A Computational Fluid Dynamics Modeling and Experimental Study of the Mixing Process for the Dispersion of the Synthetic Fibers in Wet-Lay Forming

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ABSTRACT
In this paper, we present results from a computational fluid dynamics (CFD) model for the mixing process used to disperse synthetic fibers in wet-lay process. We used CFD software, FLUENT, together with the MIXSIM user interface to accurately model the impeller geometry. A multiple reference frame (MRF) model and standard k-e turbulence model were used to model the problem. After obtaining a converged solution for the mixing tank with water, a discrete phase model was constructed by injecting spherical particles into the flow. A mixing tank with baffles and a centrally located impeller was used in experiments. PET fibers (1.5 denier, 6.35, 12.7, and 38.7 mm) at a concentration of 0.01% were mixed in water for the study. In regions behind the baffles, where the model predicted higher concentration of particles, experimental results showed a 34% higher concentration relative to the region in the high turbulence zone near the center. Instantaneous sheets were formed by rapidly dipping and removing a flat wire mesh strainer into the tank at two different locations to assess the state of dispersion in the tank. The sheets were transferred onto a blotting paper and examined under a microscope to count defects. Results show that the number of rope defects was 43% higher in sheets drawn from the region behind the baffles than in the sheets drawn from regions near the center of the tank. Changing baffles from a rectangular to a triangular cross section decreased the number of rope defects, but increased the number of log defects in the sample sheets at the same location. The CFD model can be used to optimize mixing tank design for wet lay fiber dispersion. The model provides further insight into the mixing process by predicting the effect of changes in design parameters on dispersion quality.

INTRODUCTION
Wet-laid nonwovens refer to flexible web-like structures manufactured using the papermaking process with synthetic fibers bonded together with a suitable binding material. A major objective of wet-laid nonwoven manufacturing is to produce structures with textile-fabric characteristics, primarily flexibility and strength, at speeds approaching those associated with papermaking. Specialized paper machines are used to separate the water from the fibers to form a uniform sheet of material, which is then bonded and dried. In theory, any natural or synthetic fiber could be used in the production of wet-laid nonwovens. However, there are practical limitations on the use of many fibers (cost, availability, priorities, etc). Some form of wood pulp is used in virtually all wet-laid nonwovens because of its ease of handling and forming, low cost, excellent optical properties, printability, and high opacity. Natural fibers other than wood pulp remain of interest because they have valuable properties for specialized end-uses. They suffer from unstable pricing and supply due to variations in climate, worldwide demand, and availability of competing fibers. Some natural fibers - such as cotton linters, Manila hemp and cellulose staple fibers - are used in wet-lay process. Synthetic fibers provide specialized properties, uniformity, and constancy of supply. Some are used more widely than others. For example, bicomponent fibers, which provide both a structural element and a thermal bonding capability, have been used in specialized materials despite their high cost [1]. Crimped fibers require special dispersion and bonding techniques, but make a very soft and bulky product. The use of rayon and polyester textile fibers with lengths exceeding 1.5 inches has been reported sporadically. "Synthetic wood pulp" made from very short, shear-precipitated polyolefin fibers is available and results in improved wet strength and other properties of wet-laid nonwovens. Unfortunately, synthetic fibers for use in wet-laid nonwovens are 20 to 50% more expensive than the same fiber in the form of textile staple, because the market is small relative to that for textile fibers, and special handing and cutting are required. Specialty fibers such as low-melting bicomponent fibers are even more expensive, and

their manufacturing quantity is too small to allow economies of scale to be fully realized. In general, man-made fibers are longer, stronger, more uniform, and less compatible with water than natural fibers. Their flexibility and length can mean that they entangle when they are dispersed in water, which either prevents or limits their use in nonwovens. Several approaches have been developed to overcome this problem. For example, synthetic fiber manufacturers offer fibers with proprietary chemical surface treatments, which improve dispersion by overcoming the inherent hydrophobicity of the polymers from which the fibers are made. Recently, a study of the effects of atmospheric pressure He/O_2 plasma treatment on the surface characteristics of polyethylene terephthalate PET fibers has been reported [2]. It was found that the Oxygen-based functional groups on the surface of PET increased from 27 to about 32% due to plasma treatment, and the wettability increased tenfold and the moisture regain increased threefold.

