

Computational Fluid Dynamics and Simulation of a Mixing Mould Unit of a Mini Foam Batch Production Plant

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Abstract

Polyurethane foams are found in almost every home, whether in flexible or rigid form, and the demand for this product is high since it is a vital product for every home. Thus, there is a need to improve the quality and production rate of this valuable product. In this research, simulation and performance evaluation of a mixing and mould unit of a batch foam production plant were conducted. Computational fluid dynamics was employed to determine the effect of the stirrer in adequate mixing of the foam reactant chemicals, the velocity distribution of the flow through the mixer, temperature and flow rate of the product at the outlet of the foam mixing tank. The CFX- solver, on completion of the simulation, provided the flow variables. The results obtained at the inlet of the foam mixing tank include an average inlet velocity of 0.3m/s, the average inlet pressure of 30,460 Pa, and an average mass flow rate of 0.000148 kg/s. The temperature of the fluids at the outlet corresponds to 323K showing an increase in the flow rate of the fluids after mixing with the mass flow rate of 0.000780 kg/s. Therefore, it was concluded that CFD is a viable tool in predicting fluid flow behavior in mixing equipment.

Keywords: Computational fluid dynamics, simulation, polyurethane foam, mixing and mould unit, batch production plant

1. Introduction

Polyurethane is one of the most important classes of a special polymer. Ideally, a typical polyurethane may contain in addition to the urethane linkages, aliphatic and aromatic hydrocarbons, esters, ether and other groups. Flexible polyurethane foams are one of the most important classes of cellular plastic used in the manufacture of such materials as foam mattresses, pillows, furniture, cushioning materials for automobiles, packing, recreation, shoes, etc. The research is aimed at using Computational Fluid Dynamics (CFD) and Simulation of the Mixing and Mould Unit of a Mini Foam Batch Production Plant to show the viability of CFD being a viable tool in predicting fluid flow behavior in mixing equipment. The objectives of this research include to: study the simulation software (SS) that has previously been used for prediction of fluid flow behavior during foam mixing operation in a Batch Production Plant; suggest better SS for predicting the fluid flow behavior during mixing operation in a Batch Production Plant; show the viability of the SS and conduct performance evaluation of the mixing and mould unit of the batch production plant.

2. Review of Literature

The global consumption of foam was estimated to be above 7 million metric tons in 2007 and the average annual growth rate is about 5% (Woods 1990, Avar 2008). In general, industries that produce foams use fillers to modify the material's properties in some way to achieve dimensional stability ease of retraction from the mould and service density (Saliba et al. 2005, Bartizan et al. 1999). When adding a filler to a polymer to form a conjugated biphasic material, the tension applied to the polymeric matrix will be transferred in part to the disperse filler phase since it presents properties superior to the pure polymer (Callister 2000). The use of several fillers to achieve improved

properties in foam has been widely studied [6]. Some notable ones include inorganic materials such as calcium carbonate, dolomite, aluminum silica, titanium dioxide, and talc (Nunes et al. 2000) while some of the organic materials used as filler are carbon black and natural fibers (Mothé et al. 2002, Mothé and Araújo 2000). Polyurethanes are a broad class of materials used widely in many applications. Polyurethanes are also written as PUR and also called as urethanes. They are characterized by urethane linkage -NH- C(=O) - O -. Polyurethanes are discovered by Otto Von Bayer & co-workers in 1937. The characteristic structure of urethanes is given as shown in Figure 1.

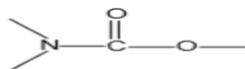


Fig.1. Structure of Polyurethane Ashida (2006)

Polyurethanes are considered as esters or amide esters of carbonic acid. They are synthesized by the reaction of polyfunctional hydroxyl compounds with polyfunctional isocyanates. Structure of polyurethane formed from di hydroxyl compound and diisocyanate is given as shown in Figure 2 below. (Ashida 2006, Oertel 1999, Szycher 1999)

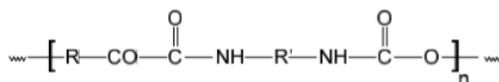


Fig.2. Polyurethane formed from di hydroxyl compound (Ashida 2006)

Polyurethane is a versatile polymer having unique chemistry with excellent mechanical and optical properties and has good solvent resistance (Matsumura et al. 2006). Polyurethane foam covers almost 29% of the total market of polyurethane (Begum, M. and Siddaramaiah. T. 2004). In flexible polyurethane foams, the fillers promote an increase in density and resistance to compression. However, they reduce resilience and contribute to the increase in permanent deformation. In addition, properties such as tear strength are significantly affected by the introduction of filler (Ashida 2006). Accordingly, it is necessary to determine the correct concentration of the filler in the polymer matrix, to obtain a product of reliable quality (Latinwo 2009). Usage of flexible polyurethane foam in Sub- Sahara Africa has been mainly for mattresses and recently, there has been a growing demand for durable and high hardness characteristic (i.e. high compression resistant) foam at low cost (Latinwo, et al. 2010). Foams with these qualities are of interest to many sectors of the economy, and therefore their preparation, characteristics, and applications are subject interest (Niemeyer et al. 2006). The availability of petro-chemical based polyol in Nigeria, which constitute the largest percentage of materials used in foam production and which possess the characteristics to induce superior mechanical properties in foam make the production of the machine a welcome development.

