by the reversed burned gases from the bottom of the fire box, so that the flame does not get into contact with the plates around the fire tube. The drops evaporation of atomized fuel is obtained from the heat of the burned gases, forming turbines at the surfaces where the flame and burned gases are separated resulting an intense fuel-air mixing and complete combustion with small amount of air excess. The returnable flame also presents an uniform charge of heat by radiation surface.

In order to avoid toxic acrolein emissions, characterized for glycerol combustion, the combustion chamber was previously heated up to 700°C using commercial diesel oil. Temperature acquisition was registered using a K-type thermocouple placed inside the combustion chamber, next to the atomization nozzle.

The NO estimations were predicted in a post-processing mode based on the numerical solution of the transport equations for nitric oxide (NO) and hydrogen cyanide (HCN). The main reactions governing the formation of thermal NO from molecular nitrogen are derived from the extended Zeldovich mechanism [3,6]:

\[
N + O \leftrightarrow NO + N_2 \quad (1)
\]

\[
N + O \leftrightarrow NO + O_2 \quad (2)
\]

\[
N + O + H \leftrightarrow NO + H \quad (3)
\]

All reaction rates were given by FLUENT database, for the case of NOx emissions.

**Computational Approach**

For the computational simulation, FLUENT commercial code was used. The spray combustion model contains a gas phase (an Euler steady model) and a liquid phase in the form of steady flux of particles which move and interact with the gas phase (heat and mass transfer in a Lagrange model). For the gas phase, the following equations are calculated: mass conservation (transport inside several chemical species), momentum balance, energy balance, turbulence model (standard k-ε model), and local combustion reaction (eddy-dissipation model).

In order to model the turbulence, the standard k-ε model was chosen. The disadvantage of this option derives from the assumption of isotropic turbulent viscosity and the assumptions made in ε-equation modeling, resulting in a less satisfactory estimation of the flow field for heavy fuel oil combustion case [5].

The combustion model was based on the conserved scalar (mixture fraction) and prescribed probability density function (pdf) approach, resulting the species mass fraction, temperature and density. The most difficult step in simulating the combustion of heavy fuel oil and its glycerol emulsions was represented by the boundary conditions, especially relating to the atomizing air inlet velocity.

The simulation domain is 2D, with a simple mesh representing an idealized combustion chamber, in which the fuel (heavy fuel oil and glycerol-heavy fuel oil emulsion, respectively) is injected together with air from the left and gases are released on the right side. The heavy fuel oil is modeled as C_{19}H_{30} molecule for both liquid and gas phase. As for the new material, glycerol-heavy fuel oil emulsion, a new database file was created, using the physical and chemical properties previously determined by experiments (named material G-HFO).

The liquid fuel combustion system considered in the computational simulation is a liquid spray of heavy fuel oil, glycerol-heavy fuel oil respectively, entering a 1 m length 2-dimension duct in which air is flowing at 650 K and 1 m/s. The Reynolds number, based on inlet conditions, is 100000 and the flow is turbulent. As the fuel evaporates, it enters the gas phase and reacts. The combustion is modeled using the mixture-fraction/PDF approach, with the equilibrium mixture containing 11 chemical species (C_{19}H_{30}, CH_4, CO, CO_2, H_2, H_2O gas and liquid, O_2, OH, solid C and N_2). The spray consists of 100 micron diameter liquid droplets injected at 300 K over a filled spray half-angle of 30 degrees on the duct centerline. The mass flow rate of fuel (heavy fuel oil and glycerol-heavy fuel oil combustion case [5].

The NO estimations were predicted in a post-processing mode based on the numerical solution of the transport equations for nitric oxide (NO) and hydrogen cyanide (HCN). The main reactions governing the formation of thermal NO from molecular nitrogen are derived from the extended Zeldovich mechanism [3,6]:

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\]

All reaction rates were given by FLUENT database, for the case of NOx emissions.
For SO$_2$, the mass fraction option was chosen, with the data for H$_2$S, S$_2$O, SO, and SO$_2$ species available in the commercial code.

**Results and discussions**

Experimental tests, shown in table 4, revealed an important decrease of pollutant emissions, of 12-20% in the case of NOx, and 5-95% in the case of SO$_2$, respectively. The phenomenon is due to the mixing with glycerol, which led to a decrease in nitrogen and sulfur content in the furnace feed, resulting in a lower combustion temperature. Hence, the NO$_x$ formation mechanism changed and thermal and fuel nitrogen, as well as sulfur oxides mechanism, had lower reaction rates. From the same reason, real test also showed a decrease in the temperature of the exhaust gas, and an increase in CO$_2$ with simultaneous decrease in CO, indicating lower soot formation. The whole improvement was also caused by the previous heat of the combustion chamber with diesel oil, done for preventing the acrolein formation.