There are three major operations in the manufacture of nonwoven bonded fabrics by the wet-laid method [3]:

• Swelling and dispersion of the fibers in water and transport of the suspension to a forming fabric or traveling screen
• Continuous web formation on the screen as a result of filtration and dewatering
• Drying and bonding of the web.

In this study, we focus on the first step of dispersion of dry chopped strand fibers in water medium before being directed to the fan pump.

BACKGROUND

A polyester fiber is a manufactured fiber in which the raw material is any long chain synthetic polymer composed at least 85% by weight of an ester of a dihydric alcohol (HOROH) and terephthalic acid (p-HOOC-C6H4COOH). The most widely used polyester fiber is made from the linear polymer (polyethylene terephtalate), and this polyester class is generally referred to simply as PET. High strength, high modulus, low shrinkage, heat set stability, light fastness and chemical resistance account for the great versatility of PET [4]. These fibers are drawn through a multiple orifice system, cooled, and cut by a flying knife. The result is fiber bundles that are arranged in parallel, in the form of bundles known as logs. Each bundle might contain 100-200 fibers. The fibers must be dispersed as uniformly as possible before forming into a sheet. This is accomplished by adding the fibers to water, sometimes with a surfactant, and mixing for sometime using an impeller. The shear stresses exerted during mixing causes the fibers to slip past each other in the bundle and eventually come free of . The shearing force generated parallel to the length of the logs is opposed by friction between the fibers, surface tension, and the forces from polymer fusion during cutting process [5]. For dispersion to occur, the following inequality must be satisfied [6]:

$$F_s > F_\sigma + F_\mu + F_f \qquad (1)$$

Where
F_s = shear force exerted on the bundles of fiber
F_σ = surface tension force
F_μ = friction force
F_f = forces from polymer fusion or incipient fusion

Bundles that do not satisfy this inequality can never be dispersed in the shear field specified by F_s. When the shear force exceeds the resistance forces, the chip (bundle) will disperse if stirred long enough, but if the shear forces do not exceed the resistance forces, the log is stable in the shear field and even an infinite mixing time will not prevent the bundle from causing a log defect in the fabric. Logs are bundles of fibers that have failed to disperse in the agitating tank and whose cut ends remain aligned. These are usually formed because of under-agitation during initial dispersion. Other types of defects include the rope defect, fused fibers, and the formation of dumbbell-like structure, known as dumbbells. Ropes are fiber assemblages that have unaligned ends and are clearly more agglomerated than the average sample dispersion. They can be formed by one of two ways: Bundles of fibers which are in the process of being dispersed, but not completely so, may get transferred on to the forming mesh before being completely dispersed, or Dispersed fibers can come together and entwine around one another and form ropes. Fused fibers are bundles of fibers fused at the cut ends or along the fiber length. These cannot be separated by the shear forces in the mixing tank. Clumps or dumbbells are assemblages of normal fibers snared by a very long fiber at its ends.

Fiber type also has a powerful effect on log dispersion rate. Improvements can be made in reducing the number of log defects by improving surface finish and fiber characteristics. Fiber diameter (denier per filament) is a somewhat weaker variable. Dispersion rate generally improves as denier increases. The fiber cut length has a weak effect on dispersion rate [7]. At any rate, log defects and their formation are quite well understood and have been characterized by equations. Rope defects, however, are not as well understood, and further work needs to be done to properly characterize their formation. Ropes form when fibers encounter a vortex that is about the size of the fiber. Under such conditions, fibers are twisted into a string, or in extreme cases, they form agglomerates resembling the strands on a rag mop. Thus fiber supply, which plays an important role in the formation of log and dumbbell defects, is not a factor is rope formation. Previous studies, such as done by Shiffler [6, 7], indicate that vortex flow has a powerful effect on rope formation. The rope-formation rate was found to be approximately 10 times greater in the vortex flow than in the rolling flow [7]. Rope formation probably does not occur on a large scale during dispersion in large commercial agitators. It is more likely that a lot of the ropes are formed in the approach piping, since these vortices are on the same scale as the fiber length. Limited experience on a 0.9-m pilot paper machine tends to confirm this hypothesis. Surprisingly, many of the ropes formed in the vortex proved to be redispersible when the vortex was removed. This effect was discovered by stirring the fibers with alternating non-vortexing and vortexing flow. Many of the ropes formed during initial dispersion will redisperse in devices such as the fan pump. These ropes will not re-form if the approach piping is free of vortices on the scale of the fiber length. Thus vortex elimination, or damping in the approach piping, is a key factor in minimizing roping.