Foaming systems are classified into three types based on the type of chemicals used in the synthesis process (i.e., one step one-shot system, quasi pre-polymer system, and full pre-polymer system). One-step system and quasi system are mostly used in foaming industries. One-step process is used majorly while the pre-polymer system was used only in the early times of the urethane industry. In one step system, the components (i.e., component A and component B) are taken separately. For instance, component “A” contains only polyisocyanate component while component “B” contains polyol, surfactant, blowing agent and catalyst. Both components are mixed which led to the formation of foam as shown in Figure 3.

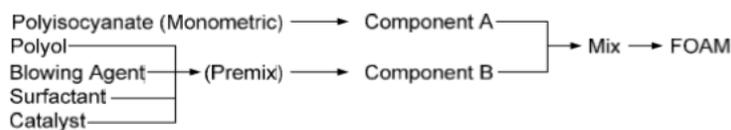


Fig.3. One step one-shot system (Ashida 2006)

Figure 4 below shows the quasi pre-polymer system, in component “A” polyisocyanate component is taken with polyol and in component “B” rest of the ingredients are added with polyol which includes a catalyst, blowing agent etc. Mixing forms, a foaming product.

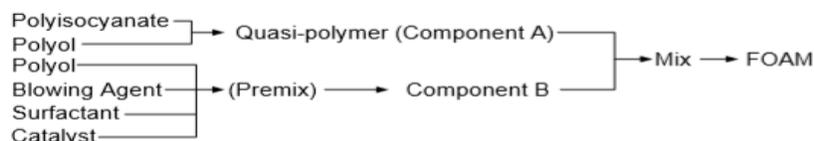


Fig.4. Quasi pre-polymer system (Ashida 2006)

In full prepolymer system in component “A” polyisocyanate component is taken and the polyol is also added in it while in component “B” polyol is not added while the rest of chemicals like blowing agents, surfactants and catalyst are taken. Components A & B are mixed as shown in Figure 5.

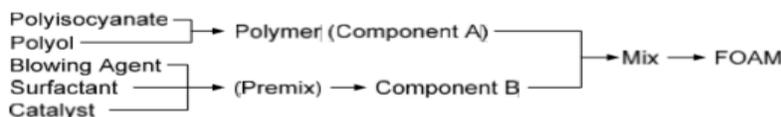


Fig.5. Full pre-polymer system (Ashida 2006)

3. Methods

3.1 Computational Fluid Dynamics

This refers to the science of predicting fluid flow, heat transfer, mass transfer, phase change (as in freezing or boiling), chemical reactions, mechanical movement and related phenomena by solving the mathematical equations that govern these processes using a numerical algorithm on a computer. Computational fluid dynamics was fully employed in this research work to determine the effect of the stirrer in the adequate mixing of the foam reactant chemicals, the velocity distribution of the flow through the mixer and temperature and flow rate of the product at the outlet of the foam mixing tank. To achieve the said goal of this CFD project analysis, the basic terminologies of computational fluid dynamics were fully studied and applied effectively. The various material properties of the foam chemicals used in creating the foam were created individually in ANSYS to form a multi-component fluid with the respective mass fractions of the fluid included, to sum up to unity. The participating fluids for the foam chemicals included Polyol, Stannous Octoate, Silicone oil, Water, Methylene Chloride and TDI (Fig.7). The various participating fluid materials were grouped to form a fixed composition mixture. This is a multi-component fluid that comprises the individual mass fractions of the foam chemicals. Figure 6 shows the computational grid of the mixing tank and inlet trough.

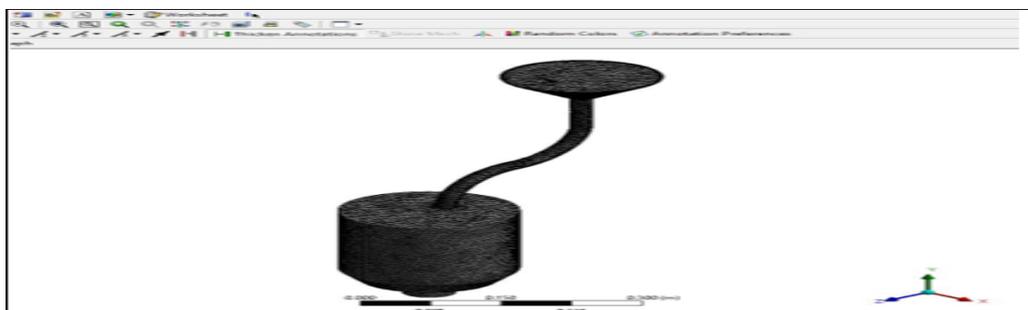


Fig.6 Computational grid of the mixing tank and inlet trough.



