SIMULATIVE STUDY ON IMMISCIBLE VISCOUS FLUIDS MIXING IN SCREW EXTRUDER

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Abstract

Single and twin screw extruders are widely used machines for the mixing of viscous fluids. The idea behind this effort is to model the mixing of two immiscible viscous fluids in screw extruder by utilizing CFD software FLUENT available at the SCME.

The subject work has wide range of applications in process industries such as polymer, food and pharmaceutical in which two immiscible fluids with one having high viscosity are mixed to achieve desired properties. The basic goal in mixing viscous immiscible fluids is to produce a mixture with a desired structure and morphology. The structure might consist of a polymer blend or the drop size distribution in an emulsion.

Mixing in viscous fluids systems is a challenging task because no turbulent eddies are present to help distribute components. Because of the high matrix viscosity, diffusion coefficients for even very small molecules are exceedingly low. Mixing can be brought about in viscous systems only by mechanical action or by the forced shear or elongational flow of the matrix. Solids with a cohesive nature (such as agglomerated particles) or other immiscible fluids (drops with interfacial tension) will require intensive mechanical stress to achieve the required diminution. The first phase in this work is the creation of geometries of single and twin screw extruders in compatible software GAMBIT and meshing of the geometries to discretize the flow domain. In the second phase, export of both geometries in FLUENT is done for simulation by solving the fluid flow equations utilizing CFD codes.

Two immiscible fluids i.e Ethylene Vinyl Acetate (EVA) and Ethylene Glycol (EG) are selected for mixing. EVA is the copolymer of ethylene and vinyl acetate. The weight percent of vinyl acetate usually varies from 10 to 40%, with the remainder being ethylene. It is a polymer that approaches elastomeric materials in softness and flexibility, yet can be processed like other thermoplastics. The material has good clarity and gloss, barrier properties, low-temperature toughness, stress-crack resistance, hot-melt adhesive water proof properties, and resistance to radiation. Ethylene glycol is mixed in ethylene vinyl acetate as compatabilizer. However viscosity ratio of continuous phase (EVA) to dispersed phase (EG) is 5.095e 03 making it difficult for mixing to be done by turbulence. To model the mixing in such system, problem is set up in FLUENT 6.2. The appropriate boundary conditions at the inlet and outlet are set. The screws are rotated at 200 rpm for both single and twin screw extruder. Multiphase mixture model

is used for transient simulations. The unsteady state simulations are done because at each time step the screw meshes are moved to a new position, overlapping the flow mesh. For each node of this new domain that lies within a given screw, a special formulation is used that imposes a velocity that matches the rotation speed of the screw.

After solution convergence, results of pressure, velocity, shear stress, volume fraction, shear rate, vorticity magnitude distributions developed in the flow domain are studied and mixing index is evaluated to observe the dispersive and distributive mixing. Simulation results indicate shear stress gradient from the tip of the screw flight near the wall to the root of the screw. The axial velocity gradient is also observed from the inlet to the outlet indicting elongational stretching. The combination of shear stress gradient and axial velocity gradient show high shear and elongational stretching necessary for the dispersive mixing. Twin screw extruder is a better choice because it generates more elongational stretching in the fluids with less shear stress.

Acknowledgements

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I would like to dedicate this work to my parents, my wife and children for their sincere prayers and compromise on time which I could not be able to provide them during my studies.

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Nomenclature

Symbols		Unit
A	Face area	[m^2]
$A_{cross\text{-}section}$	Pipe cross-sectional area	[m^2]
D	Tube diameter	[mm]
G	Mass flux	[kg/(m^2 s)]
g	Acceleration of gravity	[m/s^2]
k	Turbulent kinetic energy	[m^2/s^2]
m	mass flow rate	[kg/s]
p	Pressure	[Pa]
γ	Strain-rate tensor	1/Sec
t	Time	[s]
u, v, w	Velocity components in x, y, z-directions	[m/s]
w,v,u	Stationary mean velocity components	[m/s]
w,v,u′′′	Fluctuating velocity components	[m/s]
U	Mean flow velocity	[m/s]
V	Velocity vector	[m/s]
Γ	Diffusion coefficient	[varying]
Δt	Time step size	[s]

δ_{ij}	Kronecker delta	[-]
Ω	Vorticity magnitude	1/Sec
λ	Mixing Index	
μ_c	Continuous phase Viscosity	Pa.s
μ_d	Dispersed phase viscosity	Pa.s
ρ	Density	[kg/s]
σ	Surface tension	[N/m]
τ	Shear Stress	[N/m^2]
φ	General flow variable	[varying]
ϕ	Under-relaxation factor	[-]
ψ	Two-phase flow parameter	[-]

Superscripts

T	Transposition

Dimensionless Groups

Re	Reynolds number
Pe	Peclet number

Prefixes

∇	Del:

∂	Partial differential $\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$

Abbreviations

EVA	Ethylene Vinyl acetate
EG	Ethylene Glycol
RTD	Residence Time Distribution
CFD	Computational Fluid Dynamics

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Chapter 1

Viscous Fluids Mixing

To start the project work it is necessary to get awareness of phenomenon of viscous fluids mixing. The chapter describes the general principles involved in mixing of viscous fluids, types of viscous fluids, the mixing equipment and their type. Salient features of these mixing equipment are also included. Literature searched during project work describing experimental and computational work by the various researchers is also presented.

1.1 Background

Viscous mixing involves the many applications in processes wherein the viscosity is sufficiently high (e.g., greater than 10 Pa. s) and turbulent mixing is usually unobtainable, or the dissipation of the viscous energy involved would result in an unacceptably high product temperature. Many industrially important products, such as pastes, putties, chewing gum, soap, grease, solid propellant, and some foods, fall into this category. In mixers handling viscous materials, it is necessary to promote both lateral and transverse motion, with the material(s) being pulled, sheared, compressed, kneaded, and folded by the action of rotor(s) against vessel walls, saddles, or projecting stators. [1]

Mixing is an operation whereby the non uniformity within a mixture is reduced. Mixing in viscous systems can be a formidable task. There are no turbulent eddies present to help distribute components. Because of the high matrix viscosity, diffusion coefficients for even very small molecules are exceedingly low. [1]

Mixing can be brought about in viscous systems only by mechanical action or by the forced shear or elongational flow of the matrix. These actions in viscous mixing are termed as dispersive mixing and distributive mixing. *Dispersive mixing* is defined as the breaking of agglomerates or lumps of dispersed phase to the desired ultimate grain size of the solid particulates or the (drops) of other immiscible fluids. Thus, dispersive mixing is a consequence of imposing mechanical stresses on the mixture. *Distributive mixing* is defined as providing spatial uniformity of all the components. In general, viscous fluids mixing operations are combination of dispersive and distributive actions; *intensive dispersive* mixing is the break up of globs or agglomerates, and *extensive distributive mixing* is spreading of the broken phase throughout the co-mixture. Both phenomenon are shown in fig 1.1[1].

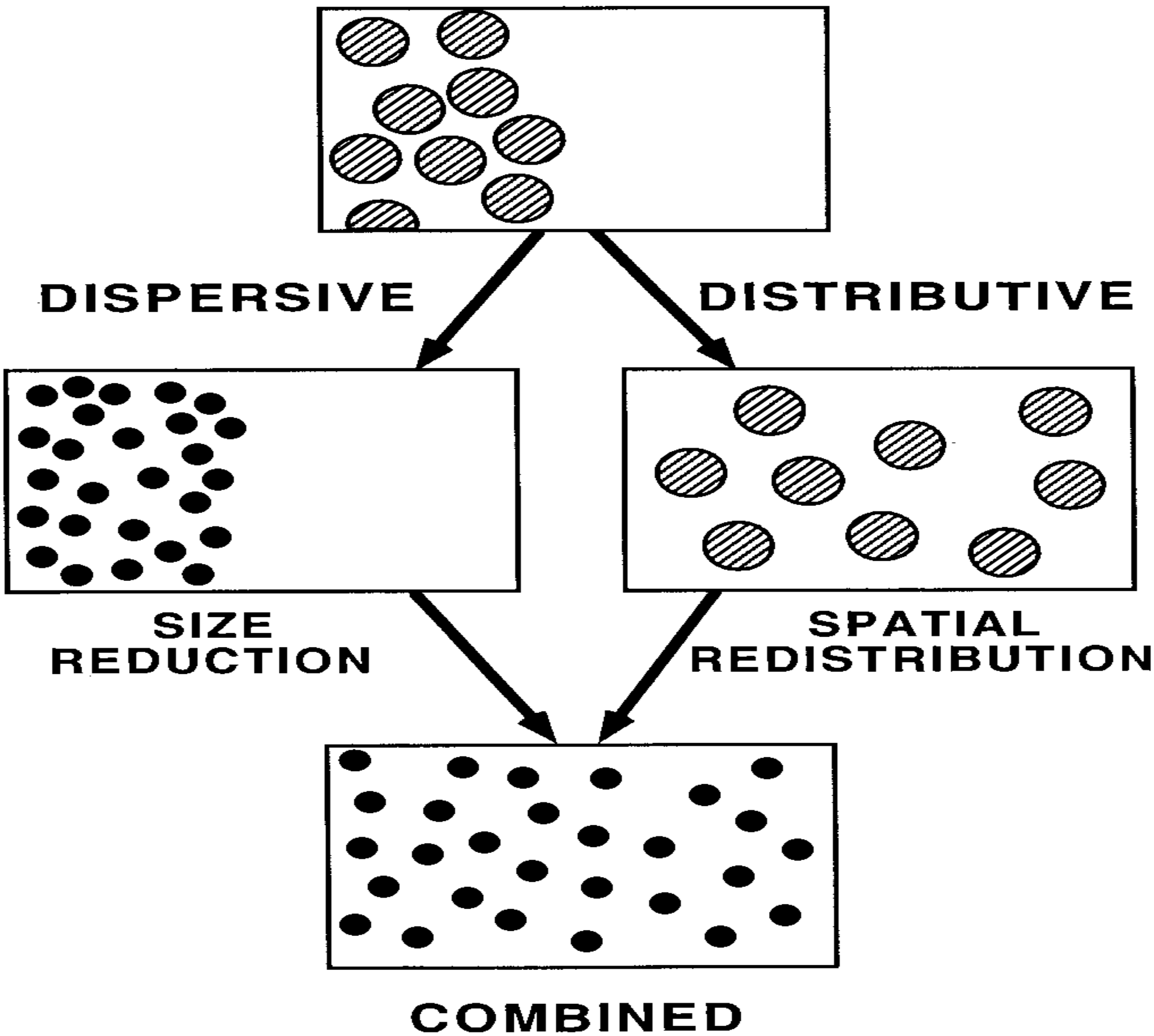

Fig 1.1 Morphology of dispersive and distributive mixing [1]

1.2 General Principles

Mixing is very important unit operation in process industry like polymer, pharmaceutical and food processing. It is employed to produce product of required specifications. Its purpose is to reduce in homogeneity in the blend or mixture of components. The in homogeneity can be one of concentration, phase, or temperature. Secondary effects, such as mass transfer, reaction, and product properties are usually the critical objectives. The basic principles involved in mixing phenomenon are laminar shear, extensional or elongational flow, distributive mixing, molecular diffusion, and dispersion. During mixing, material elements undergo continuous transient changes because shear and extensional rates vary a great deal from location to location. Mixing in highly viscous fluids is much complex issue than less viscous fluids because turbulent eddies in the mixing domain are absent to effect diffusion. The diffusion coefficient of even small molecule of viscous fluid is very low. Other complications associated with viscous fluids mixing are their Non Newtonian (means viscosity varies quickly with shear stress) behavior and temperature build up during mixing due to viscous energy dissipation. Mixing in viscous system is brought about by mechanical action or by forced shear or elongational flow of the matrix. In general, viscous mixing operations require some combination of dispersive and distributive actions. Fluids to be mixed can be miscible or immiscible [1].

1.3 Miscible Fluids Mixing

Miscible fluids possess no interfacial forces between them. Dispersed phase undergo stretching and folding to very thin lamella until complete diffusivity even though very low in matrix phase. The phenomenon is shown in Fig 1.2

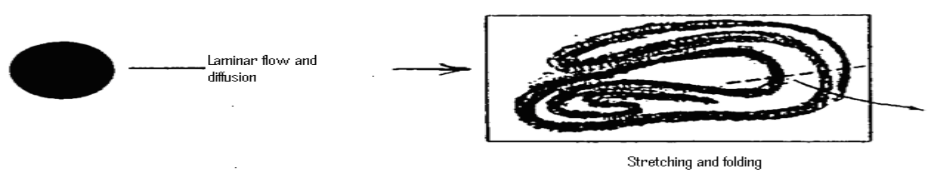

Fig 1.2 Distributive laminar mixing and diffusion with miscible fluids (no interfacial tension and very low diffusivities

1.4 Immiscible Fluids mixing

Initial mixing of viscous immiscible liquids occurs by stretching and folding of large blobs on a global scale; later stages are controlled by repeated stretching, folding, breakup, and coalescence of individual filaments or drops at local or homogeneous flow scales. In the beginning stages of mixing, large masses of the dispersed phase, d, are embedded in a continuous phase, c. The ratio of the viscosities of the dispersed to continuous phase μ_d/μ_c is denoted by p. The large masses of fluids are stretched and folded over. At this stage the capillary number, Ca, which is the ratio of the viscous forces to interfacial forces, is very large; therefore, interfacial forces do not play a significant role. As the process evolves, the capillary number decreases and the extended blobs break into many smaller drops. Concurrently, smaller drops begin to collide with each other and may coalesce into larger drops, which may in turn break again. The breakup and coalescence processes compete against each other and it is the result of this competition which determines the final drop size distribution or morphology [2]. The phenomenon is shown in the Figure 1.3.