Vortices are typically caused by:

- Orifice plates used to measure flow rates
- Butterfly valves
- Gate valves or knife valves used for metering
- Dead-end tees in the piping
- Sharp elbows
- Instrumentation probes
- Abrupt reductions in pipe diameter
- Improperly designed pumps
- Improperly designed agitators

Rope formation can be reduced through careful elimination of vortices. Viscosity boosters, which damp the violence of vortices, are also effective in reducing rope formation. Improvements in dispersion rate also may increase the occurrence of rope defects, just as they do in the case of dumbbell formation. As dispersion improves, the fibers are present in a more finely divided and thus lower-modulus form, which makes them more easily twisted.

The use of chemicals to facilitate dispersion has also been studied. Effect of consistency, pH, agitator speed, and the presence of inorganic ions, and microbiological activity on the dispersion of synthetic fibers and performance of viscosity modifiers has been reported by Brandenburg [8]. A combination of Polyethylene glycol, phthalic acid, and monomeric glycol has been claimed to improve dispersion of polyester fibers in water [9]. In another study, a cross-section change to a cruciform shape has been claimed to improve the dispersibility of synthetic fibers in water [10]. While several qualitative phenomenological understandings for the defect formation and methods for preventing them are available as discussed earlier, a systematic study to understand the relationships between the flow process parameters and the defect formation with predictability has not been reported. This requires simultaneous modeling and experimentation. Mixing times in a turbulent stirred tank by means of large eddy simulation (LES) were reported [11]. However, the study was focused on mixing of fluids and did not involve multi-phase systems. Spatial distribution of floc sized in turbulent mixing of clay particle suspensions in water was modeled using computational fluid dynamics (CFD) [12]. Results showed that the regions close to the impeller (about 15% of the tank volume), promoted floc breakup while the reminder of the volume promoted floc aggregation [12]. For wood pulp suspension mixing, the dynamics have been studied using CFD in which the suspension is treated as a Non-Newtonian fluid [13]. Their work focused on power input prediction and they qualitatively assessed the predicted flow field results by visually observing the flow in experiments. The work did not use baffles in tank. A particle-level simulation to model the floc dispersion in simple shear and extensional flows has been reported by Switzer and Klingenberg [14]. It was shown that the simple shear flow disrupts completely while in extensional flow, the initial rate of disruption is higher, the disruption reaches a plateau, and the floc fragments remain intact [14]. This may be the reason why approach flow piping should be studied to minimize the floc formation. Tafreshi and Pourdeyhimi [15] conducted a numerical study using Computational Fluid Dynamics of wet lay fiber dispersion in mixing tanks and the role of baffles. Their simulations showed that aligning the baffles along the streamlines eliminated central vortex formation while maintaining the shear at satisfactory level. No experimental verification of the influence of baffles was offered.

The objective of this paper is to study the synthetic fiber dispersion process used in wet lay nonwovens manufacturing, through computational fluid dynamics (CFD) modeling and experiments. Specifically, the dispersion of synthetic fibers in a cylindrical tank with baffles and an impeller located in the center will be modeled. The effect of the cross-section shape of the baffles on the degree of dispersion will be studied and verified with experiments. While there are several possibilities for the cross section shape for the baffles and several configurations (one continuous element to staggered discrete elements), only two cross section shapes will be modeled, namely, rectangular and triangular cross sections. Similarly, there are several shapes possible for the impeller blades including number of blades and location of the impeller with respect to the center of the tank. We will model a three blade twisted blade impeller located in the center of the tank. The degree of dispersion will be determined through the formation of instantaneous webs by dipping and retrieving a flat strainer with a steel wire cloth into the tank and counting the defects in the formed sheet visually under a microscope. The tools can be useful in evaluating the processing potential of a new fiber, fiber blend, or white water chemical additive in wet lay nonwovens before commercial machine trials.