Fig. 7 Chemicals/Reagents Used

4. Data Collection

4.1 Boundary Conditions

Boundary condition directs the motion of the flow quantities (fluxes) such as momentum, mass, heat transfer, turbulence into the computational domain. The flow is assumed to be independent of time variations or is unaffected by time changes. The fluid domain includes the region of the inlet trough, connecting piping and the foam mixing tank. The fluid domain also includes the bounded region of the fluid that is in contact with the stirrer. The stirrer is the only solid domain in the simulation, and it imparts rotational kinetic energy to the flow by the power provided by the motor that drives the stirrer shaft. The stirrer is assumed to operate at a speed of 5 revolutions per minute. This optimum speed is required for effective mixing of the foam chemicals and for imparting turbulence required for the fluids to mix properly. Due to the steady-state nature of the problem, the rotation of the stirrer was captured using the frozen rotor model. The frozen rotor model can also be referred to as the multiple reference frame model because it provides a steady-state approximation of the flow in which individual cell zones can be assigned different rotational and/or translational speed. It is very vigorous in capturing the flow field in weak rotor-stator interactions and negligible transient effects. The domains and boundary conditions are detailed in Table 1.

The computational domain or the geometries imported into Catia were extracted from the 3d model of the entire mixing machine. An accurate representation of the participating parts of the mixing tank was carefully analyzed and modeled. These include the fluid region occupied by the foam chemicals inside the tank from the inlet trough to the base or outlet of the mixing tank, the solid stirrer of the fluid which imparts kinetic energy into the fluid and causes adequate mixing and lastly a bounding fluid region which serves as a boundary between the stirrer which is a solid domain and the other parts of the fluid which is a fluid domain. The next step after importing the geometries into ANSYS design modeler was the creation of boundary labels for some specific faces where the boundary conditions would be applied.

On completion of the boundary naming operation, the individual geometries were processed into computational grid elements or meshes. In Figure 8, the Ansys Design Modeler showing the geometrical domain of the Stirrer Bounding Fluid was presented, while Figure 9 shows the Fluid domain – Foam Tank and inlet trough, Figure 10 shows the Inlet Boundary Condition – Foam Tank and Inlet Trough, while Figure 11 shows the Solid domain – Stirrer, and Figure 12 shows the Domain Interface: Stirrer – Stirrer bounding fluid.

Table 1. Domains and boundary conditions

| | | |
|----------------------------|------------------------------------|--|
| Analysis Type | Steady State | |
| Domain 1 | Foam Chemicals | |
| Domain Type | Fluid domain | |
| Material Type | Foam Chemicals | Water, Methylene Chloride, TDI, Stannous Octoate, Polyol, Silicone Oil |
| Domain Model | Reference pressure | 1 atm |
| | Buoyancy | Non-buoyant |
| | Domain Motion | Stationary |
| | Mesh Deformation | None |
| Fluid Models | Heat Transfer | Total Energy |
| | Turbulence | K-Epsilon |
| | Wall Function | Scalable |
| | Thermal radiation | None |
| Boundary Conditions | Inlet | Inlet |
| | Flow Regime | Subsonic |
| | Mass & Momentum (Mass flow rate) | 167g/s |
| | Turbulence | Medium Intensity, 5% |
| | Heat Transfer | Static Temperature (23 C) |
| | Outlet | Pressure: 0 Pa |
| Domain 2 | Stirrer | |
| Domain Type | Solid domain | |
| Material Type | Aluminum | |
| Domain Model | Morphology | Continuous solid |
| | Domain Motion | Rotating |
| | Angular Velocity | 5 revs/min |
| | Rotation Axis | Global Y |
| | Mesh Deformation | None |
| Solid Models | Heat Transfer | Thermal Energy |
| Domain 3 | Stirrer Bounding fluid | |
| Domain Type | fluid domain | |
| Material Type | Foam chemicals | Water, Methylene Chloride, TDI, Stannous Octoate, Polyol, Silicone Oil |
| Domain Model | Morphology | Continuous fluid |
| | Domain Motion | Rotating |
| | Angular Velocity | 5 revs/min |
| | Axis definition | Coordinate axis |
| | Rotation Axis | Global Y |
| Fluid Models | Heat Transfer | Total Energy |
| | Turbulence | K-Epsilon |
| | Wall Function | Scalable |
| | Thermal radiation | None |
| Domain Interface 1 | Foam Tank – Stirrer Bounding Fluid | |
| | Interface Type | Fluid – fluid |
| | Interface Side 1 | Stirrer Boundary |
| | Interface Side 2 | Fluid interfaces (foam tank domain) |
| | Interface Model | General Connection |
| | Frame Change/Mixing Model | Frozen Rotor |
| | Pitch Change | None |
| Additional Interface Model | Heat Transfer | Conservative Interface Flux |

| | | |
|----------------------------|----------------------------------|------------------------------|
| | Mesh Connection Method | GGI |
| Domain Interface 2 | Stirrer Bounding Fluid – Stirrer | |
| | Interface Type | Fluid/Solid |
| | Interface Side 1 | Stirrer Boundary |
| | Interface Side 2 | Stirrer wall |
| | Interface Model | General Connection |
| | Frame Change/Mixing Model | Frozen Rotor |
| | Pitch Change | None |
| Additional Interface Model | Heat Transfer | Conservative Interface Flux |
| | Mesh Connection Method | General grid interface (GGI) |

