Hydrodynamic cavitation of heavy crude oil in Vortex reactor using computational fluid dynamics

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Abstract. The improvement of the physicochemical properties of heavy crudes for their better use has brought the application of new technologies and processes to the oil and gas industry. Hydrodynamic cavitation consists of cavitating the working crude oil as it passes through a reactor, which operates with specific process parameters such as flow rate, hydrogen donor percentage, and temperature. In this work, we will focus on the effect of temperature on the fluid dynamics of the crude oil inside the Vortex reactor. The process started with a 3D steady-state, multiphase liquid-vapour fluid flow modelling with k-ε turbulence model and Schnerr-Sauer cavitation in Ansys Fluent software. The results obtained for the different operating temperatures in the range of 92 °F to 350 °F allowed us to analyse the behaviour of the fraction of vapour generated by cavitation. The amount of vapour produced in the reactor increased notably when a certain temperature value of the crude oil is reached, and the vortex effect becomes stronger in the fluid dynamics of the crude oil. To have a better understanding of the physical phenomena, the possibility of further investigation of this equipment with different crude oils and operating parameters is open to determine the optimal operating points of the hydrodynamic cavitation nano reactor.

1. Introduction

Cavitation occurs when the pressure of fluid drops below the vapour pressure, generating microbubbles of vapour that subsequently collapse. Designing an experiment involving cavitation, different parameters such as flow velocity, pressure and temperature must be identified [1], as in the reactor design process, where operating parameters and geometry alter the bubble dynamics [2]. The effect of temperature on cavitation has been studied using water at different temperatures to evaluate the erosion of an aluminium plate due to bubble collapse, and it was found that erosion is observed at 60 °C [3]. In another study using different operating parameters, a relationship between bubble dynamics and the fluid temperature was found [4].

Recently, cavitation has been used to improve industrial processes by implementing new acoustic cavitation and hydrodynamic cavitation technologies. The latter has been the most relevant in engineering and agribusiness projects due to its ability to generate cavitation over large areas of the fluid and the wide range of physical and chemical effects it produces [5]. Some studies on the synthesis of biodiesel from waste cooking oil using hydrodynamic cavitation have shown a reduction in reaction times, improved energy efficiency and the development of an easily scalable process [6].
Due to their simple geometry and easy experimental setup, venturi tubes have been used for experimental and numerical studies of cavitation. Among these studies are the effect of the variation of the convergence angle of the venturi tube on the fluid [7], the theoretical-experimental study of venturi geometries for different cavitation stages and zones [8], the comparison of turbulence models, Large-Eddy Simulation (LES) and Reynolds-Averaged Navier-Stokes (RANS) [9], the validation and calibration of steady-state and transient cavitating flow models [10], and the comparison between experimentally measured velocity profiles and pressure fluctuations with values obtained from computational fluid dynamics [11].

Mathematical and numerical models are extensively used to model physical phenomena for engineering applications in the oil and gas industry [12-14], and such models describing phase change and bubble behaviour can be used to simulate cavitation. One of the most used models is the Singhal method, also known as the full cavitation model, as it describes the formation and transport of bubbles, turbulent fluctuations, and the magnitude of non-condensable gases [15]. Another commonly used model is the Schnerr-Sauer method, which is a combination of the volume of fluid (VOF) technique and a model that predicts bubble growth and collapse [16].

The hydrocarbon industry has found several applications for the use of cavitation in crude oil refining processes, including enhanced recovery, water de-emulsion in crudes, desulphurization and crude oil upgrading [17]. Regarding the upgrading of heavy and extra-heavy crudes, hydrodynamic cavitation and acoustics have become attractive from an industrial point of view, where several aspects have been addressed, such as viscosity reduction, an increase of American Petroleum Institute (API) grade, reduction of asphaltenes, sulphur and metals. Despite the research carried out, there is still a lack of work to make this method profitable at an industrial level [18]. Studies on viscosity reduction in propanediol show that the capacity and efficiency of hydrodynamic cavitation processes are highly associated with the operating parameters [19].

2. Materials and methods

The numerical model was developed in 3D, as vorticity effects are considered. The geometry used was obtained using SpaceClaim, which allows the extraction of the control volume of a solid, this geometry can be seen in Figure 1(a). The selection process of the multiphase flow, cavitation, turbulence and discretization models was done through a literature review, considering an experimental study on cavitation in injectors [20]. Thanks to this study, several authors were able to compare their simulations on the cavitating flow [21-24].

Figure 1. Inner volume of the reactor. (a) isometric view; (b) front view.

The mixture model was chosen, as it is recommended for the type of flow where there is a liquid-gas interaction, where the gas is in the form of bubbles. Moreover, it has a lower computational cost than the Eulerian model, which also works for this type of flow. The cavitation model used is the Schnerr-
The Sauer model, which is numerically more robust and faster to converge than the others. In addition, this model does not consider the effect of non-condensable gases dissolved in the liquid at the inlet.

A stationary simulation was used since the importance of this work is not in the study of the bubble dynamics but the general behaviour of the fluid in cavitation. The turbulence model selected was the Realizable k-epsilon, which has better numerical performance compared to the standard k-epsilon, and its computational cost is not as high as that of an LES model. Since viscous effects near the wall are not very relevant, Standard Wall Functions were used to decrease the computational cost [21].