COMPUTATIONAL FLUID DYNAMICS MODEL

The mixing tank that was used in this study was a standard 55-gallon (208.2 liters) drum, 22.5 inches (0.5715 m) in diameter, and 31.5 inches (0.8 m) in height, with a centrally located impeller. This tank was modeled using a commercial computational fluid dynamics (CFD) software package, FLUENT (Fluent, Inc, Lebanon, NH, version 5.2) with the MIXIM [16] front end to facilitate easier and more accurate model generation for this problem. The overall framework of this general purpose code is to solve the conservation of mass and momentum equations. For the rotating flow problem, a multiple reference frame (MRF) approach [16] was used. In this approach, a rotating frame is used for the impeller while a stationary frame is used for the tank and baffles. The solution proceeds with a steady transfer of information across a predefined interface between the two frames. Only one position of the impeller relative to the tank is represented in the model. While the flow field analysis is? steady-state, this method can be used for transient analyses as well, involving other problem variables [17]. For a mixing tank with a single impeller, one can define a rotating reference frame that encompasses the impeller and the flow surrounding it, and use a stationary frame for the flow outside the impeller region. Steady-state flow conditions are assumed at the interface between the two reference frames. That is, the velocity at the interface must be the same (in absolute terms) for each reference frame. The grid does not move.

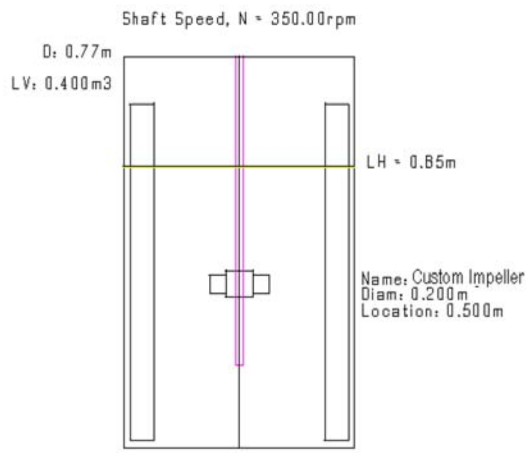

Figure 1.Tank Simulation model with four baffles

Water was used as the fluid and the standard k-e turbulence model was used for all calculations. A twisted blade impeller was used in the experiments and was modeled using the MIXIM user interface. *Figure 1* shows the dimensions chosen and *Figure 2* shows the modeled tank, baffles, and the impeller and shaft. The impeller rotates clockwise when viewed from above.

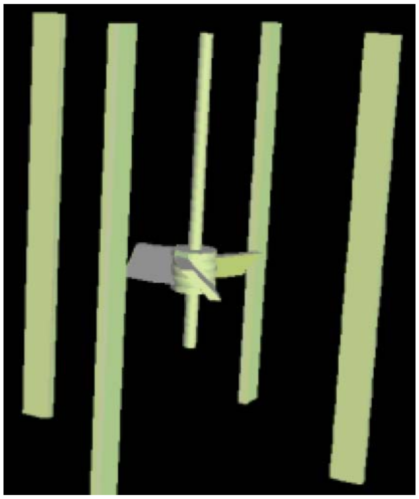

Figure 2. Model of the impeller and baffles

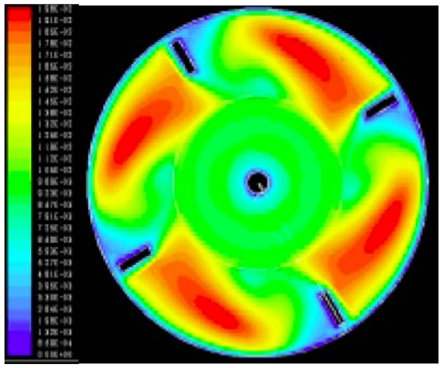

Figure 3. Kinetic Energy (KE) of turbulence above the impeller.