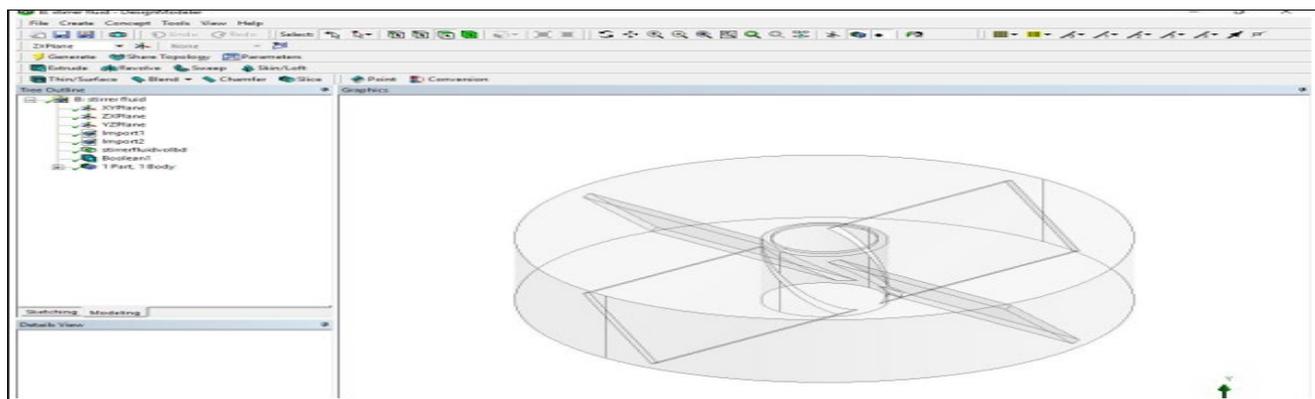


Fig. 8 Ansys Design Modeler showing the geometrical domain of the Stirrer Bounding Fluid