Two pressure boundary conditions were imposed based on operating conditions, one at the flow inlet and one at the flow outlet. In addition, the walls were treated as Wall, so, they have the condition of no-slip and zero flow through them. The pressure values taken for each model are shown in Table 1.

Table 1. Pressure boundary conditions for each model based on operating conditions.

| Model | Temperature (°F) | Inlet pressure (psi) | Outlet pressure (psi) |
|-------|------------------|-----------------------|-----------------------|
| 1     | 92               | 360.0                 | 14                    |
| 2     | 140              | 335.0                 | 14                    |
| 3     | 180              | 325.0                 | 14                    |
| 4     | 250              | 308.6                 | 14                    |
| 5     | 350              | 293.0                 | 14                    |

A mesh independence study was performed. To achieve this, the velocity values on a characteristic S line, shown in Figure 1(b), were obtained by interpolating the solution in 100 points, as shown in Figure 1. Five meshes with a number of elements between 1,179,758 and 8,474,211 were evaluated. As can be seen in Figure 2, as the mesh is refined, different values of velocity on the S line are obtained, and the behaviour of the curve also changes. However, between mesh 4 and mesh 5 there is no longer a considerable difference, therefore, we chose mesh 4 with 6,764,078 elements to perform the analysis.

Figure 2. Mesh independence.

Once the mesh was defined for the simulations, three quality parameters were evaluated: aspect ratio, skewness, and orthogonal quality. The minimum, maximum, and average values of these are shown in Table 2. As can be seen, the mesh has a good quality in all three parameters.

Table 2. Mesh quality parameters.

| Metric             | Minimum value | Maximum value | Average value |
|--------------------|---------------|---------------|---------------|
| Aspect Ratio       | 1.002         | 29.267        | 2.661         |
| Skewness           | 8.832E-9      | 0.799         | 0.166         |
| Orthogonal quality | 0.200         | 1.000         | 0.857         |

3. Results
The main variable of interest in the simulation is the vapour fraction since the viscosity reduction in the crude oil depends on it [21]. Figure 3 shows the isosurfaces for a value of 0.2 of the vapour fractions at temperatures of 180 °F and 350 °F since from this temperature onwards the amount of vapour is significant. Notice that there is an increase in the vapour fraction as the temperature increases, this is...
because the viscosity of the liquid decreases and, therefore, there is an increase in its velocity inside the reactor, which generates greater pressure drops. Thus, depending on the temperature, vapour can be generated in four different zones, each of these zones is marked with a number.

![Figure 3. Vapour fraction 0.2 isosurfaces for different temperatures. (a) 140 °F; (b) 350 °F.](image)

Zone 1 and zone 2 correspond to a type of cavitation that occurs when there is a sudden reduction in cross-sectional area and a change in the flow direction, which can cause a separation of the boundary layer from the walls of the reduction and create what is known as a vena contracta. The cavity created between the walls and the vena contracta is called the recirculation zone [25]. This phenomenon can be seen in an experiment performed on an injector nozzle, where a similar type of cavitation is generated, as the flow is sharply diverted [26]. In addition, due to the reduction of the area, the fluid accelerates, causing the static pressure to drop below the vapour pressure and cavitation is generated [25].

Zone 3 and zone 4 correspond to cavitation generated by a vortex. The vapour is generated in the centre of the vortex, as this is where the minimum pressure zone is located. This zone is created because of the centrifugal force created by the rotation of the fluid. This phenomenon occurs mainly in the suction tubes of Francis turbines [27].

To have a better understanding of the problem, the total vapour volume for different temperatures is shown in Table 3. The minimum value was obtained at 92 °F since no vapour was generated there, and the maximum value was 1.507 cm³ at 350 °F. These values can be contrasted with the isosurfaces shown in Figure 3. The first 3 temperatures do not have significant amounts of vapour, because cavitation zone 1 and zone 2 generate less vapour volume and the vortex zones of the reactor are not used correctly, which, as can be seen in the isosurfaces, is where most cavitation is generated.

| Temperature (°F) | Vapour volume (cm³) |
|-----------------|---------------------|
| 92              | 0                   |
| 140             | 0.0002              |
| 180             | 0.0068              |
| 250             | 0.1621              |
| 350             | 1.5070              |

4. Conclusions
The final mesh selected by a mesh independence analysis has 6764078 elements, with maximum values of 29.267 and 0.799, for the aspect ratio and skewness parameters, respectively, and a minimum value of 0.2 for the orthogonal quality parameter, all parameters are within the desirable range of a good mesh quality for computational fluid dynamics models.
The fluid dynamics of the heavy crude oil shows the behaviour of the volume of vapour generated when passing through the Vortex reactor, where the cavitation zones are mainly due to the abrupt reduction of the cross-sectional area and the formation of vortices. As the temperature of the crude oil increases, these are the first zones where cavitation is generated, however, their contribution in volume is reduced compared to the vortex cavitation zones.

Using computational fluid dynamics, the behaviour of the crude oil through the hydrodynamic cavitation nano reactor at different temperatures was simulated to evaluate the behaviour of the vapour fraction due to cavitation. It was found that in the temperature ranges from 92 °F to 180 °F the vapour volume did not exceed 0.00685 cm³, however, at 350 °F the vapour volume rises significantly up to 1.507 cm³.

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