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Numerical Validation of a Pressurized Batch Reactor for In-Situ Transesterification

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Abstract. Subcritical in-situ transesterification is one of the more recently developed processes that consumes less energy and is more environmental friendly than conventional methods. Diving deeper into this process, the fluid dynamics of the liquid mixture is an area of interest not studied before due to the solid, thick metal enclosure of the reactor vessel. Previous studies observed that the mixing characteristics of the agitator being used influences biodiesel yield. As commercialization of this biofuel production process is of importance in order to contribute to biofuel demand in a nation-wide scale, this study considers a reactor vessel working volume of around 1.5L, which is relatively larger than typical laboratory batch-type sizes. A numerical validation study, through mesh analyses, was performed to produce a numerically accurate model for the study. Factoring in computational time and accuracy of the solution, a steady state, multiphase model running the standard k- ϵ turbulence model was chosen. The Multiple Reference Frames approach was used for the steady state condition to be met. The validation model is of a 6.3L-volume cylinder with baffles. Glass beads served as the solids and water as the liquid in the system. The first mesh analysis was performed by comparing 11 unique mesh models. The model with a relevance of fine 30 was seen to have the closest data fit with the experimental data. It was seen that only when using the size function 'proximity' showed a slightly different velocity profile among the models. The second mesh analysis was conducted to check if the chosen mesh setting would affect this study's smaller reactor geometry before the main study's simulations are to be conducted. The model with baffle's percent error at the specified point was at an acceptable 8.2%, and its resultant velocity profile's is at 23.5% which is around the same range as that of the 1st mesh analysis' models. With this, the numerical model developed was deemed to be applicable for the main study.

1. Introduction

The current state of conventional liquid fuels is unfavorable for the long term. These fossil fuel-based energy are non-renewable and harmful to the environment. The Philippines recognizes this and has pursued strategies to attract interests in sustainable energy such as the enactment of the Philippines' Biofuels Act of 2006. The Act mandated a blend of 2% for biodiesel into the country's diesel fuel mix [1]. Current research is looking into transesterification of microalgae as it does not affect food supply. Moreover, it is easier to cultivate and has a high biomass yield compared to other terrestrial plants. The interaction between lipids contained in the feedstock and reactant produces fatty acid methyl ester (FAME) or biodiesel in a chemical reaction called transesterification [2]. The complexity of the cultivation to biodiesel production of biodiesel has led to a new methodology to reduce energy consumption and make the process more environment friendly [3].

Subcritical in-situ transesterification (SCW-ISTE) is an example of such process. It directly makes use of the wet biomass, bypassing the need to isolate the lipids through extraction, and allowing catalyst-



free transesterification to take place within the solid matrix of the mixture [4]. In using batch systems, operating parameters can be varied and optimized easier to get a complete understanding of the production process before scaling up the production level. One such promising research area is the mixing characteristics [4,5]. For smaller, laboratory scale processes, mixing is not needed to reach an acceptable yield rate [6]. At a larger production scale, the concentration of the reactant may not be equally distributed throughout the wet microalgae mixture, thus limiting the biofuel yield [7]. With an increase in reactor size, higher frequency mixing may be expected [8]. A computational fluid dynamics (CFD) model is to be simulated to quantify the magnitude of mixing that is occurring within the vessel to determine the effect of mixing on biomass dispersion within the liquid mixture. The use of conventional experimental tests is not applicable for this study as tanks used in SCW-ISTE are made up of a fully opaque, thick metal material due to the process' pressurized operating conditions. Non-intrusive methods such as those of Particle Imaging Velocimetry rely on imaging equipment [9]. In this case, light would not be able to penetrate thick metal walls. As such, experiments on fluid flow are typically done using transparent containers that have good optical properties to be able to track particles. The model will be the first to model and simulate the multiple materials and their properties involved in this chemical process. In order to investigate this area, a numerical validation study was implemented through this work. This study aims to identify an appropriate mesh strategy for a biofuel reactor model under SCW-ISTE conditions.