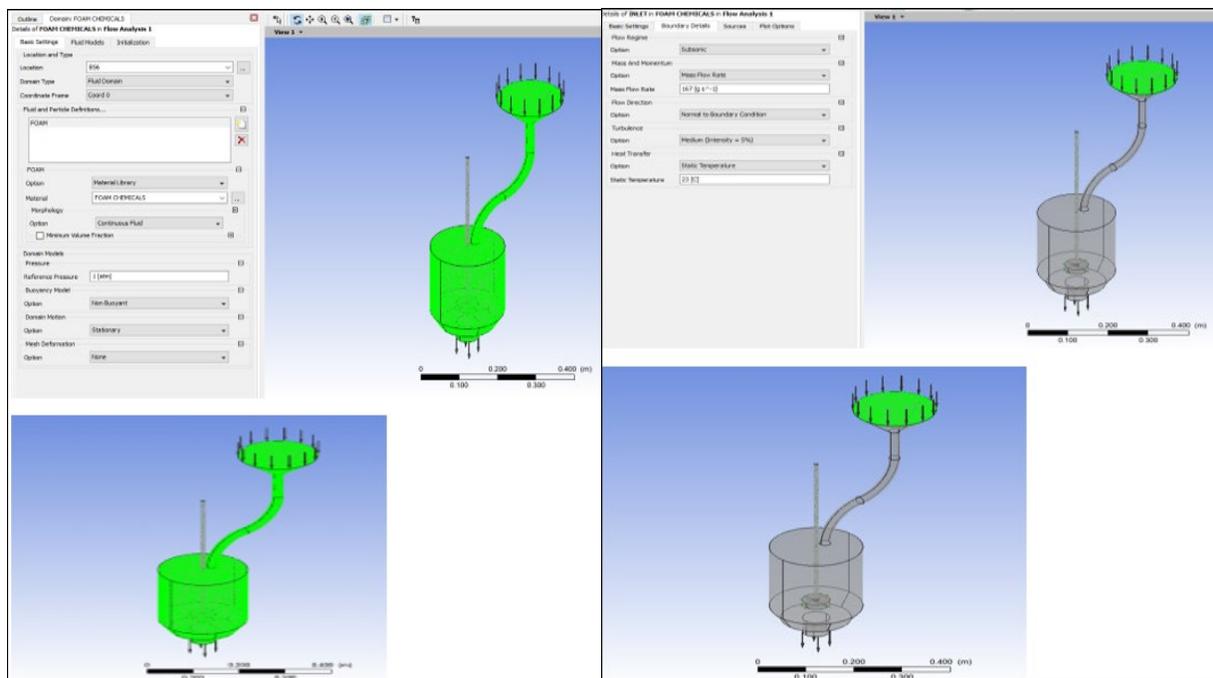


Fig.9 Fluid domain – Foam Tank and inlet trough

Fig.10 Inlet Boundary Condition – Foam Tank & Inlet

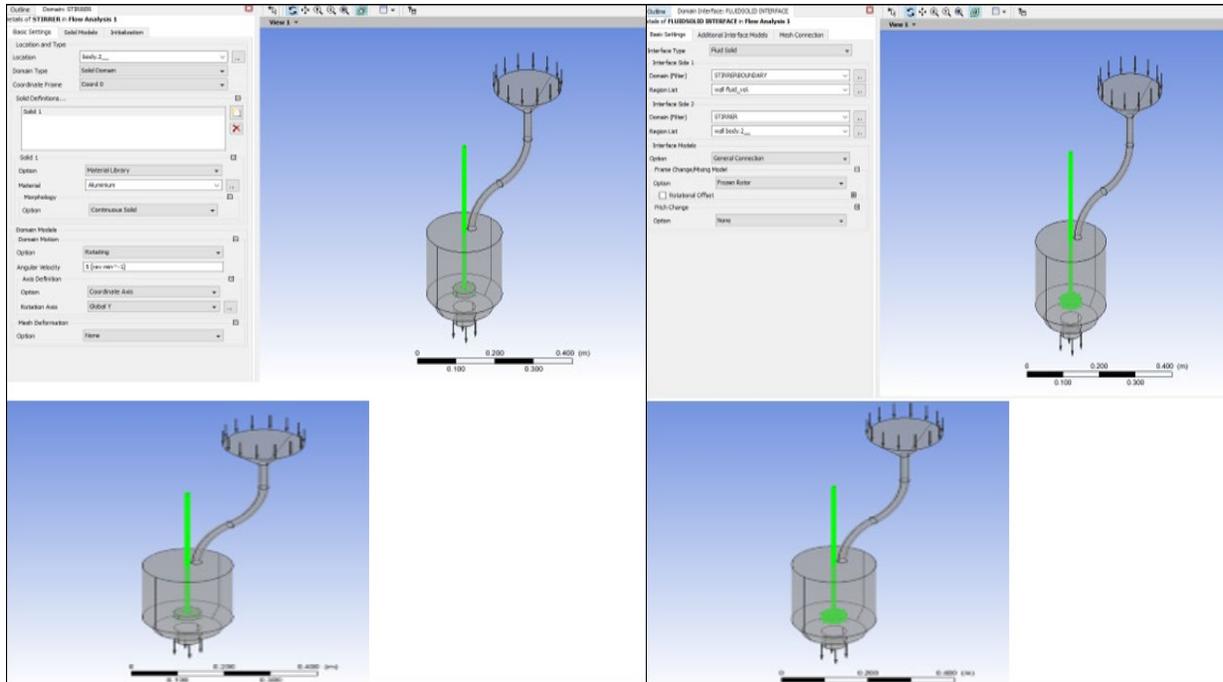


Fig.11 Solid domain – Stirrer

Fig.12 Domain Interface: Stirrer – Stirrer bounding fluid

4.2 Meshing Operation

On completion of the meshing operation, the mesh of the mixing tank and inlet trough fluid domain was linked directly into a CFX PRE-PROCESSOR component. The other meshes of the stirrer and the bounding fluid was saved and later imported into the ANSYS cfx pre-processor to merge with the mesh of the stirrer tank and inlet trough.

4.3 Pre-Processing

This is the preliminary process that involves setting up the CFD simulation. It includes operations such as geometry modeling, meshing, boundary conditions and material property definition and solver settings. The meshes of the domains required for the simulation was imported into ANSYS cfx pre and was positioned with respect to the coordinates to create the entire multi-structure domain comprising of the fluids' and solid domains. The domains, boundary conditions and the interfaces between the fluid and solid domains were created. Analysis type and solver settings were also keyed in to carry out the solution process using the CFX- Solver.

4.4 Processing and Post Processing

This is the intermediate process in the CFD simulation where the CFD solver or code analyses the input provided during the pre-processing stage such as geometry, meshes and boundary conditions and carries out iterative solutions in analyzing the flow field and flow variables. Post-processing is the act of analyzing the results of the CFD simulation using reports, integrals, graphs, and contour plots to list a few.

4.6 Solver

ANSYS CFX and ANSYS FLUENT possess robust solver algorithms that enable them to function effectively in solving a CFD simulation. ANSYS FLUENT possesses the pressure-based and density-based solver formulations while ANSYS CFX possesses the coupled solver formulation. Both software packages are effective in solving problems in single and double precision and in solving 2d and 3d CFD problems. The CFD solver applied in this analysis is the ANSYS CFX solver which is very robust and effective in handling simulations of flows such as complex mixing of multi-component fluids'. The Solver control settings oversee the convergence and completion of the simulation. The simulation continues to run until the solution is converged. The results of the simulation are further outputted to ANSYS CFD-Post Post-processing tool which enables result generation and analysis to be further carried out. On completion of the various CFX-Preprocessor inputs such as the domain creation, boundary

conditions and domain interfaces, the solver settings for the CFX processing was inputted to simulate as shown in Table 2.