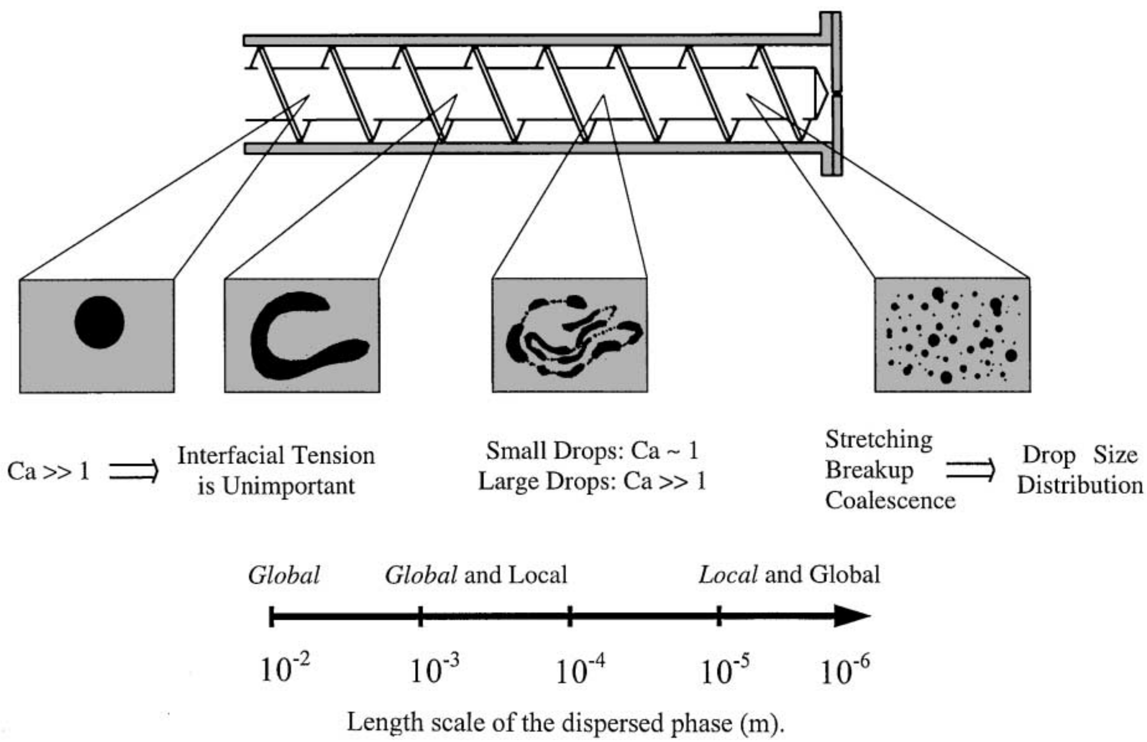

Fig1.3 Mixing of immiscible liquids starts from the initial stages in which mixing is controlled by the global properties of the flow

At the inlet of full flighted single screw extruder the Ca number is high which means viscous forces are much larger than interfacial forces and dispersed phase is present in the shape of large blob. The material is subjected to shear stress and stretching by the action of screw movement and large blob of dispersed phase is stretched into long thread and interfacial forces between phases increase and at certain stress the dispersed phase is broken into small drops .In the process of extrusion there is continuous coalescence of small neighboring drops to form large drop. This process of breaking and coalescence compete with each other to effect mixing of dispersed phase in the continuous phase.

1.5 Viscous Fluid mixing Equipment

Mixture of high viscosity i.e. >10 Pa.s can not be mixed with conventional impeller such as turbine or propeller stirrer. The high viscosity is due to the solids in slurry or high viscosity of the matrix itself. High viscosity is related with low mixing Reynolds number ($Re = \rho D^2 N/\mu$) which may be less than 100.The basic requirement of high viscous fluids mixer is to develop deformation in the fluids. The deformation is brought about by shear stress in the fluids but simple shear is inefficient and insufficient. Additional complexity in the system must be incorporated to improve mixing. The inefficient orientation of simple shear must be disrupted. When dispersion is required, region(s) of intense deformation must be created by having flow forced through narrow passageways either through passive orifices (consuming pressure drop) or between walls which move with respect to each other, such as provided by a closely fitting impeller (consuming power for rotation).[1]

Viscous fluids mixing equipment must have narrow clearance between impeller and vessel wall, high power per unit volume, relatively small volume and low impeller speed to limit heat buildup etc. There are two major classes of mixers for the viscous fluid.

1- Batch mixers

2- Continuous mixers

1.5.1 Batch Mixers

These are single stirrer mixers which may be of anchor blades or helical ribbons. The later is preferred as they provide end to end axial turnover as well and requires less power than anchor mixers. For very high viscosity fluids which are mostly Non Newtonian too, anchor blade mixers are not recommended because their central motion does not produce agitation at the vessel wall. [1]

1.5.2 Continuous Mixers

Recently these mixers are used extensively in mixing operation replacing batch mixers because of low power requirement, less material hold up in the machine, and continuous product attainment. But mixing efficiency can be reduced due to broad residence time distribution. So very accurate metering is required in continuous mixers. [1]

Screw extruders are most commonly used continuous mixer which has been classified as;

a) Single Screw Extruder

b) Twin Screw Extruder

1.5.2.1 Single Screw Extruder

In polymer processing industry, the most necessary step is to melt the polymer before further processing of mixing with other component. Single Screw Extruder converts mechanical energy of the drive into thermal energy, most of which is utilized to melt polymers. Feed is flood fed to the extruder. Feed rate is controlled by the take away capacity of the rotating screw. It has continuous helical flights, typically with lead distance (distance covered by screw in complete turn of 360 deg) normally equal to the screw diameter. The root diameter must be large enough to handle the torque. Our area of interest in this project work is the mixing section which acts as pump to drag the material forward. In screw mixer a sufficient pressure is needed to be generated at the inlet to overcome the resistance created in the machine due to presence of die at the exit. Due to this back pressure the material tend to flow back to the inlet offsetting some of the drag flow. The net capacity of the extruder is calculated as follows.

$Q = Q_d - Q_p$

Q= net capacity of the extruder

Q_d =volumetric drag flow forward

Q_p =volumetric pressure flow back the channel [1]

1.5.2.2 Twin Screw Extruder

While single screw extruder takes the advantage of friction between barrel and screw, the twin screw extruder capitalizes on interaction of two screws. They are classified as non inter meshing co rotating, counter rotating and inter meshing co rotating and counter rotating. In non inter meshing counter rotating extruders, flow in each screw channel is same as in single screw extruder with additional reorienting as flow oscillates between the screws. It achieves mixing only when it is full. It is well enough for distributive mixing but gives poor dispersive mixing. Intermeshing counter rotating extruders consists of essentially closed C-shaped chambers .There is milling effect with good elongational flow and good dispersion between the flights of one screw in cooperation with the channel of the other. These have regions of low volume under going high shear and potential over heating there by limiting screw speed and capacity.

The most commonly used extruder is co rotating inter meshing with flight tip of one rotor intermesh and wipe the channel of the other. With almost half of each screw in close contact with the barrel, the conventional intermeshing counter rotating twin screw extruder has regions of low volume undergoing high shear and potential overheating, thereby limiting the screw speed and potential capacity of this type of twin screw extruder. [1]

Over the last decade there is much increase in the study of this subject. There are number of papers available on the viscous fluids mixing describing experimental and computational work. In the following section work of some researchers is presented.

1.6 Literature Review

1.6.1 Experimental Work

1.6.1.1 Mixing of Liquid/Polymer in twin screw extruder by residence time distribution [6]

The viscous fluids mixing is very important unit operation being carried out in process industry but measurement of mixing efficiency is quite tedious task. People studied indirect methods to study mixing efficiency. P.Cassagnau, M.Courmont and others in 2005 studied the immiscible fluids mixing by measuring residence time distribution of fluids. They injected UV tracer material (Hydroxymethyl anthracene) for EVA. A master batch was prepared with 1% tracer material in molten EVA. EG tracer was also manually prepared separately. The measured RTD for each phase in the mixer is determined by employing UV fluorescence device at the outlet. The extrusion process is done in 34 mm diameter twin screw extruder with L/D ratio of 35.EVA is fed at molten state at a temperature of 140 deg C. Experiments were conducted on three geometries with slight variations to improve mixing. These variations are adding reverse conveying element after kneading section and change in the flight angle. Residence time distribution of EG was measured at different speed and at different flow rates. It was concluded that at higher flow rates the lubrication effect comes into play and increase in residence time is observed. Higher speeds will enhance shear effects and more dispersion is expected. So high flow rates and high screw speed will increase RTD and hence better mixing.

1.6.1.2 Velocity distribution and mixing measurements in Twin screw extruder [7].

This study is conducted by L. Yerramilli and M. V. Karwe in 2004. Velocity distribution in the translational region of twin screw co- rotating self wiping extruder was determined using Laser Doppler Anemometry. To know flow field and to evaluate mixing effectiveness in the kneading section of the machine, experiments were run on Newtonian fluids on three speeds of the screw to determine velocity distributions. Effects of screw pitch in screw geometry are also observed in flow field .Total shear rate distribution and flow number (mixing index) is determined. From the results it is concluded that by increasing the screw pitch and screw speed have substantial increase in mixing. It was also concluded dispersive mixing is more than distributive mixing in translational region of the extruder.

1.6.2 Computational Work:

During the last decade or so there is tremendous increase in work on modeling of the subject by solving numerical equations using CFD codes.

1.6.2.1 Computational models for strong–weak and continuous flow systems [2]

The most common way to model the initial stages of mixing is to numerically solve the Stokes equations for the two phases. A number of methods have been used for this purpose; the volume of fluid method (Zhang & Zumbrunnen, 1996, Chella & Vi˜nals, 1996), moving mesh methods (Hyman, 1984), and the marker and cell technique (Chakravarthy & Ottino, 1996). Level set methods (Sussman et al., 1999), have not been used for mixing applications but they are well suited for this purpose as well. More recently, mapping methods have been developed; it may be possible to extend this methodology to multiphase systems as well (Wetzel & Tucker, 1999; Anderson, 1999; Kruijt, 2000). All methods work reasonably well for the beginning of mixing and each has its advantages depending on the problem being solved. Manas-Zloczower, Nir, and Tadmor (1984) proposed a model for the dispersion of carbon black in an elastomer. P. DeRoussel, D.V. Khakharb, J.M. Ottino in 2001 studied mixing of viscous immiscible liquids. Computational models for strong–weak and continuous flow systems. Robin K. Connelly , Jozef L. Kokini studied mixing ability of single and twin screw mixers using 2D finite element method simulation with particle tracking. They used CFD package Polyflow with Carreau flow model to generate velocity distribution and particle trajectories for dough mixer. The mixed Galerkin FEM simulations use a rotating reference frame technique with the single paddle mixer and a mesh superposition technique in the twin paddle mixer. Differences in the velocity profiles are noted. Distributive mixing is evaluated visually as well as using the segregation scale and cluster distribution index; stretching is evaluated using the length of stretch and mixing efficiency; and dispersive mixing is evaluated using the mixing index in combination with the shear stress. [3]

1.6.2.2 Mixing efficiency in a kneading block section of a twin-screw extruder [5].

B. Alsteens1, V. Legat, Th. Avalosse in 2004 conducted the work of studying mixing efficiency in kneading section of twin screw extruder by varying geometric parameters such as stagger angle and disc width. CFD software Polyflow and finite element model of governing equations of discretization is utilized. The mixing efficiency is evaluated by comparing the residence time and the total shear distributions of a large set of virtual particles launched in the flow domain.

1.6.2.3 CFD model for viscous drop breakup [9].

L.J. Dietschea, A.C.Neubauer worked on CFD model for the viscous drop breakup in low viscous matrix phase. The process is challenging because simple shear forces alone are not capable of breaking high viscous additives into blend as capillary number (Ca) i.e ratio of viscous forces to interfacial forces is very high. Breakup mechanisms depend upon the deformation process (shear and/or extension flow fields), system and component physical properties (miscibility, interfacial tension, solubility, rheology, density, and so on). The commercial CFD code, FLUENT 6, is used to solve the system of equations needed to track the droplet phase as it travels past breakup-inducing obstacles. A volume of fluid (VOF) method is used to track the interface between the droplet and matrix phases. The model is able to predict droplet breakup and provide insights into the physics of the breakup process. Three different breakup mechanisms are hypothesized that help to explain experimental observations, including a minimum in breakup efficacy (ability to create smaller droplets) versus velocity data. Important parameters include the system rheology, velocity, cylinder size versus droplet size, and cylinder layout.

1.6.2.4 Simulation of polymeric flow in Twin screw extruder- elongational viscosity effects [4]

A. Shah and M. Gupta developed a three dimensional simulation approach in twin screw extruder using Flow Network Analysis (FAN) technique to study the effect of elongational viscosity on the flow is analyzed using independent power law models for the shear and elongational viscosities. For the purpose bench scale twin screw geometry is developed with screw tip diameter of 29.2 mm and screw root diameter of 21mm and screw lead is 30mm. The flow is simulated on fluid with three different viscosity models. Simulation results are summarized as follows. Flow of a polymer in an intermeshing co-rotating twin-screw extruder is simulated. Effect of elongational viscosity on the flow is analyzed using independent power law models for the shear and elongational viscosities. Axial component of the velocity is found to be maximum in the intermeshing region of the extruder. Axial component of velocity, which determines the throughput of the extruder, decreased as the elongational viscosity of the polymer used for the flow simulation was increased. The pressure in the extruder decreased from a very high positive value on the leading edge to a very large negative value on the trailing edge of the screw. For the same rotational speed, the pressure build-up in the twin-screw extruder is increased as the elongational viscosity of the polymer was increased.