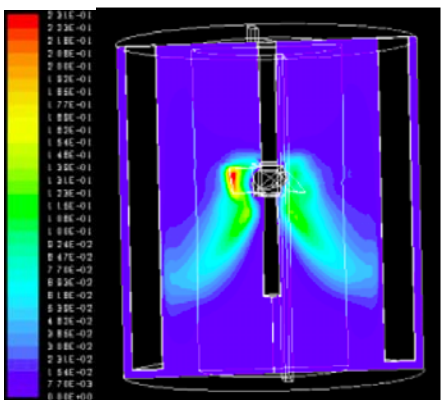

Figure 4. KE of turbulence through a vertical section

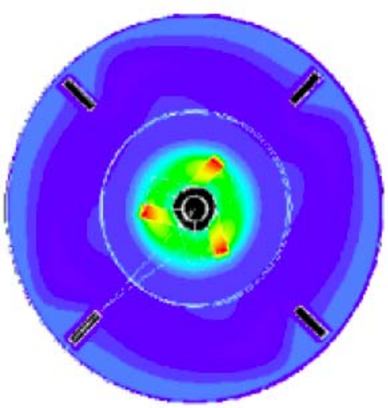

Figure 5. Velocity contours through a slice through the impeller

Figure 3 shows the KE of turbulence plotted for a horizontal slice above the impeller and *Figure 4* shows the KE of turbulence distribution on a vertical symmetry plane. *Figure 5* shows the velocity contours for the flow for horizontal section through the impeller. It can be seen that the areas of lowest turbulent kinetic energy were observed at the corners behind the baffles in the tank. These points are potential stagnation points. The installed baffles effectively break up the large central vortex observed in unbaffled mixing tanks (not shown). Local eddies are formed in the wake of each baffle as seen through the velocity profiles. These points are close to the stagnation points behind the baffles. This increases the residence time of the fluid element in by decreasing the kinetic energy in these areas. In the next step, particle tracking was attempted to visualize the accumulation of particles.

Discrete Phase Model

After obtaining a converged solution for the mixing tank described above, the solution was used to construct a discrete phase model. This is the injection of a solid phase into the flow domain to study the behavior of the injected particles in the turbulent flow as a post-processing operation (i.e., it is assumed that the presence of the solid phase does not affect the behavior of the much more dominant fluid phase). A 1.5 denier/filament, 0.25" chopped PET strand (6.35 mm) fiber was used as the solid phase. However, the software only accepts rigid spherical particles in particle tracking simulation. Hence, the fiber was approximated as a spherical particle with an equal volume and density. This is admittedly an oversimplification and the results can only predict accumulation of particles in localized regions and cannot account for the shape effects. However, with the knowledge of the flow field and accumulation, a particle-level simulation similar to the one cited [14] that takes into account the geometry of the fiber, and the mechanical properties of the fibers, can be used to predict tangling and formation of ropes in the flow. Particle tracking was performed for the fiber-representative spherical particles in the solved flow domain (fixed continuous phase flow field) using an uncoupled, stochastic approach. In this approach, the introduction of particles does not change the fixed continuous phase flow. FLUENT predicts the turbulent dispersion of particles by integrating the trajectory equations for individual particles, using the instantaneous fluid velocity, along the particle path during the integration [16]. The Discrete Random Walk (DRW) model is used. In this model, the fluctuating velocity components are discrete piecewise constant functions of time. Their random value is kept constant over an interval of time given by the characteristic lifetime of the eddies. By computing the trajectory in this manner for a sufficient number of representative particles, the random effects of turbulence on the particle dispersion are accounted for. The purpose of the particle tracking is to demonstrate the possibility that the particles may preferentially accumulate in different regions and not to directly quantify concentration profiles.

