Microfluidic Dynamics coupled with Populational Balance Equations to further describe Water/diesel Microemulsions.

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Abstract

Reducing the environmental impact of pollution emissions stemming from diesel engine combustion is a pressing concern. One promising approach is the utilization of water/diesel (W/D) microemulsions that mitigate pollutant emissions due to the microexplosion process. It also elevates combustion efficiency, improves the piston performance, and does not require adaptations on the engine. In a novel work, a phenomenological model was developed to produce (W/D) microemulsions through mechanical agitation aided by emulsifiers. This methodology effectively characterizes the distribution of water droplets through a population balance evaluation, and it allows a precise depiction of the micrometric scale through a refined model. However, a shortcoming of this approach is that the vessel geometry cannot be accounted by only using a populational balance methodology. Therefore, this study aims to apply microfluidics concepts together with the population balance equations. The computational fluid dynamic (CFD) studies were conducted in Ansys Fluent software and the partial differential equations related to the population balance were coupled in the simulation. The mathematical model approach and the software developed in Python were validated by comparing the results obtained with other computational/experimental data. It is worthwhile highlighting that the proposed simulation described in more detail the emulsification process and the impact of the vessel’s geometry could be evaluated.

**Keywords**: Computational fluid dynamics, Population balance, Breakage functions, Fuel upgrading.

* 1. Introduction and objective

The main advantages of diesel engines are their high energy efficiency, allowing for their use in heavy vehicles. However, the main disadvantage of diesel combustion is the high emission of polluting gases. (Debnath et al., 2015). Especially the nitrogen monoxide (NO) reaction, which occurs at temperatures around 1300 °C (Equation 1) (Driscoll, 1997).

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| --- | --- |
| $$N\_{2}+O\_{2}\rightarrow 2NO (T\~1300°C)$$ | (1) |

The emission of nitrogen monoxide can be prevented by lowering the combustion temperature. However, this can affect the engine's performance. Consequently, efforts are made to employ techniques that reduce the temperature without compromising engine efficiency. Diesel upgrading by using a water microemulsion is an effective method to decrease pollutant emissions. This process involves a microexplosion, which lowers the combustion temperature due to the water vaporization's endothermic nature (Patel and Dhiman, 2021).

The water/diesel (W/D) microemulsions can be formed through various processes, but agitation coupled with emulsifiers stands out (Supriyanto et al., 2021). The manufacturing of this microemulsion depends on the operational and physical variables of the process, and these can influence the engine efficiency and pollutant emissions. Experimental tests were employed to examine the W/D microemulsions and their combustion, but there was limited exploration into the formulation of phenomenological models. Recently, an article addressed the use of modeling based on population balances to describe the formation of W/D microemulsions through mechanical homogenization using the Python programming language (Khouri et al., 2023). In general, Khouri et al. (2023) considered the following hypotheses to model the micro-droplets of water in diesel:

* Use of a simplified population balance (Figure 1)
* Test of two breakage functions (g(v)) applied to emulsions consolidated in the literature (Coulaloglou and Tavlarides, 1977; Andersson and Andersson, 2006) to determine the most suitable for the water/diesel system.
* Numerical solution by the Discrete Method.



**Figure 1:** Simplified populational balance and its considerations.

As modeling results revealed, the breakage function by Coulaloglou and Tavlarides (1977) is suitable only for emulsions at larger scales. Additionally, the breakage model by Andersson and Andersson (2006) did not represent any of the data sets (micrometric and nanometric) – this unsatisfactory result stems from limitations in the model, where only the breakage of millimetric droplets is represented. Therefore, an adjustment was made to the second model to depict the breakage of micrometric droplets. Consequently, the adjusted model yielded reasonable results.

Expanding the models of the W/D system are important, as the combustion process and pollutant emissions can be analyzed in more depth after developing a tool that further describes this formation. Advancements in phenomenological studies can be achieved by extending the modeling through computational fluid dynamics (CFD). Thus, the scope of this work focused on the application of CFD coupled with population balances (PB) in the Ansys Fluent to simulate an agitation system that produce a W/D microemulsion. By using simulation techniques with CFD, the direct influence of the system's geometry and fluid viscosity could be evaluated, addressing limitations of the methodology that solely relies on population balance equations (Becker et al., 2014).

* 1. Methodology

The simulation was performed in the Ansys V14.5 software, and the objective was to compare it with the results obtained by Khouri et al. (2023). The operational and physicochemical conditions of W/D emulsion homogenization used in this work are described by Table 1 (Dataset A).

**Table 1:** Dataset A (Rastogi et al., 2019) conditions and results of the W/D microemulsification.

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| --- | --- |
| **Water volume fraction** | 5.3% (v/v) |
| **Emulsifier composition** | 50% Tween© 80 + 50% Span© 80 |
| **Interfacial tension** | 3.8 × 10-3 N/m |
| **Mixing time** | 2 min |
| **Rotational speed** | 2500 rpm |
| **Dispersing element diameter** | 8 mm |
| **Temperature** | 25°C |
| **Final droplet size diameter** | 6 ± 2 μm |

Initially, the geometries were constructed in CAD (computer-aided design) format using the *Design Modeler* environment. According to the information from Dataset A, the process was conducted in a 10 mL glass vial with a mixing element of 8 mm. Therefore, a cylinder with a diameter of 20 mm and a height of 50 mm was used to represent the glass vial, along with an impeller of a diameter equal to 8 mm. Additionally, in the region around this impeller, a cylinder was added to define and characterize the rotation in the subsequent steps. In other words, the geometry was separated into two cell zones: a stationary domain (outer\_fluid) and a mixing domain (inner\_fluid).