1.7 Objective of Work

The basic objective of this project is to study the mixing of viscous fluids computationally utilizing CFD codes. Single and twin screw extruders are selected machines. CFD software FLUENT 6.2 is utilized for modeling. The other objective is to learn CFD concepts and mechanism of software to apply CFD codes. To fulfill these objectives single and twin screw extruder geometries are developed in compatible software GAMBIT and after proper meshing these are simulated in FLUENT. The system selected for the mixing is based on experimental data available in literature [6]. Study of dispersive and distributive mixing is done by studying pressure, shear stress, strain rate, velocity and vorticity contours developed after convergence.

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Chapter 2

Computational Fluid Dynamics (CFD)

2.1 Introduction

The project relates with the computational study utilizing CFD codes. It is worth while to present the introductory information regarding CFD.

Computational fluid dynamics, or CFD, is the numerical simulation of fluid motion. While the motion of fluids in mixing is an obvious application of CFD, there are hundreds of others, ranging from blood flow through arteries, to supersonic flow over an airfoil, to the extrusion of rubber in the manufacture of automotive parts [4]. Numerous models and solution techniques have been developed over the years to help describe a wide variety of fluid motion.

2.2 The Structure of CFD

CFD codes are all structured around the numerical algorithms that will solve the fluid flow problems. The CFD code consists of the following three fundamental features [1];

1. Pre-processor
2. Solver
3. Post-processor

1 Pre-processor

The task for the pre-processor is to gather the essential information needed for the solver to tackle the problem, i.e the in-data. This involves;

• Generation of the grid that defines the geometry of interest, i.e. the computational domain.

• Specifications of the physical and chemical phenomenon that need to be modeled.

• Definition of the fluid properties.

• Specifications of appropriate boundary conditions.

2 Solver

The aim for the solver is to carry out the numerical calculations necessary to produce satisfactory simulations of the flow problem. The solver can be based on the following three techniques: finite difference, finite element and spectral methods. The main differences between these techniques are based on how the variables of flow are approximated and, on the discretisation process. FLUENT uses a technique called the finite volume method (FVM). This method was originally developed as a special finite difference formulation and will be discussed in the following section [1].

3 Post-processor

The post-processor returns the results of the simulation calculated by the solver. Today, most of the available CFD programs have developed graphical tools, which make it possible to receive a visualization of the calculated data. Examples of this follow below:

• Vector plots of the velocity field.

• The ability to track the path of a particle through the domain.

• Contour plots

• Animations of the fluid flow.

• View manipulation (translation, rotation, scaling etc.)

2.3 Governing Equations of Fluid Flow

Fluid flow is governed by three basic conservation equations, which are conservation of mass, momentum and energy. All CFD software including FLUENT 6.2 is used to perform calculations of the fluid flow field of concern. The governing equations of fluid flow are as follows.

2.3.1 Equation of Continuity (conservation of mass)

Consider the infinitesimal fixed control volume shown in Figure 2.1:

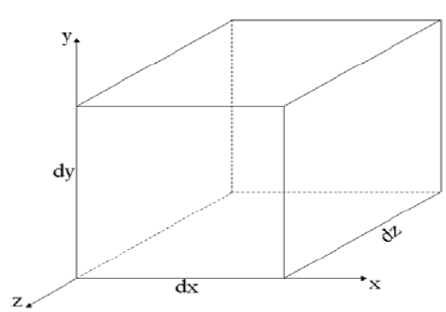

Figure 2.1: Infinitesimal fixed control volume.

The following equation can be derived if a mass conservation is applied on the volume:

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$$\frac{\partial u_i}{\partial x_i} = 0 \qquad \textbf{(2.1)}$$

This is the equation of continuity, which, in its present shape, is valid for situations when the flow is incompressible and no source or sink singularities exist within the volume

2.3.2 Equation of Momentum

The differential momentum equation valid for any fluid in any general motion is obtained by applying Newton's second law of motion on the control volume above:

$$\rho g_i - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j} = \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} \qquad (2.2)$$

$$s_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \qquad (2.3)$$

Equation (2.2) can now be rewritten as the famous Navier-Stokes´ equation:

$$\rho g_i - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\mu s_{ij}\right) = \rho \frac{\partial u_i}{\partial t} + \rho \frac{\partial}{\partial x_j}\left(u_j u_i\right) \qquad (2.4)$$

2.4 Models for multiphase fluids mixing In FLUENT

The subject project deals mixing of two immiscible fluids making two phase system. The problem can be modeled utilizing multiphase model. There exist two different approaches for modeling multiphase flows by the way of numerical calculations: The Euler-Lagrange approach and the Euler-Euler approach. Short introductions to these approaches are given below [2].

2.4.1 The Euler-Lagrange Approach

The Euler-Lagrange approach treats the fluid phase as a continuum by solving the time-averaged Navier-Stokes equations while the dispersed phase is solved by tracking a large number of particles, bubbles or droplets through the calculated flow field. The dispersed phase can interact with the fluid phase by exchanging momentum, mass and energy.

The approach computes the trajectories of the particles or droplets at specified intervals during the fluid phase calculation. This makes it ideal for flow problems involving spray dryers, coal and liquid fuel combustion and some particle-laden flows. A fundamental assumption made by the Euler-Lagrange approach is that the dispersed second phase occupies a low volume fraction making it inappropriate to model flow problems involving liquid-liquid mixtures, fluidized beds or any other application where the second phase is not negligible.
FLUENT possesses one model that adopts the Euler-Lagrange approach:

- The Lagrangian discrete model

2.4.2 The Euler-Euler Approach

The Euler-Euler approach treats the different phases as interpenetrating continua. The concept of phasic volume fraction is introduced in this model because the volume of one phase cannot be occupied by other phases. The sum of these volume fractions is equal to unity in every cell and they are assumed to be continuous functions of space and time.

There are three basic models available in FLUENT for modeling of multiphase fluids based on Euler-Euler approach. These are [2]

- Volume of Fluid (VOF) Model
- Mixture Model
- Eulerian Model

2.4.2.1 Volume of Fluid (VOF) Model

The VOF model can model two or more immiscible fluids by solving a single set of momentum equations and tracking the volume fraction of each of the fluids throughout the domain. Typical applications include the prediction of jet breakup, the motion of large bubbles in a liquid, the motion of liquid after a dam break, and the steady or transient tracking of any liquid-gas interface. The VOF formulation in FLUENT is generally used to compute a time-dependent solution, but for problems in which you are concerned only with a steady-state solution, it is possible to perform a steady-state calculation. A steady-state VOF calculation is sensible only when your solution is independent of the initial conditions and there are distinct in flow boundaries for the individual phases. The limitations of VOF model are as follows [2].

1- Only segregated solver can be employed.

2- Flow control volume is filled with one fluid or other or combination of both .There is no void region in the flow domain.

3- Only one of the phases can be defined as a compressible ideal gas. There is no limitation on using compressible liquids using user-defined functions.

4- The LES turbulence model cannot be used with the VOF model.

5- The second-order implicit time-stepping formulation cannot be used with the VOF model.

2.4.2.2 Mixture Model:

The mixture model is a simplified multiphase model that can be used to model multiphase flows where the phases move at different velocities, but assume local equilibrium over short spatial length scales. The coupling between the phases should be strong. It can also be used to model homogeneous multiphase flows with very strong coupling and the phases moving at the same velocity. In addition, the mixture model can be used to calculate Non-Newtonian viscosity. The mixture model can solve n phases (Fluid or particulate) by solving momentum and continuity equations for mixture, volume fraction equations for secondary phases. The mixture model is a good substitute of full scale Eulerian model because it can perform like Eulerian model by solving less number of variables though results may not be accurate as of Eulerian model.

2.4.2.3 Eulerian Model:

The Eulerian multiphase model in FLUENT 6.2 allows for the modeling of multiple separate, yet interacting phases. The phases can be liquids, gases, or solids in nearly any combination. An Eulerian treatment is used for each phase, in contrast to the Eulerian Lagrangian treatment that is used for the discrete phase model. With the Eulerian multiphase model, the number of secondary phases is limited only by memory requirements and convergence behavior. Any number of secondary phases can be modeled, provided that sufficient memory is available. For complex multiphase flows, however, you may need that your solution is limited by convergence behavior. This model differs from mixture model in the sense there is no global distinction between fluid fluid flow or fluid solid (granular) flow. A granular flow is simply one that involves at least one phase that has been designated as a granular phase. The solution is based on the following.

-A single pressure is shared by all phases.

_ Momentum and continuity equations are solved for each phase.

- Several inter phase drag coefficient functions are available, which are appropriate for various types of multiphase regimes.

2.5 Choosing a General Multiphase Model:

The VOF model is appropriate for stratified or free-surface flows, and the mixture and Eulerian models are appropriate for flows in which the phases mix or separate and/or dispersed-phase volume fractions exceed 10%. Flows in which the dispersed-phase volume fractions are less than or equal to 10%, can be modeled using the discrete phase model. To choose between the mixture model and the Eulerian model, one should consider the following

If there is a wide distribution of the dispersed phases (i.e., if the particles vary in size and the largest particles do not separate from the primary flow field), the mixture model may be preferable (i.e., less computationally expensive). If the dispersed phases are concentrated just in portions of the domain, one should use the Eulerian model instead. If inter phase drag laws that are applicable to the system are available (either within FLUENT or through a user-defined function), the Eulerian model can usually provide more accurate results than the mixture model. Even though one can apply the same drag laws to the mixture model, as for a non-granular Eulerian simulation. If the inter phase drag laws are unknown or their applicability to your system is questionable, the mixture model may be a better choice. For most cases with spherical particles, then the Schiller-Naumann law is more than adequate. For cases with non-spherical particles, then a user-defined function can be used. If you want to solve a simpler problem, which requires less computational effort, the mixture model may be a better option, since it solves a smaller number of equations than the Eulerian model. If accuracy is more important than computational effort, the Eulerian model is a better choice. Keep in mind, however, that the complexity of the Eulerian model can make it less computationally stable than the mixture model.

2.6 Selection of Mixture Model:

Our problem relates with mixing of immiscible high viscosity copolymer Ethylene vinyl acetate(EVA) with low viscosity Ethylene glycol .The ratio of continuous phase viscosity to dispersed phase viscosity is the range of 5.095e 03 ,so system may be treated as dispersed phase of ethylene glycol embedded in continuous phase of ethylene vinyl acetate(EVA). On this basis discrete phase model, mixture model and Eulerian model can be selected. As volume fraction of dispersed phase i.e ethylene glycol is more than 10%, so discrete phase model is rejected. Mixture model and Eulerian model can be selected .Due to time constraint mixture model is selected because of simplicity and requirement of less computational effort. More over complexity of the Eulerian model can make it less computationally stable than the mixture model.

2.7 The Finite Volume Method (FVM)

Due to the fact that FLUENT attacks physical or engineering problems by using the finite volume method, a short description of this method will be given. The numerical algorithm of FVM has the following structure:

1. Exact integration of the governing equations of fluid flow over all the control volumes within the solution domain.

2. Discretization involves substitution of a variety of finite difference-type approximations for the terms in the integrated equation representing the flow processes. The terms in question are convection, diffusion and source terms. By doing this the system of integral equations are transformed into a system of algebraic equations that can be solved numerically.

3. Solution of the algebraic equations by an iterative method.

It is the first step that differs the finite volume method from the other numerical techniques. The finite volume method expresses the conservation of relevant properties for each finite size cell. It is this clear relationship between the numeric algorithm and the physical principal of conservation that makes the finite volume method easier to apply and understand than finite element and spectral methods.

With the finite volume method the conservation of a general flow variable, φ, can be described as a balance between different processes which tend to increase or decrease φ. In other words:

Rate of change of ϕ in the control volume with respect to time	=	Net flux of ϕ into the control volume due to convection
	+	Net flux of ϕ into the control volume due to diffusion
	+	Net rate of creation of ϕ inside the control volume

Below, a brief run-through of the three steps from which the finite volume method is build.

The general equation of transport, which serves as a starting point for computational procedures in the finite volume method, is written in the following form:

$$\frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x_i}(\rho\phi u_i) = \frac{\partial}{\partial x_i}\left(\Gamma\frac{\partial\phi}{\partial x_i}\right) + S_\phi \qquad (2.5)$$

Where Γ is a diffusion coefficient, e.g., thermal conductivity, ρ is the density [kg/m^3] and S_φ is a source term.

For a more straightforward and easy explanation a stationary, one-dimensional convection and diffusion problem will be considered. To make it even more basic there will be no production of φ inside the control volume (i.e. S_φ=0).

These simplifications make it possible to write equation (2.5) in the following manner:

$$\frac{d}{dx}(\rho u\phi) = \frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right) \qquad (2.6)$$

Mass conservation yields:

$$\frac{d}{dx}(\rho u) = 0 \qquad (2.7)$$

1. Integration of the Equation of Transport over a Control Volume

Consider a one-dimensional control volume shown in Figure 2.2 below. The node of interest is P and the neighboring nodes are W and E. The control volume for which P represent the centre is restricted by faces w and e.