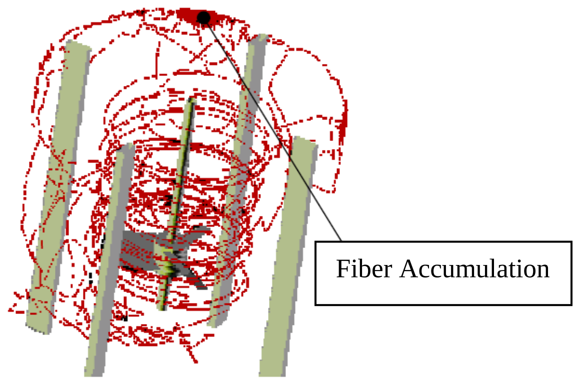

Figure 6. Particle trajectory and points of accumulation

Figure 6 shows a region of accumulation behind the baffle towards the top of the tank. The residence time for the solid phase was the longest in this area of the tank as observed earlier in the velocity profile. These regions are prime candidates for the generation of rope defects in practice, where a bunch of dispersed fibers have sufficient time and proximity to each other to entangle themselves in a loosely connected structure, namely, the rope structure.

Baffle Design

While a radial baffle, as studied, is effective in increasing the kinetic energy of turbulence and breaking up large vortices, the stagnation regions behind the baffles cause rope defects. We attempted a non-rectangular section for baffle cross-section and simulated the flow. *Figure 7* shows the velocity profiles around a rectangular radial baffle and *Figure 8* shows a triangular cross section providing a smoother transition or a smaller radial velocity gradient.

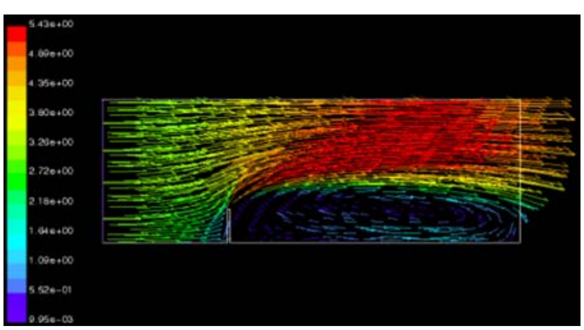

Figure 7. Velocity contours for flow past a rectangular baffle

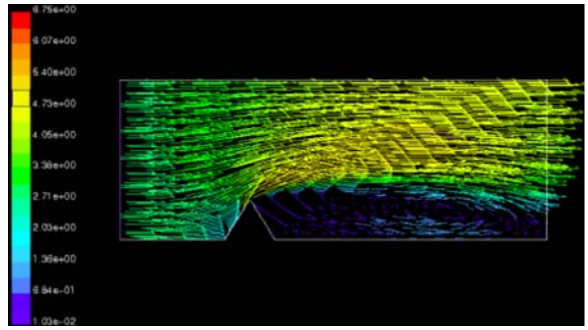

Figure 8. Velocity contours for flow past a triangular baffle

EXPERIMENTS

The following experiments were performed in an attempt to validate the results obtained from the simulations described in the previous section. A 55-gallon (208.2 linters) disposable mixing tank was obtained and four baffles were installed in it. A Lightnin mixer was installed in the center of the tank. The tank was filled with water, and PET fibers (0.25 inch (6.35 mm) long, 1.5 denier) were added to it at a concentration of 0.01% by weight. In the first set of experiments, the conventional baffles were used with a width of $1/12^{th}$ the diameter of the tank (Baffle width: 1.875 inches (43.2 mm); baffle height: 31.5 inches (0.80 meters)). Fibers were dispersed for fifteen minutes before the first sample was collected, although after about eight minutes, the fibers seem to have dispersed fairly uniformly. Two beakers of 400 ml volume were used to simultaneously obtain samples of the medium periodically from a point behind one of the baffles where local eddies were observed (point A) and from a point close to the center of the tank (point B) as shown in *Figure 9*. Since the flow itself has a steady upward circulation in addition to axial rotation, the samples are well mixed and represent the state of fibers into the depth of the tank.