Next, the system mesh was generated by discretizing the geometry in the *Meshing* environment. Micro-mixing systems can be described using tetrahedral elements using cells in the order of 6.105 (Shiea et al. 2022). The Advanced Size Function was set to 'On: Proximity and Curvature' to refine mesh quality. The sizing specified for this geometry is detailed in Table 2. Skewness and orthogonality criteria were considered to assess the quality of the generated mesh. Skewness quantifies the shape of the elements to determine if they possess an equilateral property. Ansys recommends that the skewness must be lower than 0.95. Orthogonality evaluates the angle of the faces/edges of the elements. In the simulator, orthogonal quality varies in values from 0-1, and it is recommended to use values greater than 0.1.

**Table 2:** Mesh sizing information and characteristics.

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| --- | --- |
| **Num Cells Across Gap** | 3 |
| **Min Size** | 4×10-3 mm |
| **Proximity Min Size** | 4×10-3 mm |
| **Max Face Size** | 0,4 mm |
| **Max Size** | 0,8 mm |
| **Growth Rate** | 1,2 |
| **Minimum Edge Length** | 0,250 mm |
| **Inflation** | Program Controlled |

After the mesh generation, the CFD simulation can be implemented in *Fluent*. In summary, the setup used was:

* **General:** transient and gravity of -9.8 m/s².
* **Models:** Multiphase (Eulerian), Viscous (Standard k-epsilon), Population Balance (Discrete).
* **Materials/Phases**: diesel (first phase) and water (second phase).
* **Cell Zone conditions:** Mesh motion = 2500 rpm in the mixing domain (inner\_fluid).
* **Mesh interfaces** – contact region between the stationary (outer\_fluid) and mixing domain (inner\_fluid).
* **Boundary conditions** – none, due to the transient state (i.e., no inlets or outlets were defined).
* **Solution Methods** – Phase Couple SIMPLE.
* **Solution Initialization** – Gauge pressure = 1 atm, Water volume fraction = 0.053, 0-bin fraction = 1, Time step size = 1s, Number of steps = 120, Max iteration/time step = 100.

The population balance was included through the 'addon-module' present in the Fluent library. To use this module, it was necessary to activate the Multiphase (Eulerian) model. The population balance was solved using the discrete method to compare with the results obtained by the baseline study (Khouri et al., 2023). The breakage function used was the Luo model, considering the influence of interfacial tension – an important parameter for the system (Khouri et al., 2023). Flow definition and calculation of its parameters were also developed at this stage. It was observed that the turbulence in systems with homogenization could be adequately represented by the k-epsilon model (Becker et al., 2014). After defining the operational and physical variables according to Table 1, it was possible to obtain the results of the CFD simulations.

* 1. Results and Discussion

The mesh generated from the data in Table 2 successfully met all the necessary criteria to ensure its quality (Table 3). In other words, the generated elements were above the order of 105, the maximum skewness was below 0.95, and the minimum orthogonality was above 0.1. The average and standard deviation of the skewness and orthogonality were also within reasonable values for the system's application.

**Table 3:** Mesh statistics and quality parameters.

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| **Nodes** | 303886 |
| **Elements** | 1402469 |
| **Min Skewness** | 1.182×10-6 |
| **Max Skewness** | 0.848 |
| **Average Skewness** | 0.227±0.122 |
| **Min Orthogonality** | 0.183 |
| **Max Orthogonality** | 0.999 |
| **Average Orthogonality** | 0.867±0.088 |

The CFD simulation obtained a water droplet distribution of 3.698±1550 μm(Figure 2). The residual values during the iterations had a transient behavior. In the final set, the continuity presented a residual of 3×10-5 and the bin-fractions residues were in the order of 10-4, indicating an acceptable convergence. The performance of the Luo-model to describe the formation of W/D microemulsions has a Standardizes Mean Difference 1.312 in comparison to the only‑population balance model (Khouri et al. 2023).

**Figure 2:** Population distribution of the water droplets in the CFD simulation.

Thess results reflects the potential in using Ansys to represent the W/D microemulsions, but further studies should be conducted to improve the results. A suggestion is to implement the adjusted model in the breakage kernel by using a User-Defined Function (UDF). The challenge to apply this UDF is that Ansys only accepts coding in C language. Therefore, the adjusted model must be re-structured and adapted since its original format is in Python. Other improvement that could be employed in this case, is to use the Standard Method of Moments (SMM) to achieve a convergence in a shorter processing time. The Discrete solution method can be computationally exhausting to systems that require a more refined distribution to be represented, (i.e., number of bins).

* 1. Conclusion

Therefore, the Ansys Fluent software is a capable approach to describe the behavior of W/D microemulsion by using the Population Balance available in the “addon-module”. The proposed simulation described the emulsification process more adequately by considering the impact of the vessel’s geometry and the mixture viscosity. Further studies could implement an UDF to represent the breakage and solve by the SMM to refine the results.

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