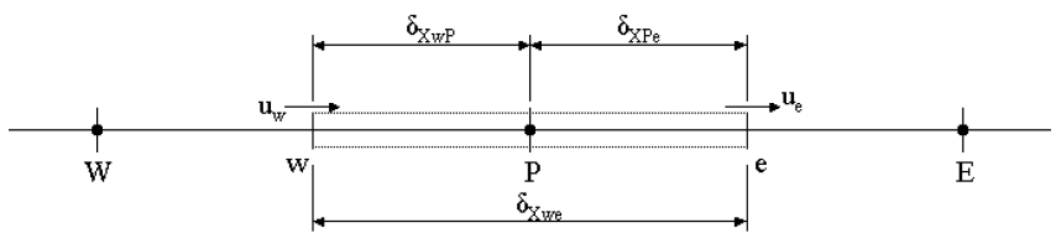

Figure 2.2: Control volume around node P

Integration of equation (2.5) and (2.6) over the control volume gives the equation (2.7a and 2.7b)

$$(\rho u A \phi)_e - (\rho u A \phi)_w = \left(\Gamma A \frac{\partial \phi}{\partial x}\right)_e - \left(\Gamma A \frac{\partial \phi}{\partial x}\right)_w \qquad (2.7a)$$

$$(\rho u A)_e - (\rho u A)_w = 0 \qquad (2.7b)$$

2. Discretisation

The terms in equation (2.7a) must be approximated in order to achieve discretised equations. It has been found convenient to define two variables F and D to represent the convective mass flux per unit area and diffusion conductance at cell faces, respectively:

$$F = \rho u$$
$$D = \frac{\Gamma}{\delta x}$$

The variables F and D at the different cell faces can be expressed as

$$F_w = (\rho u)_w, \qquad F_e = (\rho u)_e \tag{2.8}$$

$$D_w = \frac{\Gamma_w}{\delta x_{WP}}, \qquad D_e = \frac{\Gamma_e}{\delta x_{PE}} \tag{2.9}$$

Using the central differencing scheme, the following expressions are achieved:

$$\left(\Gamma A \frac{\partial \phi}{\partial x}\right)_e = \Gamma_e A_e \frac{\phi_E - \phi_P}{\delta x_{PE}} = D_e A(\phi_E - \phi_P) \tag{2.9}$$

$$\left(\Gamma A \frac{\partial \phi}{\partial x}\right)_w = \Gamma_w A_e \frac{\phi_P - \phi_W}{\delta x_{WP}} = D_w A(\phi_P - \phi_W) \tag{2.10}$$

$$(\rho u \phi A)_e = (\rho u A)_e \frac{\phi_E + \phi_P}{2} = \frac{F_e}{2} A(\phi_E + \phi_P) \tag{2.11}$$

$$(\rho u \phi A)_w = (\rho u A)_w \frac{\phi_P + \phi_W}{2} = \frac{F_w}{2} A(\phi_P + \phi_W) \tag{2.12}$$

The integrated equation of mass conservation can be written as:

$$F_e - F_w = 0 \tag{2.13}$$

By inserting equations (2.9) to (2.12) into equation (2.7a) the following expression is achieved:

$$\left[\left(D_w + \frac{F_w}{2}\right) + \left(D_e - \frac{F_e}{2}\right) + (F_e - F_w)\right]\phi_P = \left(D_w + \frac{F_w}{2}\right)\phi_W + \left(D_e - \frac{F_e}{2}\right)\phi_E$$

which can be rewritten in the following fashion:

$$a_P \phi_P = a_W \phi_W + a_E \phi_E \tag{2.14}$$

where

$$a_W = D_w + \frac{F_w}{2}, \quad a_E = D_e - \frac{F_e}{2}, \quad a_P = a_W + a_E + (F_e - F_w)$$

Due to this the variable φ in the node, P can now be described with the values in the neighboring nodes W and E.

The central differencing possesses one major weakness, which is revealed for flows where convection is not negligible compared to diffusion. The relationship between convection to diffusion is often measured with the Peclet number, Pe, which is defined as

$$Pe = \frac{F}{D} = \frac{\rho u}{\Gamma / \delta x} \quad [-] \tag{2.15}$$

Figure 2.3.2 shows the distribution of φ depending on different values of Pe.

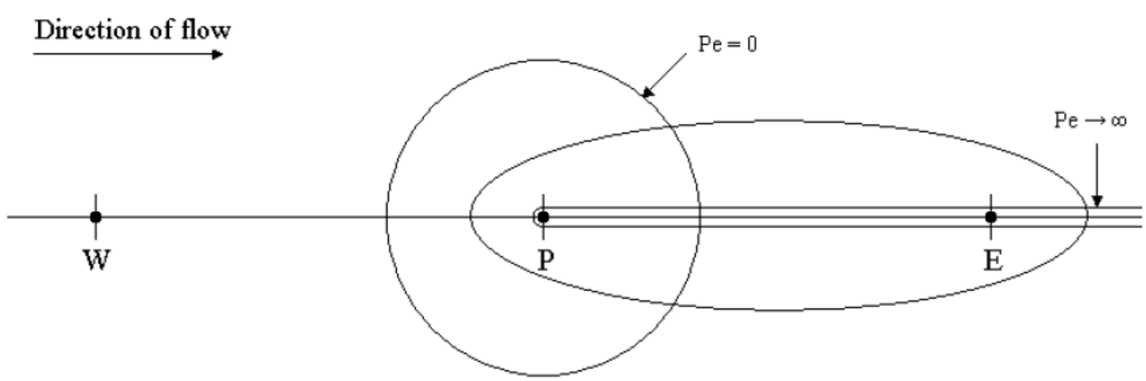

Figure 2.3.2: Distribution of φ at different Pe numbers .

For the case where Pe = 0 (i.e., pure diffusion) conditions at node E will be influenced by those upstream at node P but also by those further downstream. As Pe increases the conditions at E will be more influenced by those at P and less by those further downstream. In the case of pure convection (Pe → ∞) the conditions at E will be equal to those at P.

The central differencing scheme assumes equal influence from all neighboring nodes when calculating the value at P. This will cause some serious problems for flows where the value of Pe is not negligible. Therefore, CFD codes utilize the central differencing scheme only for the discretization of the diffusion terms, i.e., the terms on the right hand in equation. The convective terms are discretized by so- called upwind schemes. FLUENT supports four different upwind schemes for the user to utilize: First Order Upwind, Power Law, Second Order Upwind and QUICK. Please consult references for more details on these schemes.

3. Solution

When the equations of interest have been discretized, the problem is solved with iterative methods. An example is the TDMA method, which stands for Tri-Diagonal Matrix Algorithm. It is considered to be computationally inexpensive and to require a minimum amount of storage. This has made it very popular and is thus widely used in CFD programs, FLUENT included.

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Chapter 3

CFD Modeling of Viscous Fluids Mixing

Viscous fluid mixing is very important unit operation in industries like polymer, food and pharmaceutical. The major applications of the process are addition of additives in matrix to improve properties and appearance of desired product, to produce homogeneous blend of medicines and eatables. In solid rocket fuel motor casting, mixing of constituents play very vital role in performance of rocket. Mixing becomes complex phenomenon when it deals with very high viscous fluids as very high stresses are required to cause deformation in the fluids necessary to mix with each other. In recent years many researchers worked extensively for solving viscous fluids mixing problem. Experimental work is expensive and time consuming. Now the mode is shifted towards modeling of viscous fluids mixing using CFD codes. Although the results obtained are only prediction but many researchers proved that results are closed to experimental ones. It allows such detailed performance information without experimentation which allows process engineers to design advanced and more efficient process equipment with confidence [1].CFD modeling therefore saves time and money required for the designing of mixing equipment. This chapter narrates a brief description of CFD modeling techniques for viscous fluids. Parameters for mixing efficiency are also discussed.

3.1 CFD Modeling Techniques

Finite element method and finite volume method is usually used in modeling the viscous immiscible fluids mixing. Fluent employ finite volume method for system modeling. The salient features of finite volume method are described in chapter 2. The CFD software polyflow has employed finite element method for the system modeling. At SCME FLUENT 6.2 is available which uses finite volume method.

In finite element method piecewise linear or quadratic functions to describe the variation of the variable φ within a cell is used. By substituting the selected function into the conservation equation for each cell and applying the boundary conditions, a linear system of coupled equations is obtained. These equations are then solved (iteratively) for the unknown variable at all storage sites.

In literature most people carried out 2D simulation of screw extrusion mixing because of the complex nature of screw geometry and flow domain. 3D simulations require lot of time and algorithm modifications to get worth noting results. The commonly used CFD software for the mixing of viscous immiscible fluids is Polyflow developed by FLUENT Inc which utilizes Finite element technique .This software is specially designed for the simulation of flow in the complex geometry of extruder .To ease the setup of a three dimensional unsteady twin-screw extruder, a technique referred to as *mesh superposition* (MST) has been developed This robust technique greatly simplifies the meshing of the geometric entities and does not present the complexities and limitations of other commonly used techniques. A mesh is generated for each part of simulation domain, one for the domain and one for the screw. For each node of this new domain that lies within a given screw, a special formulation is used that imposes a velocity that matches the rotation speed of the screw[1].Some researchers also utilized CFD software FLUENT 6 to model mixing of such fluids. One example is "Computational fluid dynamics model of viscous droplet breakup" [8] conducted by L.J. Dietschea, A.C.Neubauerb in 2008. In carrying out this sort of simulation people treated high viscous fluid as non Newtonian and problem set up is developed by incorporating modified models such as Carreau flow model, Bird–Carreau model, Oldroyd-B model and Phan-Thien Tanner model. However to simplify the problem, fluids may be considered as Newtonian which makes the simulation process easier and faster. *B. Alsteens, V. Legat, Th. Avalosse [5] conducted modeling of viscous fluids mixing in twin screw extruder assuming fluids as Non Newtonian. Then simulations were run by considering the same fluids as Newtonian. The boundary conditions for both cases were same. The simulations results for both cases were compared. The results revealed that the global pressure drop between the inlet and the outlet section is not significantly affected by the rheological model [5]. The modified rheological model for the Non Newtonian fluids significantly increases the cost and time of the calculation without any major difference in the flow features, so Newtonian model can be used for the systems having moderate flow rates to save cost and time.*

We utilize FLUENT 6.2 present at SCME to under take the task in 3D simulations of viscous immiscible fluids. Due to time constraint and complications in solving CFD codes following simplifications are incorporated.

1) Modeling of conventional single and twin screw extruder mixing section is done.

2) No mixing enhancer is included in the geometry.

3) Separate mixing head and die are not incorporated at the inlet and outlet of the mixing element respectively.

4) Fluids are considered to be Newtonian as flow rates in the system are low.

3.2 Selection of Fluids System

Literature has been surveyed for the selection of fluids system for our problem. For the subject purpose two immiscible fluids (Ethylene vinyl acetate EVA) and (Ethylene glycol EG) are selected [6]. The system is selected on the basis of work done by P Cassagnau; M Courmont; F Melis; J P Puaux who conducted the experimental study of mixing of liquid polymer in twin screw extruder by residence time distribution. We undertake this study computationally utilizing CFD codes for both single and twin screw extruder mixing section. High viscosity co polymer is taken in molten state while ethylene glycol is low viscosity liquid. The ratio of zero shear viscosities i.e μ(EG) to μ(EVA) is in the range of 1.96e-04. In this case of unequal viscosities and phase ratios, the restorative action of interfacial tension (σ) will cause the stretched-out regions to break into segments. In simple shear flow there is a maximum viscosity ratio, p (p equals the ratio of the dispersed phase viscosity, μd, to continuous phase viscosity, μc), beyond which a liquid droplet cannot be broken up by shear alone. Weber or capillary number, or the ratio of viscous forces to restorative forces, $\gamma\mu_c r/\sigma$., and the minimum dispersed phase drop radius can be achieved where the viscosity ratio p is close to unity, but dispersion by shear flow is not possible if p exceeds 4 or reduced below 0.25. This limit may be different for viscoelastic fluids. When the viscosity is high, the mixing Reynolds number ($Re = \rho D^2 N/\mu$) is probably less than 100. In our case Reynolds Number at screw speed of 200 rpm is 0.0056. In such cases, mixing can occur only by viscous forces, and turbulence will play no part. In our case the matrix phase i.e EVA possess very high viscosity as compared to dispersed phase i.e ethylene glycol, so very high shear stress and elongational stretching is required to affect mixing in the system. Study is conducted on the conveying screw geometry and kneading disc element geometry at the same screw speed to record effect on mixing efficiency.

3.3 Study of mixing parameters

Mixing can be evaluated from the simulation results by studying graphics of solution domain and graphics of flow field function [1].

3.3.1 Graphics of solution domain

Mixing phenomenon can be visualized with the help of graphics of solution domain which include geometry outline, surfaces, grids etc.

Geometry outline: The simplest method for displaying machine geometry. The outline consists of equipment features and internals [1]. For 2D simulations, either a side view or dotted lines (or both) can be used to represent the impeller and the location where the experimental data are applied to represent it. For 3D simulations modeled using the explicit geometry, all edges are shown [1].

Surfaces: In addition of outline, surfaces are also necessary to be shown to study simulation results. In case of solid surfaces of the mixer one can not see mixer internals unless opening in the side or at the top or alternatively solid surfaces are used for the internals and translucent surfaces for the outer wall. [1]

Grids: Grids are excellent way to express accuracy level of simulation results. A coarse grid can not display accuracy in the results despite of its convergence. A fine grid, however, has the potential to deliver a much better resolved flow field, assuming that the solution is converged adequately [1].