Computational test confirmed that heavy fuel oil droplets evaporate quickly close to the burner. The predicted temperature distribution with the k-å model for 5% glycerol and 95% heavy fuel oil is shown in figure 2. Temperature measurements are available in table 5. Accordance could be easily observed.

Soot did not have a great effect on the temperature fields, and no comparative graphical representation could be conclusive. The local decrease in temperature was found to be of 30% in the same zone, inversely proportioned with the increase of glycerol content from zero to 95%, for both experimental and computational tests.

<table>
<thead>
<tr>
<th>Output</th>
<th>Heavy Fuel Oil U.M.</th>
<th>Emulsion 5% glycerol</th>
<th>Emulsion 50% glycerol</th>
<th>Emulsion 95% glycerol</th>
</tr>
</thead>
<tbody>
<tr>
<td>O$_2$</td>
<td>% 18.4</td>
<td>17.2</td>
<td>14</td>
<td>12</td>
</tr>
<tr>
<td>CO+</td>
<td>0.003</td>
<td>0.003</td>
<td>0.002</td>
<td>0.001</td>
</tr>
<tr>
<td>Gas temperature</td>
<td>°C 315</td>
<td>310</td>
<td>305</td>
<td>300</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>% 2</td>
<td>2.5</td>
<td>3.5</td>
<td>3.5</td>
</tr>
<tr>
<td>NO</td>
<td>ppm 70</td>
<td>62</td>
<td>57</td>
<td>51</td>
</tr>
<tr>
<td>NO$_2$</td>
<td>ppm 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>SO$_2$</td>
<td>ppm 17</td>
<td>12</td>
<td>10</td>
<td>4</td>
</tr>
<tr>
<td>SO$_3$</td>
<td>ppm 70</td>
<td>62</td>
<td>57</td>
<td>54</td>
</tr>
<tr>
<td>Lambda</td>
<td>8.08</td>
<td>5.81</td>
<td>4</td>
<td>3.42</td>
</tr>
<tr>
<td>Air temperature</td>
<td>°C 22.1</td>
<td>23</td>
<td>22.5</td>
<td>22.2</td>
</tr>
</tbody>
</table>

**Table 4**

**GAS ANALYSIS RESULTS**

<table>
<thead>
<tr>
<th>Observation</th>
<th>Heavy Fuel Oil</th>
<th>Emulsion 5% glycerol</th>
<th>Emulsion 50% glycerol</th>
<th>Emulsion 95% glycerol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flame temperature</td>
<td>°C 1317</td>
<td>1278</td>
<td>1181</td>
<td>1051</td>
</tr>
<tr>
<td>Flame color</td>
<td>dark orange</td>
<td>light orange</td>
<td>light orange</td>
<td>light orange</td>
</tr>
<tr>
<td>Flame size</td>
<td>Normal</td>
<td>Shorter/thinner</td>
<td>Shorter/thinner</td>
<td>Shorter/thinner</td>
</tr>
</tbody>
</table>

**Table 5**

**VISUAL OBSERVATION DURING THE COMBUSTION EXPERIMENTS**

![Fig. 2. Static temperature contour of 5% glycerol-95% heavy fuel oil combustion](image)

![Fig. 3. Static temperature plot for the combustion simulation of 95% glycerol-5% heavy fuel oil mixture](image)
Computational distribution of the species molar fractions along the furnace gave a satisfactory approximation for the experimental case, though certain discrepancies were expected in the predicted molar fractions the $k$-$\varepsilon$ model in the vicinity of the furnace axis and near the burner. Altogether, the representation of the chemical species, calculated with the mentioned fuel flow rate, helped a better understanding of the complex phenomenon of combustion. Figure 4 shows the mass fraction of the emulsified fuel containing 95% glycerol represented on the furnace axis.

As for the gases formed during the combustion, the simulation did not show any difference from the experimental tests. Most of the NO was derived from the fuel, just as $\text{SO}_2$. The predicted concentrations for both chemical species did not vary from the experimental results.

Conclusions

Glycerol-heavy fuel-oil-based emulsions proved to be a viable alternative for heating facilities, due to the decrease in pollutant emissions, which derives from the shortage of the flame and carbonaceous residue. It also represents a wise choice of both bio- and petro-residual integrated management.

This work proved the feasibility of such combustion material, with both experimental and computational means. Accordance was found between combustion tests of the heavy fuel oil and its glycerol-emulsified forms, while showing a decrease in temperature from approximately 1300 to 1050°C, in NO of 12-20%, from 5 to 95% glycerol, and a decrease of 5-95% for $\text{SO}_2$ for increasing glycerol content from 5 to 95%.

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