2. Methodology

Two mesh analyses were performed to create and determine whether the mesh generated is acceptable by comparing this study's CFD results to that of the literature's experimental data results. The most appropriate mesh was chosen and applied to this study based on solution accuracy and computational time. The first mesh analysis uses the validation paper's geometry, while the second one was performed to determine if the mesh setting is still appropriate for the main study's geometry which will have a smaller tank size and lower agitator position. A maximum tolerance of 10% error relative to the past literature's experimental results is considered. The experimental technique used by [10] is the computer automated radioactive particle tracking (CARPT) technique on a baffled, agitated, and transparent vessel. Moreover, the selected model should have an average error of its velocity profile lower than that of the past literature's numerical model. The computations are all with respect to the experimental data. A 6-bladed rushton agitator rotating counterclockwise serves as the source of mixing inside a baffled tank. The work simulated the whole tank geometry using the steady state Euler-Euler numerical model with the standard $k-\epsilon$ turbulence model as provided in the CFD software, ANSYS CFX. The materials used are water of density = 1000 kg/m^3 and spherical glass beads of density = 2500 kg/m^3 and particle diameter = 0.3 mm. The tank is fully filled with the water-solid mixture, where an initial condition of solids volume fraction of 1% (v/v) was used. For the purpose of continuing this work, only half of the tank was modelled to reduce computational effort while still retaining the same solution accuracy. This was attained through the use of rotational periodicity function in the software. This function is applicable to mixing tank models with a symmetrical figure. The full geometry of the tank is shown in figure 1.

2.1. Geometry

A steady state approach to rotating models such as that of a stirring tank's may be modelled using the Multiple Reference Frames (MRF) approach. For this approach, a relatively small portion of the fluid volume is defined to be rotating relative to the remaining, stationary fluid volume. A periodic condition called the frozen rotor model is utilized, where each numerical computation is done at each frame of reference of the model. The algorithms implemented in CFX ensure that the calculation of the imbalances at the wall interfaces is fully implicit and mass, momentum, energy, and the like are conserved. The MRF boundary is represented by a smaller cylindrical body encapsulating the agitator and part of the shaft. The Boolean subtract feature was used to separate the fluid volume of the MRF region and the rest of the tank's. This was done to facilitate the frozen rotor method, where only fluid located in the MRF zone is rotating while the rest of the fluid is stationary. Finally, face split was applied to the cut surface of the half tank, with the cutting plane perpendicular to the surface, to facilitate rotational periodicity.

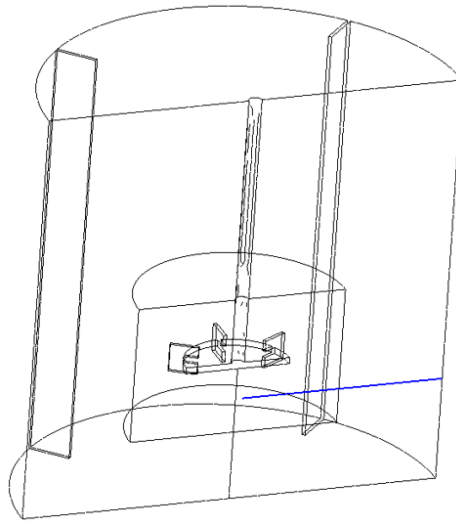


Figure 1. Wireframe model of the geometry.

2.2. Meshing

Tetrahedral meshes are used for geometries with varying angles but are of a non-complex nature, while hex elements have more faces, thus are used for more complex bodies such as the agitator. Element midside nodes were kept as this is shown to improve solution accuracy. By implementing this, elements are treated as quadratic rather than linear, which means that the mesh will have a higher degree of freedom with this feature. A total of 11 mesh settings by varying 4 mesh parameters were considered for the mesh analysis. A mesh setting basis was first created and named 'curv', standing for the mesh parameter chosen --- size function 'curvature' with fine 50 as its relevance. Its other parameters are: medium smoothing, slow transition, fine span angle center, a max face size of 2.80 mm, and a max tet size of 3.20 mm. Succeeding meshes will only have 1 parameter changed to determine the effect of a parameter in the mesh setting to the simulation result. The parameter changed reflects the name assigned to the mesh file for easy recognition. The relevance was tested from a value of 30, 40, 60, 70 and 80. Size function was set to either curvature or proximity (prox). Smoothing was set to either low or high. Span angle center was set to either coarse or medium.

Mesh quality was also taken into consideration. Mesh with good quality produces more accurate results than that of ones with low quality. The mesh quality metrics provide information to the quality of the mesh generated. This will inform the researcher whether a very refined mesh will not produce a significant difference in the solution compared to a relatively coarser mesh, thus a coarser mesh can be used to balance between solution quality and computation time. The resulting mesh metrics will be compared with ANSYS standards as defined in [11]. It is recommended that for the mesh to be a good representation of the model, skewness must be not greater than 0.8 and orthogonal quality must be at least 0.2.

2.3. Setup and Post-processing

In the solver settings, the high resolution option was chosen for both the advection scheme and turbulence numerics. The global dynamic model control was also applied. For a better convergence, the volume fraction was set to coupled under the multiphase control as recommended in [12]. Under the output control's monitor tab, imbalances were chosen and set to full. The solution is said to be converged when RMS residuals reach or drop below 1×10^{-5} . The timescale control was set to a physical timescale of 0.01s as this initialization value was seen to produce residuals that are least bouncy. A line is generated along the horizontal axis on the middle, cut surface of the tank at a tank bottom clearance = 50 mm. The resultant vector of the dry biomass along this line was then obtained. This line is portrayed in Figure 1. To compare this study's results with the work of [13], their experimental and numerical

results for the velocity axial (u), radial (v), and tangential (w) vectors at the location of the line were re-plotted on a spreadsheet, and the resultant velocities (U) were computed.