3.3.2 Graphics of flow field

There are many ways to examine the flow field results, some of which are described below.

Velocity vectors: These are used to describe magnitude and direction of flow field through out the solution domain. For 2Dsimulations, a plot of all velocity vectors gives an overall picture of the fluid behavior. For 3D simulations, a plot of all vectors in the domain is too crowded to be useful [1].The velocity vectors are shown in fig 3.1

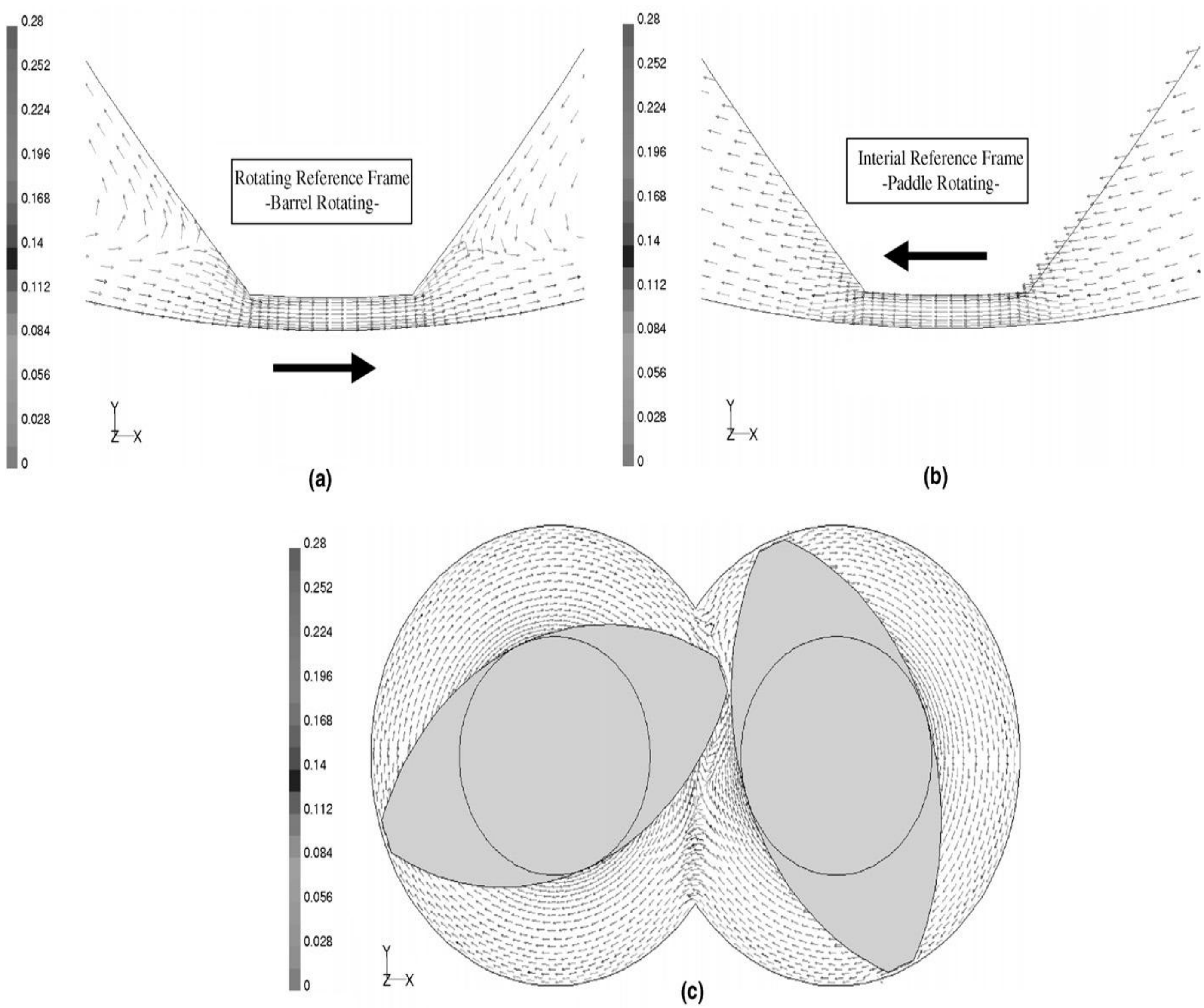

Fig 3.1 Velocity vectors showing direction of the flow and colored by the magnitude of the velocity (cm/s). (a) Single screw mixer rotating reference frame where the barrel is rotating counterclockwise and the paddle is fixed. (b) Single screw mixer in the inertial reference frame where the barrel is fixed and the paddle rotates clockwise. (c) Twin screw mixer after the paddles have turned clockwise 67.5_ from the initial position.

Contours: Contours are lines where chosen variables have constant value. Line contours, filled contours, plotted on an entire 2D domain or on a surface in a 3D domain, are also very useful for showing the maximum and minimum values as well as local gradients. Contours of a tracer species are shown on a cross-section through a 3D domain in fig 3.2

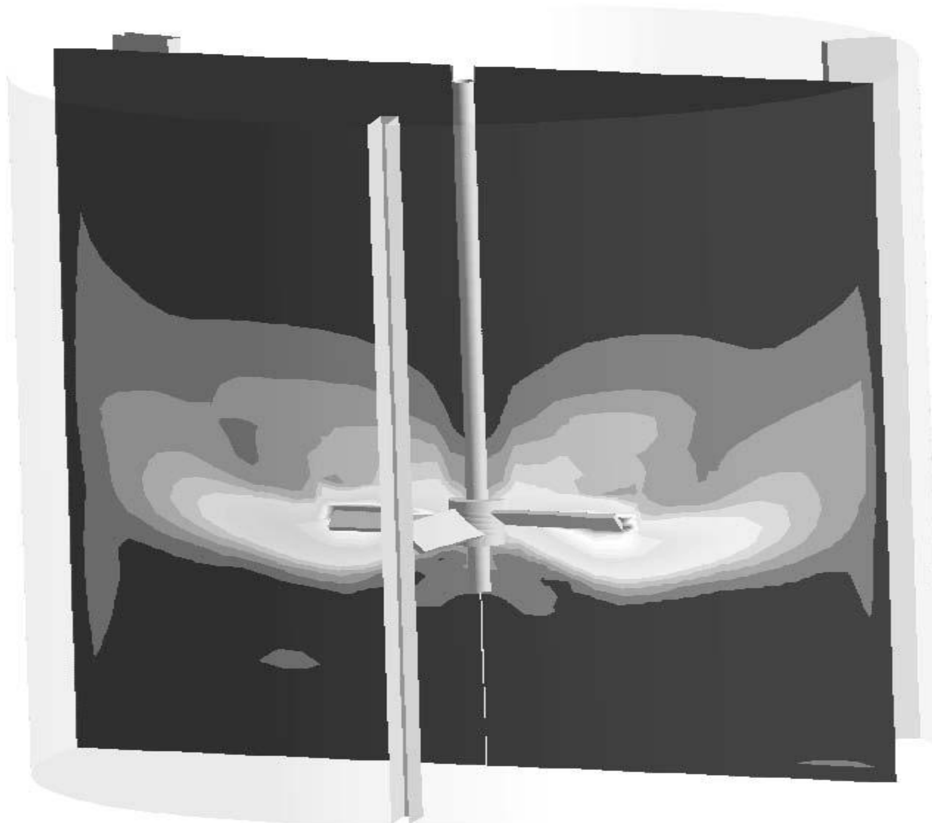

Fig 3.2 Filled contours of a tracer species shown on a planar surface in a 3D domain.

3.3.3 Useful Solution Variables

In multiphase flows, the volume fraction of the phases is the most useful tool to assess the distribution of the phases in the mixer. During the mixing of highly viscous materials, laminar shear, elongational flow and distributive mixing produce a reduction in the scale of segregation, while molecular diffusion (which takes place only at a very small scale) and dispersion act to reduce the intensity of segregation [7]. During mixing, material elements undergo continuous transient changes because shear and extensional rates vary a great deal from location to location.

The magnitudes of the rate of deformation and vorticity tensors are used to calculate the Manas-Zloczower **mixing index (λ_{MZ})** [7]. Mathematically it is written as

$$\lambda_{MZ} = |\boldsymbol{D}| / |\boldsymbol{D}| + |\Omega|$$

$|\boldsymbol{D}|=$ Rate of deformation (strain tensor)

$|\Omega|=$Magnitude of vorticity

The Manas-Zloczower mixing index (λ_{MZ}) indicates the type of mixing and nature of flow. The extent of elongational and rotational flow components with values from 0 for pure rotation to 0.5 for simple shear to 1 for pure elongation. The mixing index of 0.6~0.7 shows good dispersive mixing.

Magnitude of Vorticity ($|\Omega|$): Vorticity, a vector quantity is a measure of rotation of fluid. A non zero vorticity means that fluid is rotating as it moves [1]. The vorticity is defined as curl of velocity vector (U).

$\xi = \nabla \times \mathbf{U}$

In 2D flows vorticity direction is normal to the plane of simulation i.e vorticity is always in circumferential direction.

$\xi\theta = \partial Ux/\partial r - \partial Ur/\partial x$

In a 3D simulation vorticity can take on any direction, and plots of vorticity magnitude, rather than the individual components, are often the most helpful. The units of vorticity are S^{-1}, the same as those used for shear rate [1].

Rate of deformation (strain) tensor: The rate of deformation or strain rate tensor is a collection of terms that together describe the complete deformation of a fluid element in motion. The deformation can be the result of linear strain, which gives rise to a linear deformation or stretching of the element, and shear strain [1].

Mixing in extruders can also be evaluated by studying parameters like power number and flow number. In many cases these parameters are determined from CFD results .However these can also be determined from mathematical expressions.

Power Number is a dimensionless parameter determined the power requirement in the operation of impeller. $N_P = P/\rho N^3 D^5$

P= Power applied to the impeller

D= diameter of impeller

ρ= Density of fluid

N= impeller speed in hertz

The power delivered to the fluid is the product of the impeller speed, 2πN, in rad/s, and torque, τ, which is obtained by integration of the pressure on the impeller blade:

$P = 2\pi N\tau$

Reports are usually available for the torque delivered to the fluid by the impeller. In some cases, reports of power or even power number can be obtained from the software.

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Chapter 4

Problem Modeling Approach

This chapter describes the steps involved in modeling of selected system. Starting from basic concepts of viscous fluids mixing, practical work on software GAMBIT was carried out to learn the creation of geometries of different equipment in 2D and in 3D. Work on FLUENT was also continued to have a feel of software approach in simulating different problems. With the guidance achieved through soft wares learning, geometries of single and twin screw extruders were developed with appropriate meshing to discretize them. The inlet, outlet, and screw faces were designated with appropriate boundary conditions. The geometries were then exported in FLUENT for simulations. Following are the steps involved in this project work.

1. Creation of Geometries of single and twin screw extruders in software GAMBIT.
2. Extraction of flow domain in the geometries.
3. Meshing of flow domain for discretization to solve the continuity and momentum conservation equations by iteration.
4. Labeling of inlet, outlet and screw faces.
5. Export of geometries in FLUENT 6.2 for simulation.
6. Selection of appropriate model to solve the problem.
7. Defining the properties of fluids and phases involved in mixing.
8. Setting the boundary conditions.
9. Setting the convergence criteria.
10. Simulations and discussion on results.

4.1 Geometry/Grid Creation

Geometry/Grid creation is the first phase in this work. At SCME, FLUENT compatible software GAMBIT is available for this purpose. Due to complex nature of extruder geometry, lot of time and efforts has been spent for its creation. After many trials and literature survey geometries of single and twin screw extruders are created. From literature survey it is revealed that people worked on the modeling of viscous fluid mixing used bench scale extruder. Robin K. Connelly 1, Jozef L. Kokini in 2004 carried out 2D simulations that neglect flow along the length of the barrel were run on geometries based on the barrel and paddles of the co-rotating, twin screw, 2 inch in diameter[7]. B. Alsteens1, V. Legat1, Th. Avalosse2 in 2004 studied mixing efficiency in a kneading block section of a twin-screw extruder. They used Ishikawa kneading disk extruder of diameter 20mm and mixing length of 40mm [6].In the subject work dimensions of extruders are taken from A. Shah and M. Gupta paper regarding Simulation of polymeric flow in twin screw extruder. The dimensions of both single and twin screw extruders are as follows [1];

Barrel Diameter =30.0mm

Screw tip diameter =29.2mm

Screw root diameter =21.0mm

Screw lead =30.0mm

Centerline distance =26.0mm

Flow domain is extracted and discretized with tetrahedral mesh elements with 0.001 mesh spacing .The information of nodes, cells and faces generated of single screw extruder is as follows

Level	Cells	Faces	Nodes	Partitions
0	93004	196862	20969	1

The geometry information of twin screw extruder is as follows.