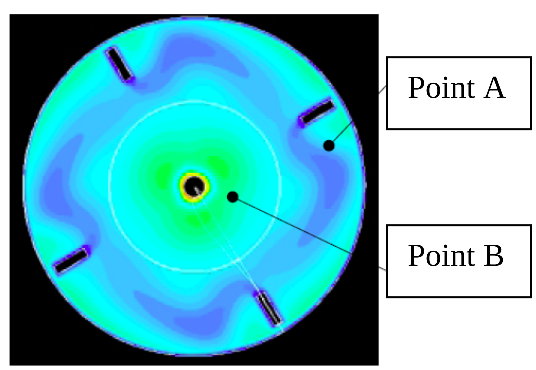

Figure 9. Sampling locations in the tank.

The fibers in each sample were extracted and weighed as a measure of instantaneous local fiber concentration. As predicted, samples from point A had higher concentration than samples from point B. It was observed that the weight of the fibers obtained from point A was about 36% greater than the weight of the fibers obtained from point B. For quantifying the defects in the suspension, it is required to get instantaneous samples of the sheet from the tank. The sample capturing device was fabricated using a stainless badminton racquet frame supporting a stainless steel wire cloth, 16 x 16 mesh, and 0.023 inch (0.5819 mm) wire diameter. The shape of the racquet head is an oval with major axis length of 261 mm and a minor axis length of 191 mm. By dipping the device into the tank at specific times quickly and removing it, a sheet is formed on the stainless steel wire instantaneously. The sheet is transferred to a blotting paper for further analysis of log and rope defects. Log and rope defects are defined by Vaidya et al [18]. A log defect is one where the chopped strand of fibers have not dispersed at all and look like a “log” with well-defined ends and length of the log is same as the fiber length. A micrograph of a portion of the sheet containing a log defect is shown in *Figure 10.*

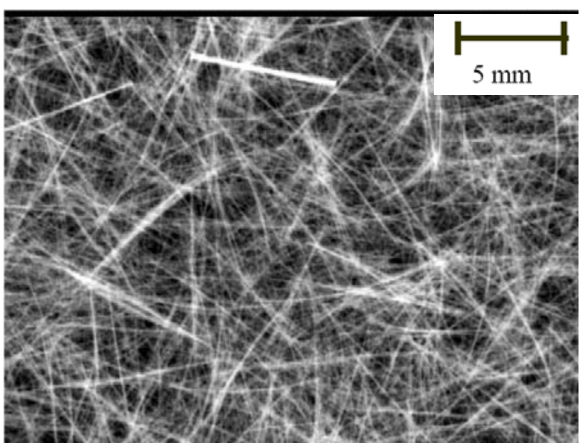

Figure 10. A log defect shown on a sample of 6.35 mm, 1.5 denier PET fiber sheet

The rope defects, on the other hand, are loosely connected fibers, substantially axially oriented, but the rope is substantially longer than individual fibers in the rope. The ropes may be partially dispersed fiber logs or formed by recombining previously dispersed fibers in recirculation zones. Example of rope defects are shown in *Figure 11*.

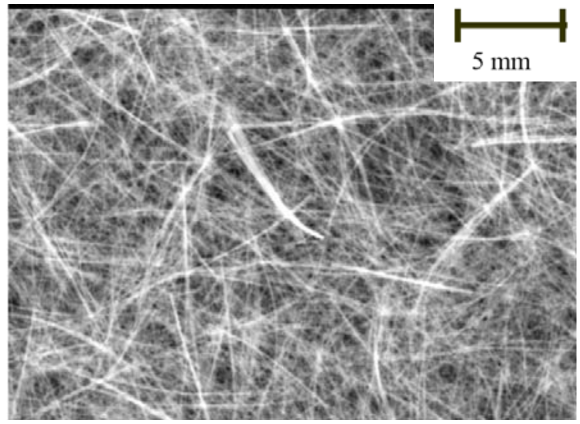

Figure 11. Rope defect in a sample sheet of 6.35 mm, 1.5 denier PET fiber sheet

Samples were collected at different dispersion times of 15, 23, 30, 37 and 45 minutes. A second set of experiments was conducted, replacing the standard baffles with modified baffles, with a triangular cross-section. Both sets of fibrous web samples obtained from the experiments were analyzed for log and rope defect counts, under a microscope. An area of 150 mm x150 mm in the center of the sheet was used for image analysis and defect counting. The sheet was weighed and the number of defects per 100 grams of fiber was calculated in every case. It was observed that points of local eddies (point A) were significantly more conducive to rope formation and precipitated a larger number of rope defects (43% increase) than points towards the center of the tank (point B). Modifying the baffles to a triangular cross section can result in increased log count, as shown in *Figure 12*. This is because of a decrease in shear stress exerted on the fiber bundles by the flow. Triangular cross-section baffles decrease velocity gradients in the flow field and hence, the shear stress.