Table 2. CFX solver settings

| | | |
|-------------------------|-------------------------|------------------------|
| Solver Control | Steady State | |
| | Advection Scheme | Specified Blend Factor |
| | Blend factor | 0.7 |
| | Timestep Initialization | Automatic |
| | Turbulence Numerics | First-order |
| Convergence Control | Min. iterations | 1 |
| | Max. iterations | 1000 |
| Fluid Timescale Control | Timescale control | Auto Timescale |
| | Lengthscale option | Conservative (1.0) |
| Solid Timescale Control | Timescale control | Auto Timescale |
| | Lengthscale option | Conservative |
| Convergence Criteria | Residual Type | RMS |
| | Residual Target | 1e-04 |

5. Results and Discussion

5.1 Numerical Results

The flow variables provided from the onset of the simulation include the inlet temperature (i.e., the ambient temperature of 23°C) and the mass flow rate of the component fluids into the tank (167g/s). The various component fluid material properties were also provided for each material case. The CFX- solver on completion of the simulation provided indefinite flow variables which were not made available. The CFD simulation carried out was outputted to ANSYS CFD-Post for post-processing. The results of the simulation were analyzed in relation to the goal of the CFD simulation which includes the following: Obtaining a velocity distribution of the flow inside the mixing tank (Fig. 13-Fig.15); obtaining the temperature distribution of the flow inside the mixing tank to decipher the location of efficient mixing of the foam chemicals (Fig. 16 and Fig.17); temperature distribution plot against the travel distance, i.e. from the inlet to the outlet of the mixing tank; plot of the velocity distribution against the distance along the foam mixing machine i.e. from the inlet to the outlet of the mixing tank; estimating the flow rate, velocity and temperature of the mixed chemicals at the outlet of the mixing tank.

The following results were obtained at the inlet of the foam mixing tank on completion of the CFD simulation. They include average inlet velocity of 0.3m/s, average inlet pressure of 30,460 Pa, and average mass flow rate: 0.000148 kg/s. The average temperature and velocity of the fluid at discrete set points within the fluid domain was obtained using a plane and the function calculator in CFD-Post. The average integral value of the quantities was used to predict the rate of mixing of the fluid. The data extracted in set distances along the inlet trough and the foam mixer outlet is given by Fig. (18) and Fig. (19).