3. Results

During the computations in CFX, using the initial timestep throughout the simulation did not result in a converged solution; the residuals flattened out a few values before reaching convergence. Therefore, when the residuals stabilized, the timescale had to be changed every few iterations until the solution reached convergence. Timescales between 0.001-1s were tested to determine the ideal numerical computation interval for the multiphase model's residuals to converge. It was found that the range of 0.01-0.5s led to convergence. Convergence is inherently difficult for multiphase simulations as compared to single phase [14]. Each simulation's number of iterations ranges from 180-580.

3.1. 1st Mesh Analysis

Most of the model's mesh quality are rated 'very good', while a few were able to reach the excellent range. Variation in the timesteps during simulation introduces noise into the solution, thus the mesh setting modelled is used for the mesh analysis instead of the number of elements. The resultant velocity profiles for each simulation is shown in figure 2. It can be seen here that among the models simulated, only the prox model has a noticeably different velocity profile in the first 1/3 portion. The other models seem to have a relatively similar velocity magnitude along the radial distance of the tank. It is observed that the CARPT experiment showed two recirculation loops for the volumes above and below the line. A stronger/faster fluid movement is seen at the recirculation loop created below the agitator blade compared to the one generated above the blade. However, the CFD models were not able to capture the profile of the upper recirculation loop. For the upper loop in the CFD models, a rigid change in solid motion was observed where the change in fluid flow direction was around 90°, which should have been more of a circular loop than a square pattern. The magnitude of the lower recirculation loop was also not completely captured by the numerical models. The simulated models underestimated the magnitude of the solid velocity, which reflects on the average percent error discussed below.

Among the 3 velocity components, the numerical models' axial velocities are the closest with CARPT's data. The authors of [13] also noted that even compared with the Large Eddy Simulation, which is a transient unsteady flow simulation, and is composed of a significantly larger mesh size, the 'Euler' model performed better with regards to the solids' axial velocity. This velocity component is the most important for this study as solid suspension would depend on this variable. Therefore, the Euler numerical approach for mixing tank was deemed numerically accurate.

Data at $z = 0.5$ (halfway point between the middle of the tank and the tank's outer wall) were taken as the basis for data comparison. This point is located at $y = 50$ mm and $z = 50$ mm. The 'Euler' mesh name is the numerical model developed by [13], while the other meshes are modelled by the authors. From these set of data points, it is evident that the authors' models are closer to the experimental data's than the 'Euler' model is. The percent error of each model with respect to the CARPT data was then computed. Most of the models are within the acceptable 10% maximum error at the specified point, with only the '70' and 'smooth low' meshes not qualifying under this criterion.

On the average percent error of each model compared to the CARPT data, which is the main criterion for choosing the mesh to be applied to this study, a high deviation from the experimental data was seen. Notably though, all of the simulated models show a better fit with the experimental data's. The average errors were in the range of 30-41%, while the past literature's numerical model is at 44%. The model that is closest to the CARPT model is the 'prox' model. However, the computational time for this model was the longest among the models at around 4 hours, and is found to have a hard convergence rate. Following this, the 30 model has the next lowest percent error and was evaluated next. Its ease of convergence is good at 2 hours, and based on the said criteria and these considerations, the model was the most appropriate mesh setting.

3.2. 2nd Mesh Analysis

Based from the smaller geometry of the model generated for the 2nd mesh analysis, the new agitator tip speed was calculated to be 2659.88 mm/s. The 2 models created are labelled as 'without baffle' and

‘with baffle’. Both models’ skewness and orthogonal quality fall within the ‘very good’ range. At the same midpoint along the radial direction, it can be seen in figure 3 that the created model with baffles is well within the values of the Euler and CARPT data. Whereas the model without baffles has a 3.5 times higher solids resultant velocity than the CARPT’s. The cause for this deviation in results is in the presence of baffles, which impede the natural swirling action of the fluids to deter the formation of vortices.