Level	Cells	Faces	Nodes	Partitions
0	155041	330081	35874	1

The geometries of single and twin screw extruders are shown in fig 4.1 & fig 4.2 respectively

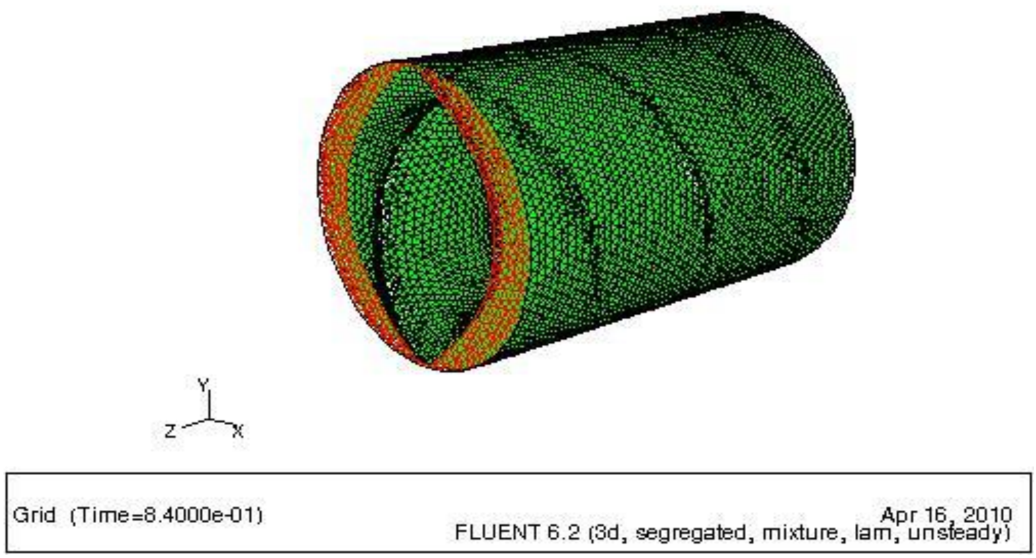

Fig 4.1 Single screw extruder geometry

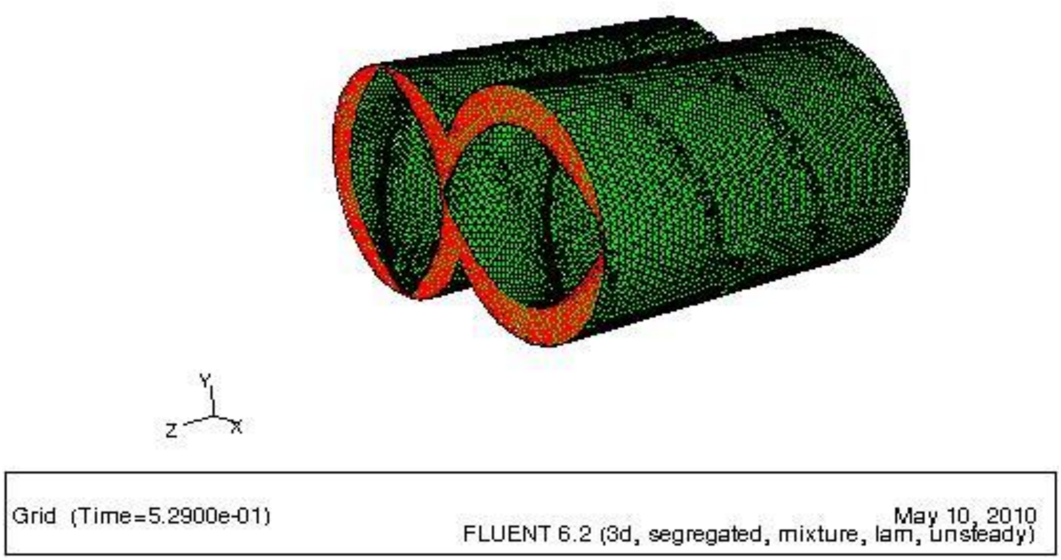

Fig 4.2 twin screw extruder geometry

4.2 Simulation approach

The selected system consists of two immiscible fluids i.e Ethylene Vinyl Acetate EVA28420 (28%VA with melt index of 420gm/10 min) and Ethylene glycol (EG).The properties of interest are given below in table 4.1.

Table 4.1

Sr No	EVA28420	EG
μ(zero shear stress viscosity)at 140 ^{0}C	80 Pa.s	0.0157 Pa.s
ρ Density	930 Kg/m3	1111 Kg/m3
Volume fraction	0.7	0.3

The primary phase EVA is highly viscous taken as continuous phase while EG is low viscous phase taken as dispersed phase. P Cassagnau; M Courmont; F Melis; J P Puaux in 2005 conducted Mixing of EVA/EG in Twin Screw Extruder by Residence Time Distribution experimentally[2] .Our effort is to study the system through CFD modeling. The ratio between zero stress viscosities of the continuous phase to dispersed phase is in the range of 5.095e03 and Ca (Capillary number i.e Ratio of viscous to interfacial forces) is very high requiring high shear stresses to affect dispersion of dispersed phase.

Multiphase mixture model is selected because of high volume fraction of dispersed phase, simplicity, and less computational effort requirement. Unsteady, segregated solver is selected. Because of very low Reynold Number (Re = $\rho D^2 N/\mu$) i.e 0.0041, laminar flow is assumed. Another assumption is that fluid is considered as Newtonian. (Viscosity does not change with high shear stresses) Reason is described in section 3.1. Only mixing section is selected for the problem solution. Simulations were run by setting following boundary conditions

Inlet= velocity inlet (linear velocity is calculated on the basis of screw speed i.e 200 rpm).The screw tip velocity comes out to be 0.31m/sec for both phases. The volume fraction of dispersed phase is set at 0.3 at the inlet. This is set on the basis of maximum flow rate of 1.4 kg/hr of EG against the 4.0 Kg/hr of EVA as set by. P Cassagnau; M Courmont; F Melis; J P Puaux. The solubility of EG in EVA is 0.15g/g .At the lower volume fraction of EG, a miscible solution is immediately formed which does not mean complete dispersion of components. To increase the dispersion a lubrication effect is required which means that non miscibility induces coalescence of dispersed phase in contact with barrel. This will enhance shear rate and more dispersion. The volume fraction of dispersed phase is 0.3 is taken on the basis of lubrication effect and more dispersion.

Outlet= Outflow having mixture rating of 1 Kg/hr with both phases coming out with zero EG backflow volume fraction.

Convergence criteria for the residuals drop on continuity, and velocities was set at 1 e-03 as referred in Computational Fluid Mixing by Elizabeth Marden Marshall and André Bakker Unsteady simulations with time step size of 0.001 were run and convergence is obtained at about 1000 iterations for the single screw extruder and 1200 iterations for the twin screw extruder.

Pressure, velocity, shear stress, strain rate, vorticity magnitude, velocity vectors contours are studied and mixing index is evaluated to observe mixing efficiencies in both geometries. Difference in both results is discussed and suggestions for the future work are also given in the next chapter.

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Chapter 5

Results and Discussion

Simulations are run in FLUENT 6.2 on the grids of single and twin screw extruder after giving appropriate boundary conditions. The screw speed is set at 200 rpm which makes the screw tip velocity of 0.31 m/sec. From simulations results, it is observed that values of shear stress, strain rate are comparatively lesser in twin screw extruder than single screw extruder but better dispersive mixing is observed because of more elongational stretching due to high fluids axial velocity in the intermeshing region of the two screws. It can be said that for better mixing twin screw extruders are preferred because they take the advantage of intermeshing nip region of screws to create additional redistribution and fluids stretching due to positive displacement action of the two screws. This action is due to change in the phase angle of the two lobes of the screws. This creates deformation in the fluids without high wall stresses. Velocity magnitude is increased from inlet of the screw to the outlet indicating increased elongational stretching along the flow domain and indicating dispersive mixing in both mixers. Distributive mixing is also better in twin screw extruder because of additional reorientation of fluids in the inter meshing zone.

5.1 Pressure Distribution

The pressure distribution generated in extruders indicates that pressure is decreased from very high value at the inlet to very low at the exit. The positive pressure is necessary at the inlet to push the fluid forward against the wall shear stress and to produce velocity gradient in the flow domain necessary for deformation in the fluid. This deformation in the fluid causes dispersive mixing. The movement in the forward direction against wall shear stress is provided by the movement of the screws and pressure energy at the down stream is converted into kinetic energy. The total pressure contours for the single and twin screw extruders are shown in fig 5.1 & 5.2.

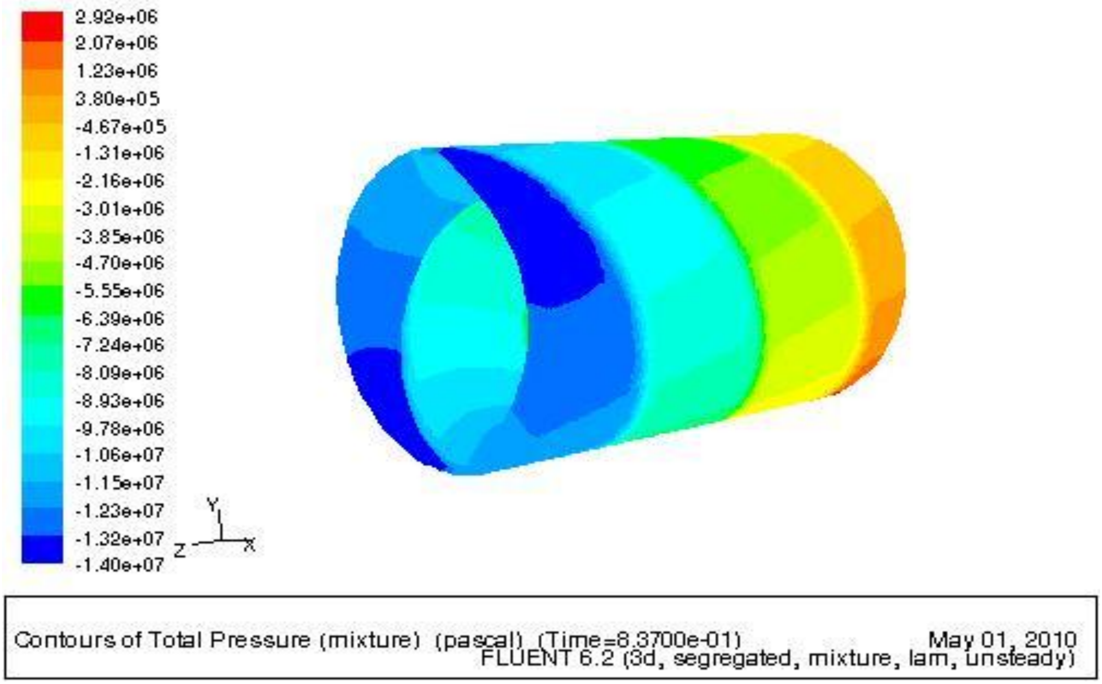

Fig 5.1 Total pressure distribution in single screw extruder.

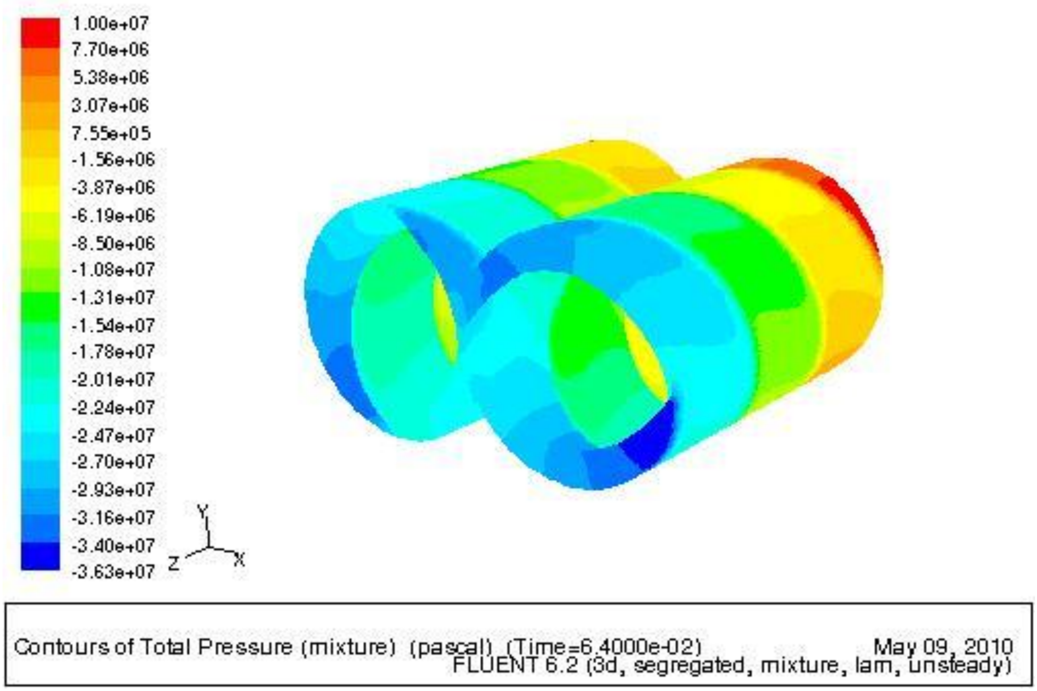

Fig 5.2 Total pressure distribution in twin screw extruder

The pressure distribution in the flow domains are verified by the force balance across the elements. Three forces act on the fluids in screws channel. The upstream pressure force pushes the fluid in the forward direction; the downstream pressure force which pushes against the flow now becomes the additional propulsive force due to screw movement. These pressure propulsive forces are balanced with the third retarding drag force which creates high wall shear stresses. So force balance across the extruder is;

Propulsive Forces acting in flow direction = Retarding drag Force acting against the flow

$$\pi r^2 P_{up\ stream} + \pi r^2 P_{down\ stream} = 2 \pi r L \tau_w \quad (5.1)$$

Putting values of radius (r), extruder length (L), and upstream/down stream pressures (P) in equation (5.1), the maximum wall shear stress for the single and twin screw extruder comes out to be 9.5 e05 and 2.3 e06 respectively which almost match with the stress indicated in shear stress contours. From this it can be concluded that by increasing the screw speed up stream and down stream pressure gradient is increased and high shear stresses can be generated which enhance deformation in the fluids and hence better mixing may be obtained.