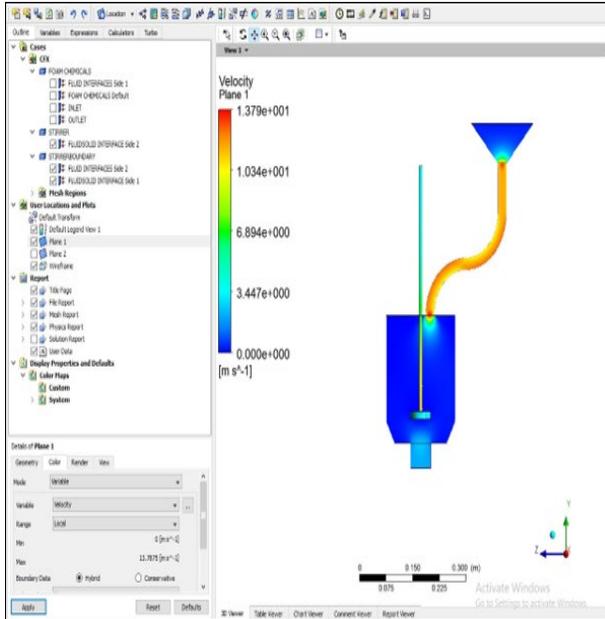


Fig.13 Fluid velocity distribution along vertical plane inside the foam mixer

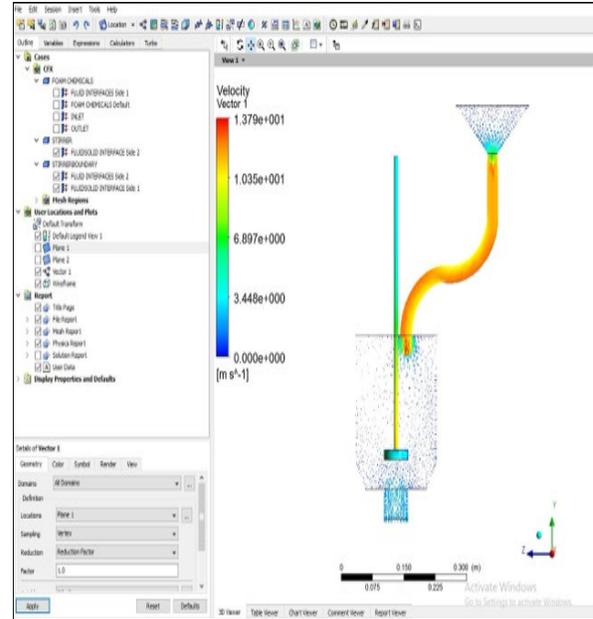


Fig.14 Fluid velocity vector plots inside the foam mixer

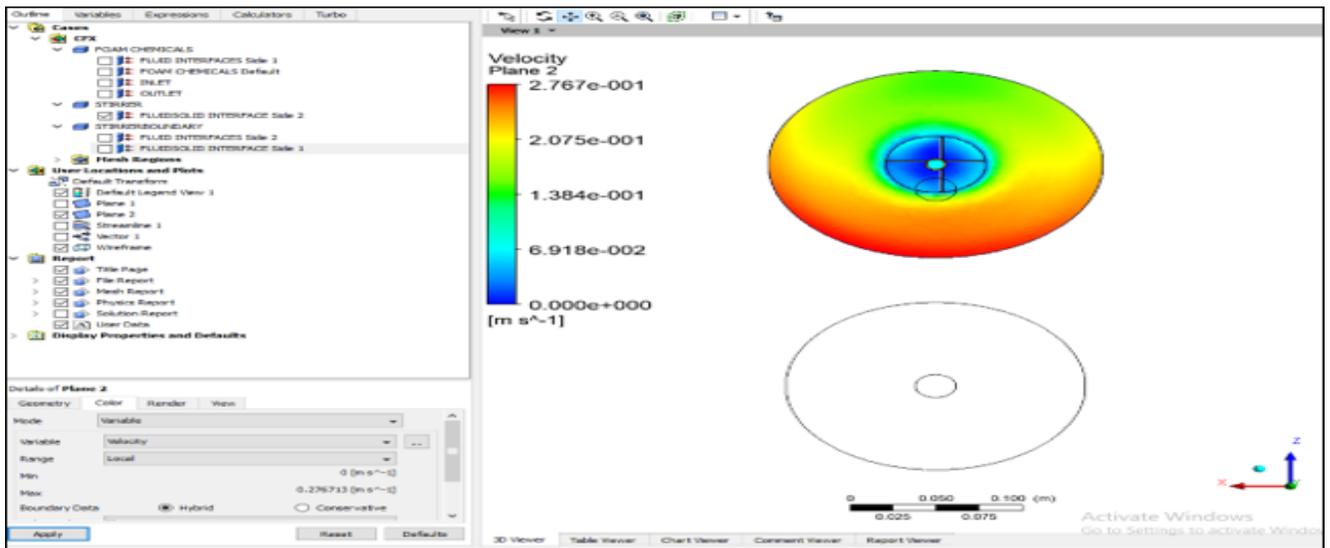


Fig.15 Fluid velocity distribution along a horizontal plane inside the foam mixer