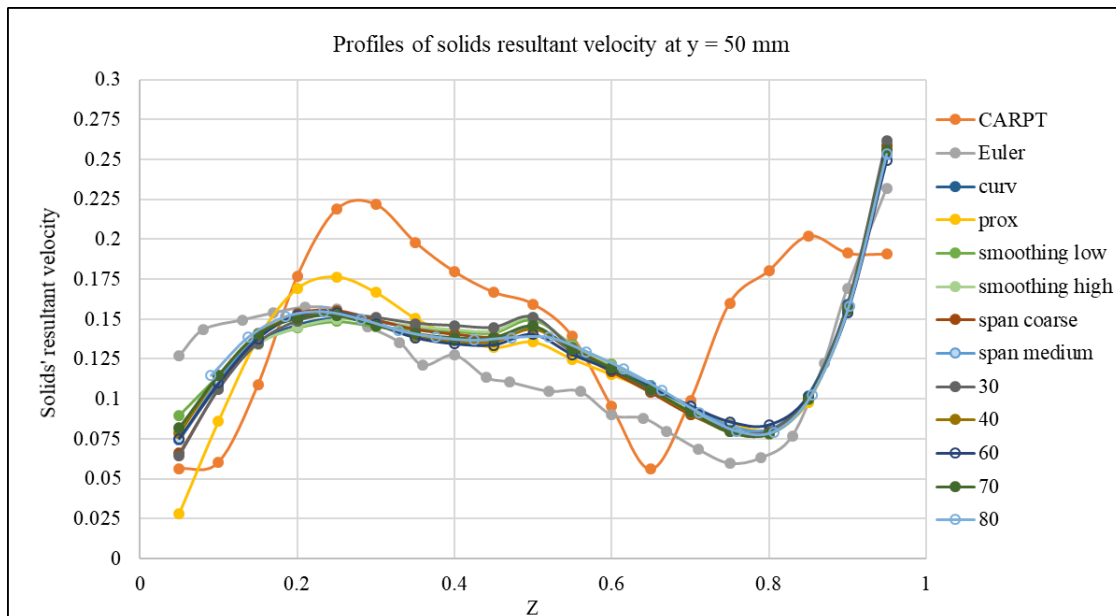


Figure 2. Resultant velocity profiles of the models for the 1st mesh analysis.

These results translate to the ‘with baffle’ model having a significantly lower percent error compared to the Euler’s. This is also the case for the average percent error, which bases from the velocity profile.

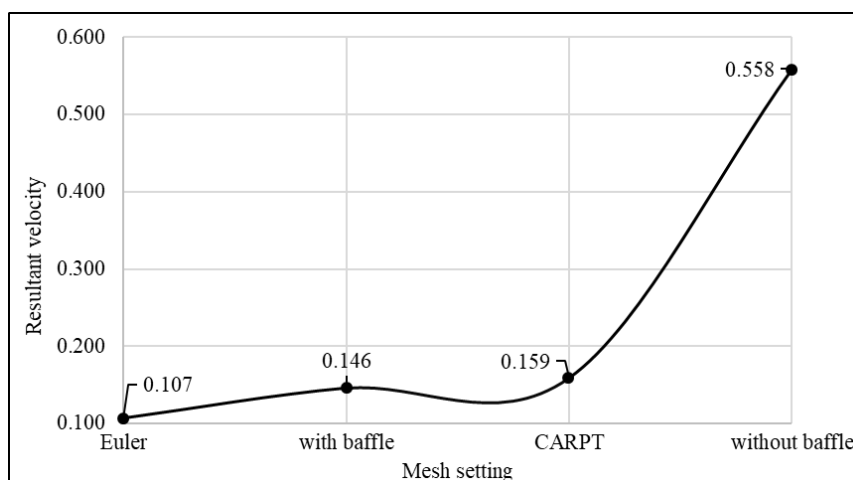


Figure 3. Resultant velocity of the 2nd mesh analysis for each model at a point.

4. Conclusion

A validation study was conducted for this study to have an accurate CFD model to use. After applying the recommended parameters for mixing tanks from the literature of [13], the recreated model was simulated. Results showed that the generated model, labelled as ‘30’, showed a more favorable average percent error of the velocity profile, equal to 31.05%, with respect to the experimental data as compared

to the error of the past literature's numerical model. With respect to the percent error at the specified point, this model was the closest fit at 4.8%. The 'prox' model yielded the lowest error at 30.47%. However, its residuals took a significantly longer time to reach the convergence criteria. Therefore, the next best model was chosen which is the '30' model. The models simulated have a similar resultant velocity profile, only varying in magnitude. Mesh analyses were done to determine if the mesh parameters available in ANSYS CFX affect the results. A total of 11 models were simulated, where only the 'prox' model showed a slightly different velocity profile. A second mesh analysis was conducted to check if the chosen mesh setting would affect this study's smaller reactor geometry before this study's actual model simulations are to be conducted. The model with baffle's percent error at the specified point was at an acceptable 8.2%, and its resultant velocity profile's is at 23.5% which is around the same range as that of the 1st mesh analysis' models. These results show a good fit with respect to the past literature's experimental data.

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