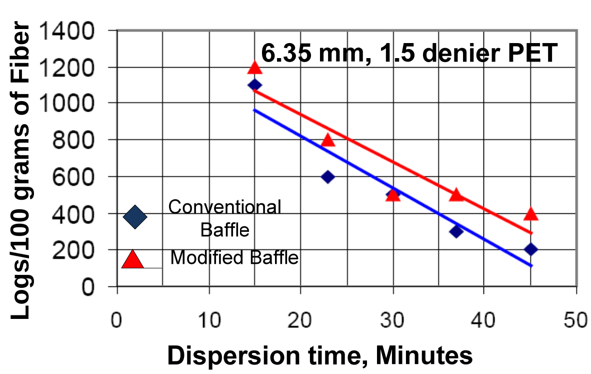

Figure 12. Log defects vs. dispersion time.

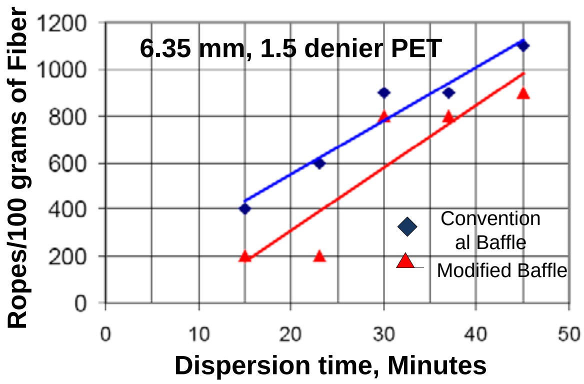

Figure 13. Rope defects vs. dispersion time.

Modifying the baffle cross section to a triangle instead of a rectangle, results in reduced rope formation at various dispersion times. This is because of the lower intensity and kinetic energy of the vortices formed behind the modified baffles. *Figure 13* shows rope defects versus dispersion time for the conventional and modified baffles. It is seen that the modified baffles result in lower rope defects. The experiments were repeated with two other fiber lengths, namely, (1.5 inch (38.7 mm), 1.5 denier), and (0.5 inch (12.7 mm), 1.5 denier). It was observed that the results had the same trends shown in *Figures 12* and *13*.

CONCLUSIONS

A complete 3D computational fluid dynamics analysis of the mixing tank with baffles and impeller was conducted using the FLUENT software. The geometry of the impeller was modeled accurately using MIXIM user interface. It was observed that the areas of lowest turbulent kinetic energy were located at the corners behind the baffles in the tank. These points are stagnation points. The installed baffles effectively break up the large central vortex observed in unbaffled mixing tanks in which recirculating flow is dominant. Local eddies were formed in the wake (behind the baffle, relative to fluid flow direction) of each baffle. These points are close to the stagnation points behind the baffles.

Spherical particles representing PET fibers by equivalent volume were injected into the 3D model mentioned above, and the motion of these particles in the flow domain was studied. The spherical equivalent particles show a tendency to collect at the stagnation points behind the baffles -- The residence time of the particle was greatest at points of stagnation behind each baffle in the tank. Experimental studies with the mixing tank and sampling at points near the center and behind the baffles found more rope defects in the sample behind the baffles. The log defect increases with lowering of the KE of turbulence while the rope defect decreases with the decrease in the velocity gradient, accomplished by two different baffle designs. Thus, it is possible to design the baffle geometry to obtain optimal mixing and dispersion while minimizing rope formation. CFD Model is useful in identifying the source and mechanism of defect formation, and offers a direction towards optimal process equipment design.

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