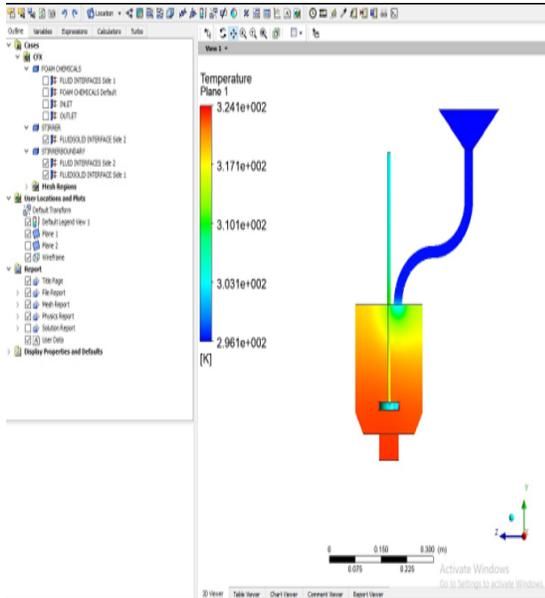


Fig.16 Fluid Temperature distribution along vertical plane inside the foam mixer

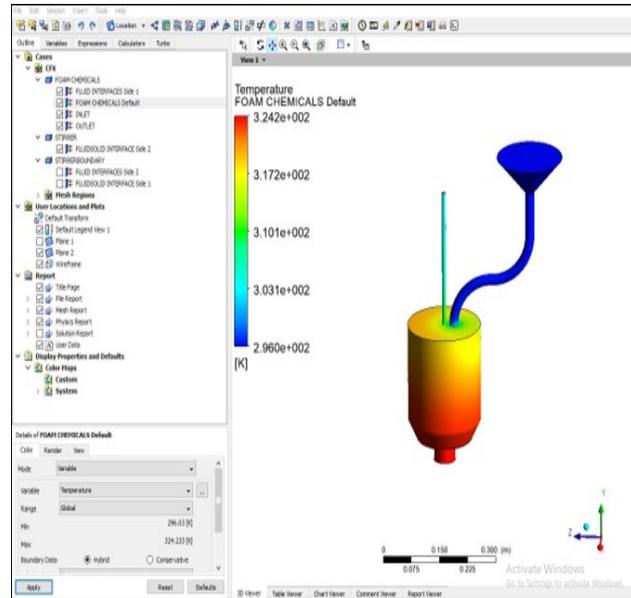


Fig.17 Fluid Temperature contour plot of the foam mixer

5.2 Graphical Results

The CFD simulation of the foam mixing machine was carried out to study the flow behavior of the fluids within the machine and to study the performance of the machine in carrying out efficient mixing of the fluid. The effect of the stirrer which was incorporated to impart kinetic energy into the fluids' and ensure that the various individual fluid materials are properly mixed before exiting the machine was also considered. The results obtained from the simulation provides a graphical insight into the operation of the fluid mixing process. The flow of fluid at the inlet of the foam mixing machine was carried out at 23°C which is referred to as the ambient or normal room temperature. It can be deduced from the results extracted in distances of 50mm variations that there was a steady increase of the fluids' temperature from the inlet of the tank up until 300mm before the fluid enters the foam mixing tank. At about 350mm there was a sudden rise of the fluids' temperature from 304k to 315.97k at 400mm inside the tank, a difference of 50mm. This is indicative of the increased turbulence and kinetic energy imparted on the fluid by the rotating shaft of the stirrer. The fluids' become more chaotic and thus there's a sudden temperature rise. At this point, the mixture becomes very effective because more molecular fluid interactions occur at higher temperatures than at lower temperatures observed earlier. The temperature of the fluid continues to increase sharply to the fluids' outlet (Fig.18). The temperature of the fluids at the outlet corresponds to 323K (50 degree Celsius). At this elevated temperature, the liquid multi-component foam mixtures have achieved maximum and adequate mixing and can thereby exit the mixing tank. The resulting temperature difference from the inlet and outlet temperatures is 27 °C.

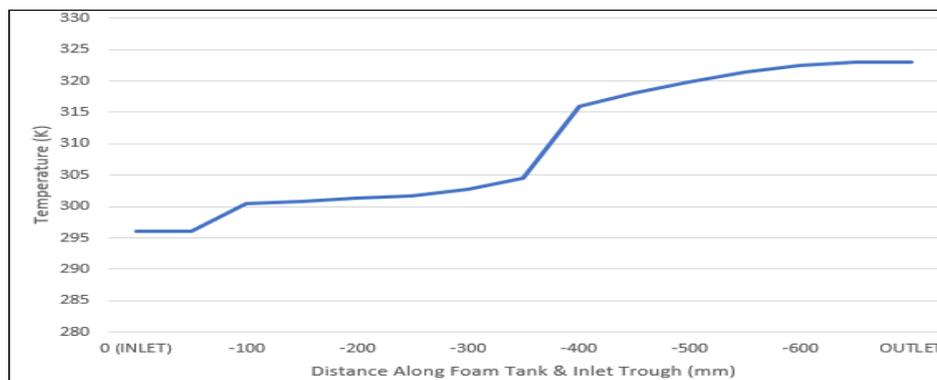


Fig.18 Plot of temperature against distance along with foam tank and inlet trough.

Another reflection of the effective design of the foam mixing machine is the constriction of the pipe that supplies the foam chemicals into the mixing tank. For efficient mixing to occur, there must be high turbulence of the fluids. This was improvised in the design by creating a wider inlet trough or funnel to allow inflow of the foam chemicals and then constricting the inlet diameter to a smaller size with respect to the trough. This would force the fluids through the trough down into the foam mixing tank thereby creating random chaotic fluid movements and disturbances. At the point where the inlet trough connects their pipe leading to the mixing tank, there occurs a sudden rise in the fluids' velocity through the pipe. This continues up until the point the fluid enters the foam mixing tank. At that point, their velocities drop drastically. However, it can be noticed that the velocity of the fluids' increases as the fluid nears the rotating stirrer's impeller blades and exit through the outlet (Fig.19). This is due to the kinetic energy contributions from the rotation of the stirrer. The average outlet velocity is 2m/s. This also reveals that there's an increase in the flow rate of the fluids after mixing. This is evident from the computed mass flow rate of 0.000780 kg/s. Thus, it can be concluded that CFD is a viable tool in predicting fluid flow behavior in mixing equipment.

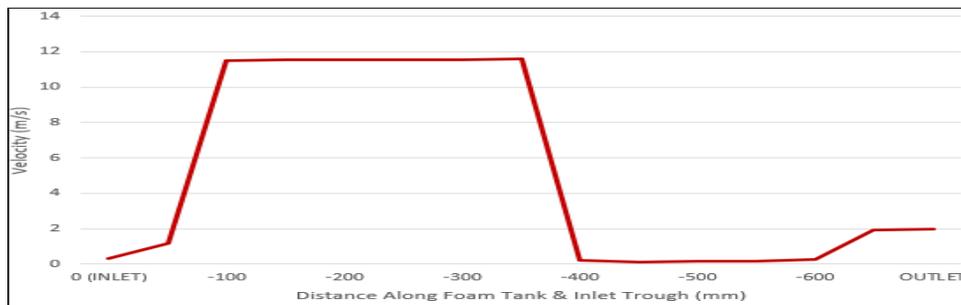


Fig.19 Plot of velocity against distance along with foam tank and inlet trough.

6. Conclusion

The results obtained from the simulation is an exposition and demonstration of the working principle and operation of the fluid mixing process. The following results were obtained at the outlet of the foam mixing tank on completion of the CFD simulation. They include average outlet velocity of 2.0 m/s, average outlet pressure of 11.46 Pa, average mass flow rate of - 0.000780 kg/s (negative sign indicates mass flow out of domain), and average outlet temperature of 323 K. Besides, there was an increase in the flow rate of the fluids after mixing. This is evident from the computed mass flow rate of 0.000780 kg/s. Thus, it can be concluded that CFD is a viable technique for effective prediction of fluid flow behavior in mixing equipment.

Acknowledgement

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