5.2 Wall Shear stress distribution

The selected system is highly viscous and very high magnitude of shear stress is required to disperse the phases mutually. Stresses play an important role in dispersive mixing. Extruder achieves dispersive mixing by forcing portions of the material repeatedly through small gaps between barrel and screw tip. High shear stresses and normal stress differences are exerted on the material. It leads to a breakup of agglomerates or size reduction of the material [7]. The simulations results are indicative of this phenomenon. The wall shear stress distribution contours of both geometries are shown in fig 5.3 and 5.4

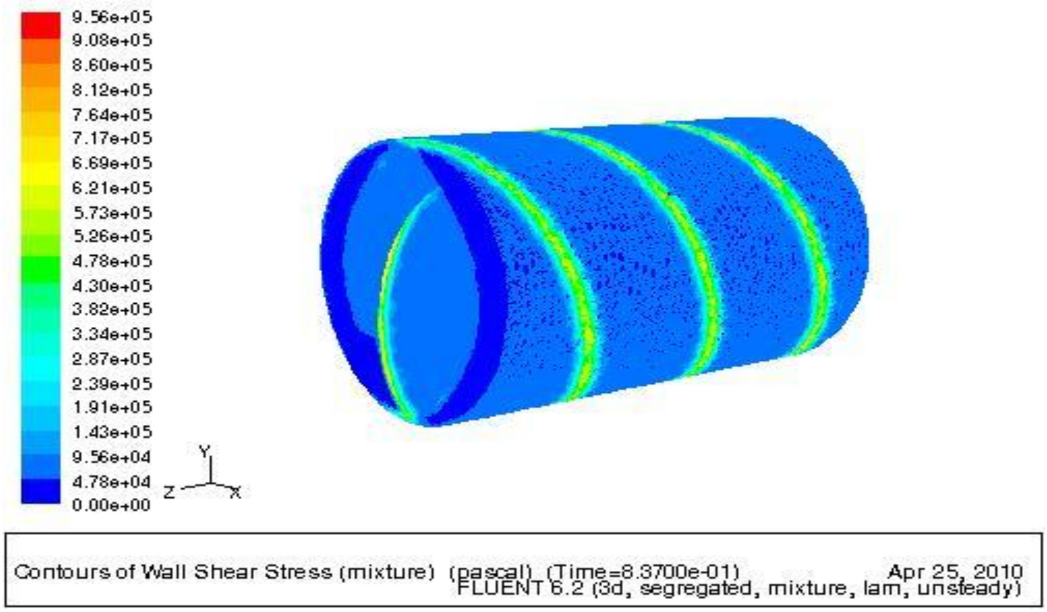

Fig 5.3 wall shear stress contour of single screw extruder

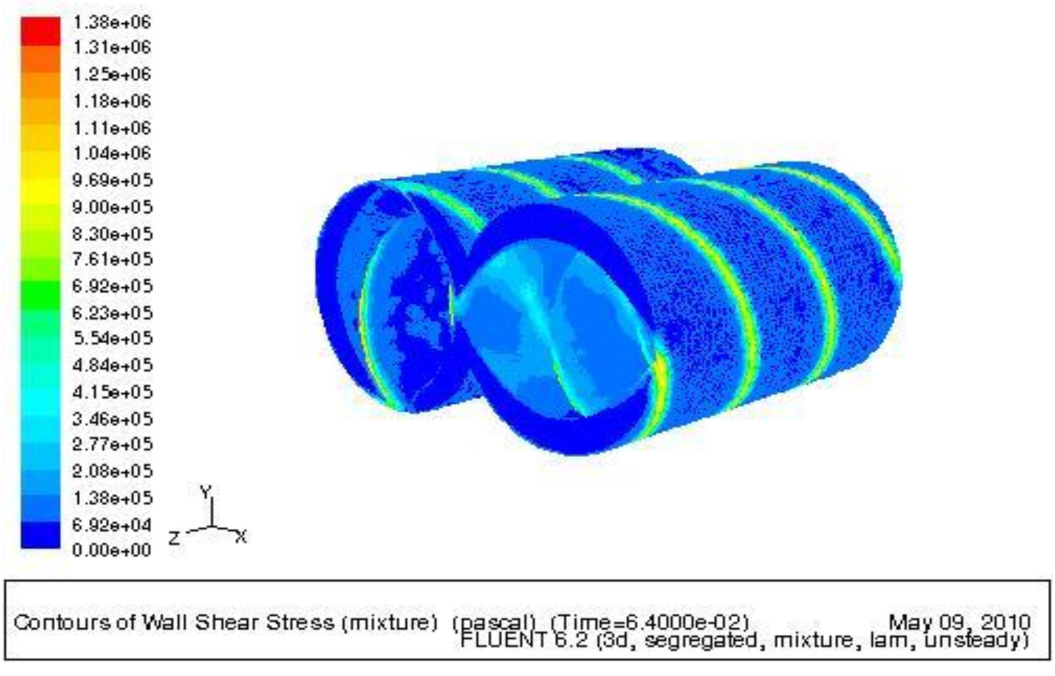

Fig 5.4 wall shear stress contour of twin screw extruder

The maximum wall shear stresses of single and twin screw extruders are up to the magnitude of 9.56e05 Pa and 1.38e06 Pa respectively. The strong stress gradient is also seen from the screw tip to the screw root channel indicating high strain rate which produces deformation in the fluids causing dispersive mixing. Almost same wall shear stress is observed at the screw tip of single and twin screw extruder which is about 9 e05 Pa.

5.3 Velocity distribution

The contours of velocity distribution of single screw extruder at 200 rpm are shown in fig 5.5 a, 5.5 b

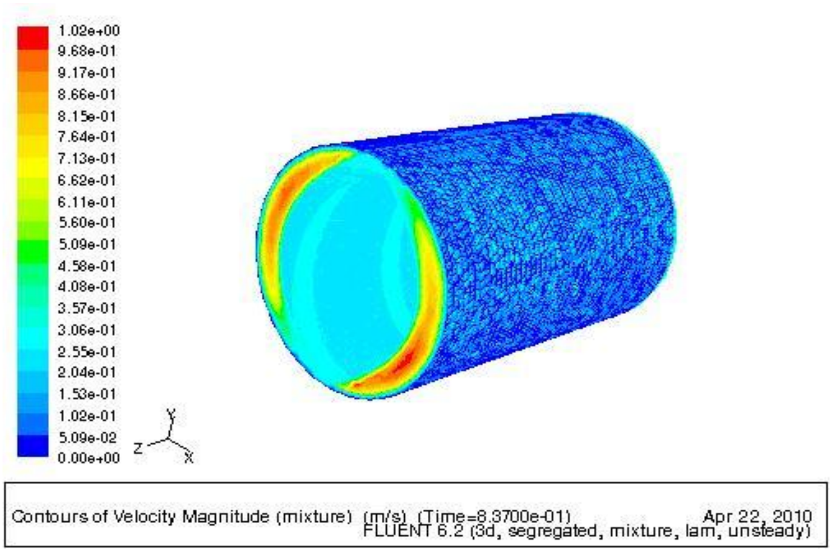

Fig 5.5 a) Velocity magnitude at outlet

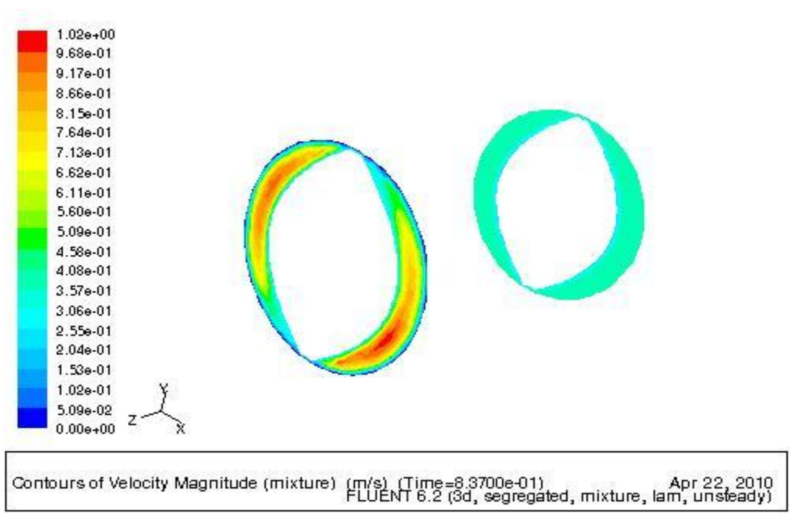

Fig5.5 b) velocity magnitude at inlet and outlet

Velocity in the extruder's element increases from the inlet to the outlet and maximum velocity is seen at the middle of flow domain at the outlet indicating flow is in the forward direction and elongational flow enhances the stretching in the fluid. The increase in velocity is due to the propulsive force provided by the rotating screw to the fluid. Velocity gradient is also observed from the barrel wall to the screw channel indicating high shear rate due to velocity gradient and maximum velocity at the middle of screw channel. The combination of normal velocity gradient and elongational stretching due to axial velocity gradient causes dispersive mixing in the machine. Velocity distribution in the twin screw extruder is shown in fig 5.6 (a) & (b)

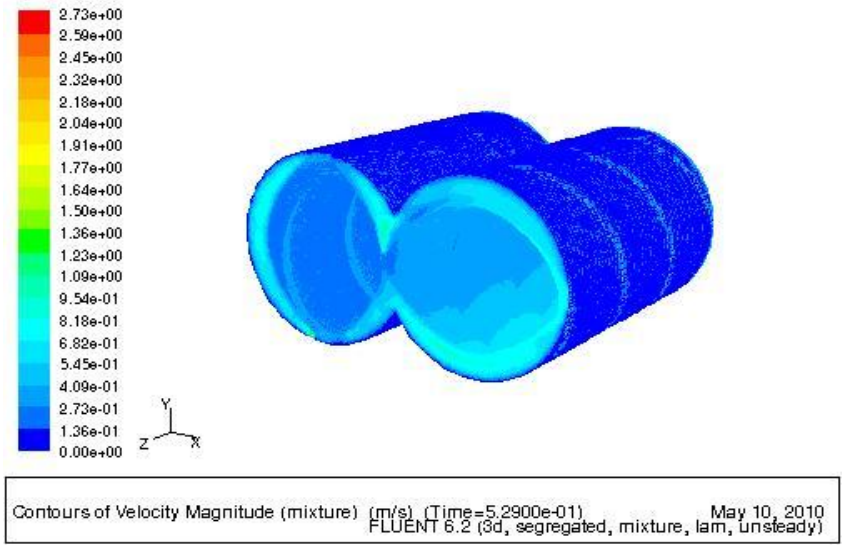

Fig 5.6 (a) velocity magnitude contour in twin screw extruder

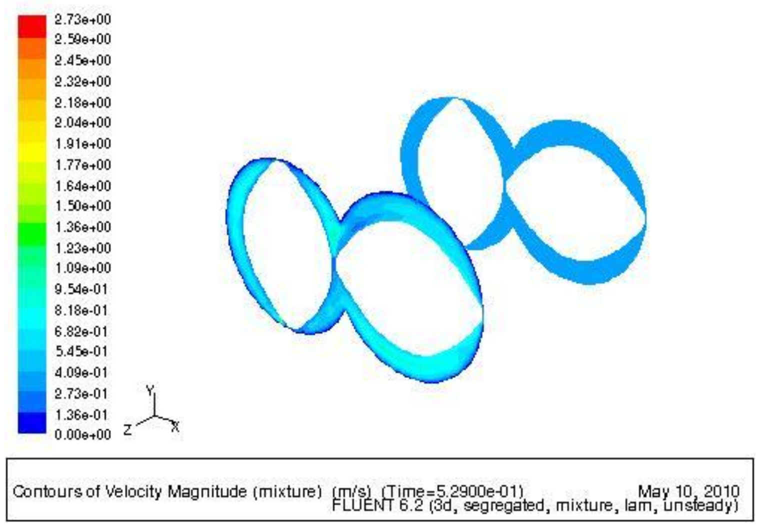

Fig 5.6 (b) velocity magnitude at the inlet/outlet contour in twin screw extruder

Flow domain of twin screw extruder is classified in two hypothetical regions, one in which two screws intermesh (nip or intermeshing region), and the other away from the nip region is called translational region. The flow in the translational region is considered similar to single screw extruder [7]. Velocity in that region is almost same for single and twin screw extruder. The advantage of twin screw extruder over the single screw extruder is attributed to the nip region which is considered to have positive displacement character [7]. The velocity distribution in nip region is different. The maximum axial velocity is observed in the nip region as fluid accelerates in that region due to positive displacement character of screw flights which is attributed to phase difference in the angular position of two lobes. This difference results in shift of channel. As material is transferred from one screw to another, it is pushed forward in a way like positive displacement pump. Higher axial velocity and maximum shear stress in nip region of twin screw extruder produces more elongational stretching in the fluids than single screw extruder.

5.4 Vorticity Magnitude (Ω)

It is defined as measure of rotation of fluid in extruder. It is the difference between velocity gradients in two dimensional flows in circumferential direction.Vorticity in flows creates due to the viscosity effects of fluids. A zero vorticity means that flow is irrotational. Laminar flows are rotational everywhere except at the centerline where velocity gradient is almost zero and fully developed flow exists.Vorticity magnitude is maximum at the walls to minimum at the centre where flow is totally axial and no velocity gradient in the circumferential direction exists. In our case of 3D simulation, the plot of vorticity magnitude is used to calculate mixing index.

The contours of vorticity magnitude of single and twin screw extruders verifies the mechanism in the flows as vorticity magnitude is maximum at the barrel wall and decreases to minimum at the screw root where velocity gradient in minimum. The contours are given in Fig 5.7 & 5.8

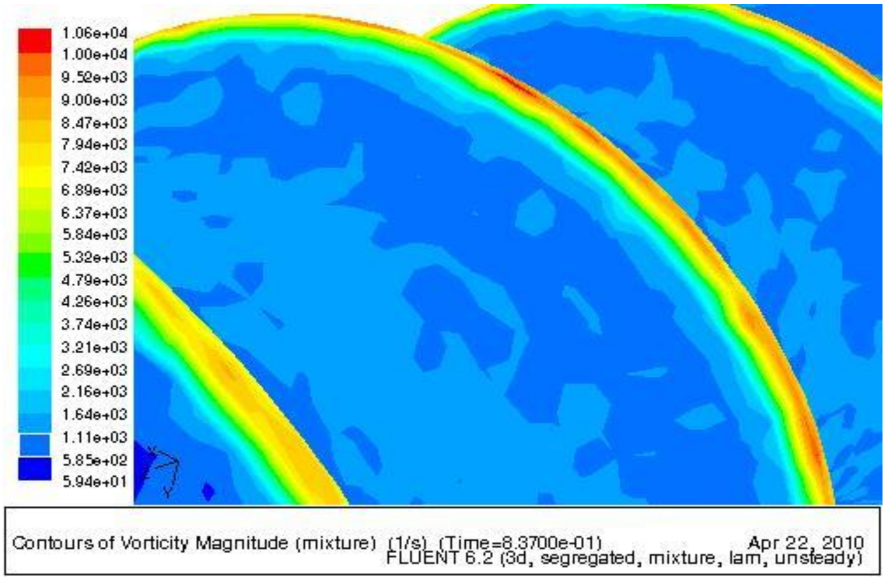

Fig 5.7 Contours of vorticity magnitude of conveying element

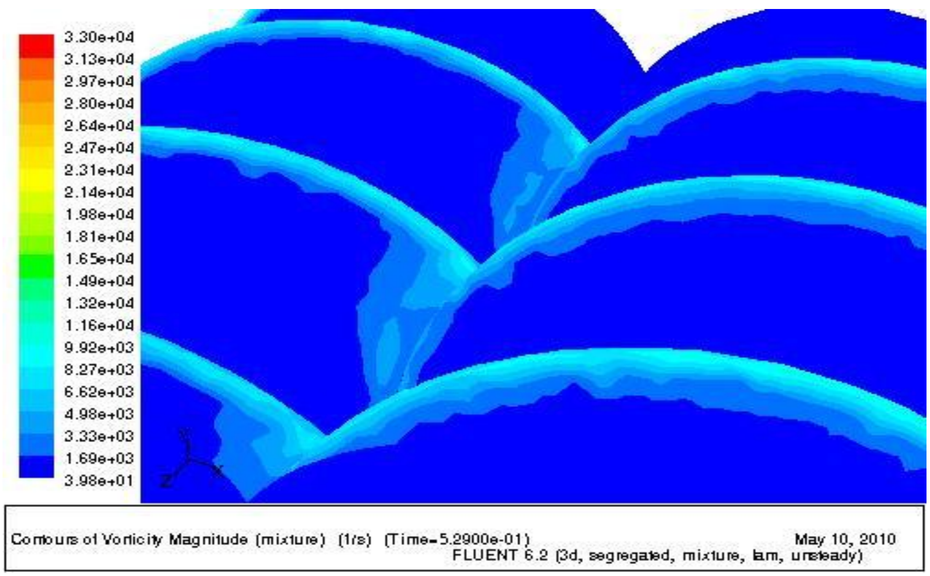

Fig 5.8 Contours of vorticity magnitude of twin screw extruder

a) Vorticity magnitude distribution for single screw extruder ranges from 59.41/sec from screw root to 10600 1/sec at screw tip

b) Vorticity magnitude distribution for twin screw extruder ranges from 39.8 1/sec from screw root to 10000 1/sec at screw tip

5.5 Shear (Strain) Rate distribution

Mixing in machine depends upon strain rate developed because it describes the complete deformation of a fluid element in motion. Regions with a high strain rate play an important role in liquid dispersion. The data of strain rate collected from the simulations results will be utilized to evaluate mixing index. The contours of strain rate for the single and twin screw extruder are shown in fig 5.9 & 5.10 respectively.

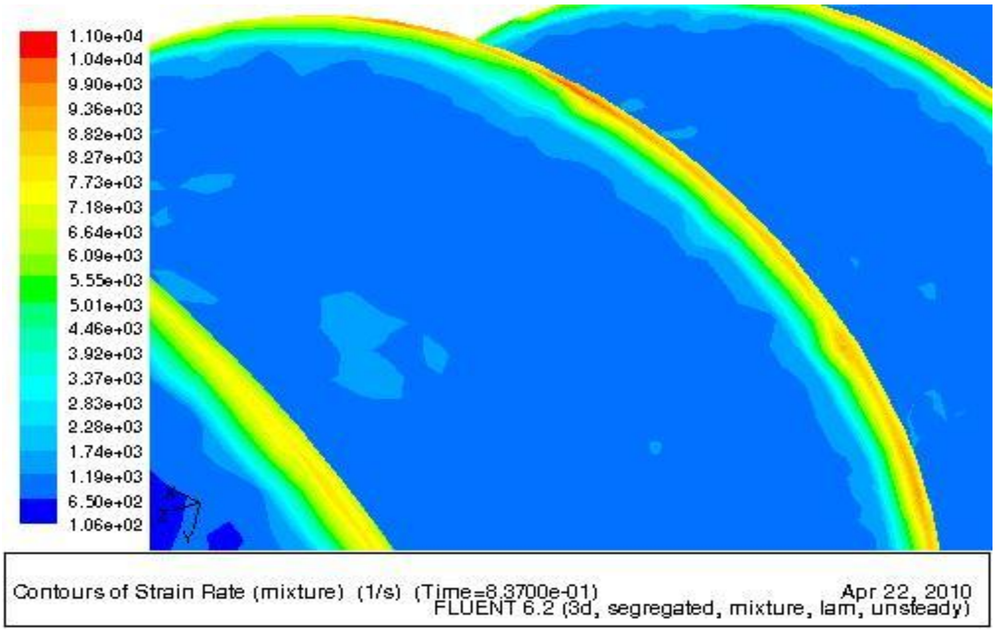

Fig 5.9 Strain rate distribution of single screw extruder

The range is106 1/sec from screw root to 11000 1/sec at screw tip.

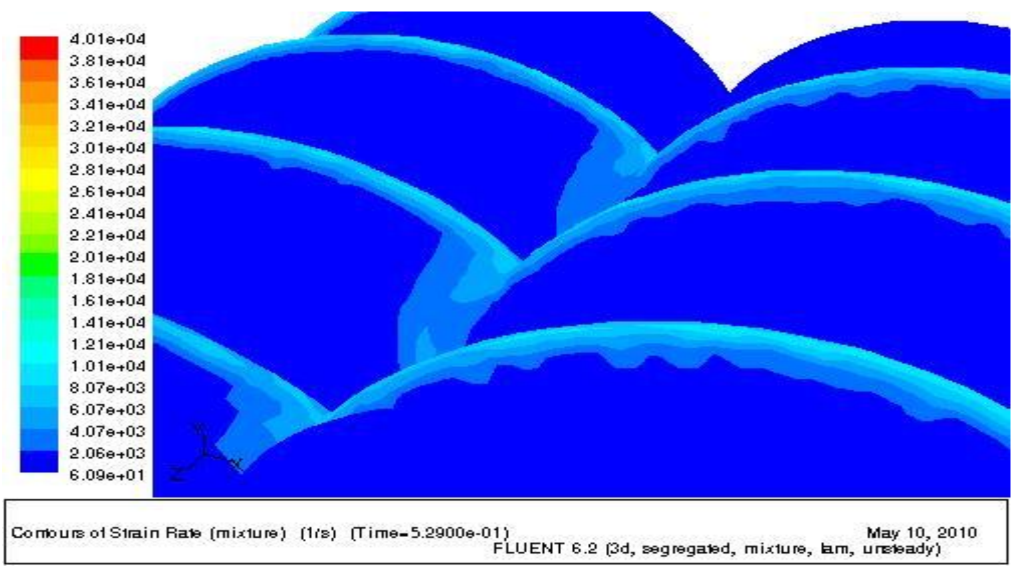

Fig 5.10 Strain rate distribution from kneading disc element .

The range is 60.9 1/sec from screw root to 9000 1/sec at screw tip

The strain rate is maximum at the barrel wall and decreases towards centre where large volume of fluid is present and also minimum velocity gradient at the center. Despite comparatively less strain rate in twin screw extruder better mixing is observed because of more elongational stretching due to positive displacement character in the nip region of the screws.

5.6 Mixing Index (λ) Evaluation

From the vorticity magnitude and shear rate distribution results after simulations of single and twin screw geometries, mixing index (λ) or flow number is calculated and given in tables 5.1 and 5.2 respectively. The values of both parameters for calculations are taken from the screw tip to screw channel.

Table 5.1 Single screw extruder

Sr No	Vorticity Magnitude (Ω) S^{-1}	Strain rate (γ) S^{-1}	Mixing Index (λ)= (γ)/ (Ω)+ (γ)
1	10600	11000	0.509
2	8470	8820	0.510
3	6370	6640	0.510
4	4260	4460	0.511
5	2160	2280	0.513
6	59.4	106	0.640

Table 5.2 Twin Screw Extruder

Sr No	Vorticity Magnitude(Ω) S^{-1}	Strain rate (γ) S^{-1}	Mixing Index (λ)= (γ)/ (Ω)+ (γ)
1	8270	10000	0.547
2	6620	8070	0.549
3	4980	6070	0.549
4	3333	4070	0.549
5	1690	2060	0.549
6	39.8	60.9	0.608

Mixing index has a range of 0~1 with 0.5 being shear flow and 1 being pure elongational. [3].The systems having mixing index ranges from 0.6~0.7 has very good dispersive mixing. In single screw extruder, the mixing index ranges from 0.51~ 0.64 indicating shear flows and elongational mixing. This shows a reasonably good component dispersive mixing. The mixing index in twin screw extruder ranges from 0.55~0.61 also showing shear to elongational stretching for dispersive mixing but more efficient than single screw extruder because of stress availability and more axial velocity at the intermeshing region of the screws.

5.7 Velocity vectors

Velocity vectors plots are also one of the post processing simulation results which illustrate the magnitude and direction of the flow field throughout the solution domain. For 3D simulations, a plot of all vectors in the domain is too crowded to be useful. In our simulation results, velocity vectors direction are from the inlet to the outlet of the flow domain and vectors are not diverging which shows that our work is in right direction. The velocity vectors contours for the single and twin screw extruder are shown in Fig 5.11 & 5.12 respectively.

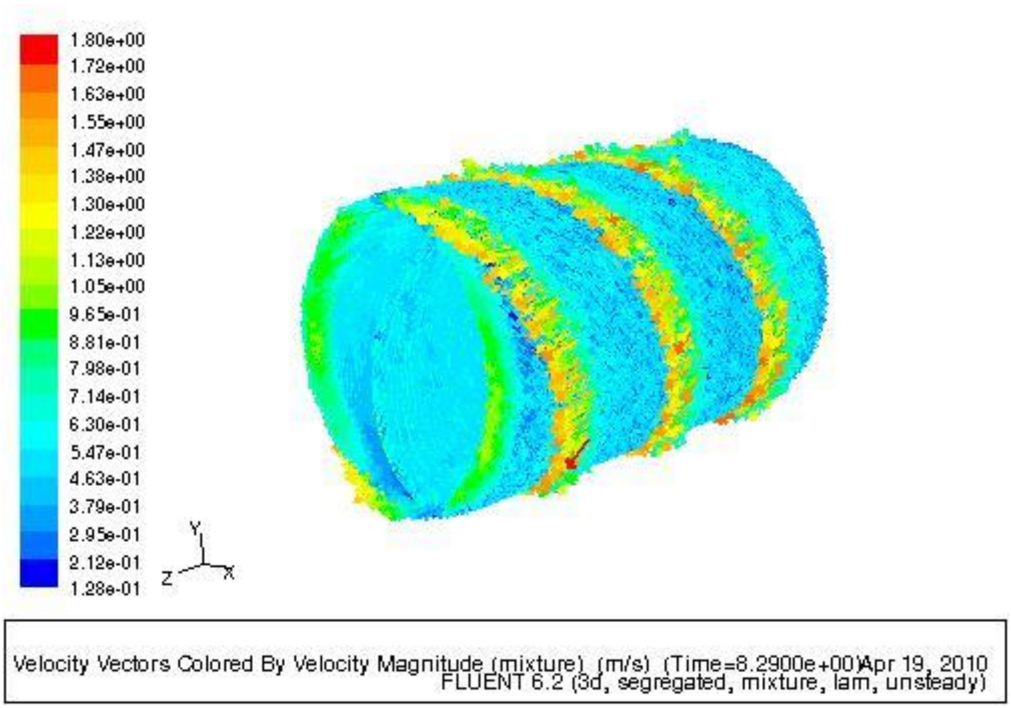

Fig 5.11 Contours of velocity vector of single screw extruder

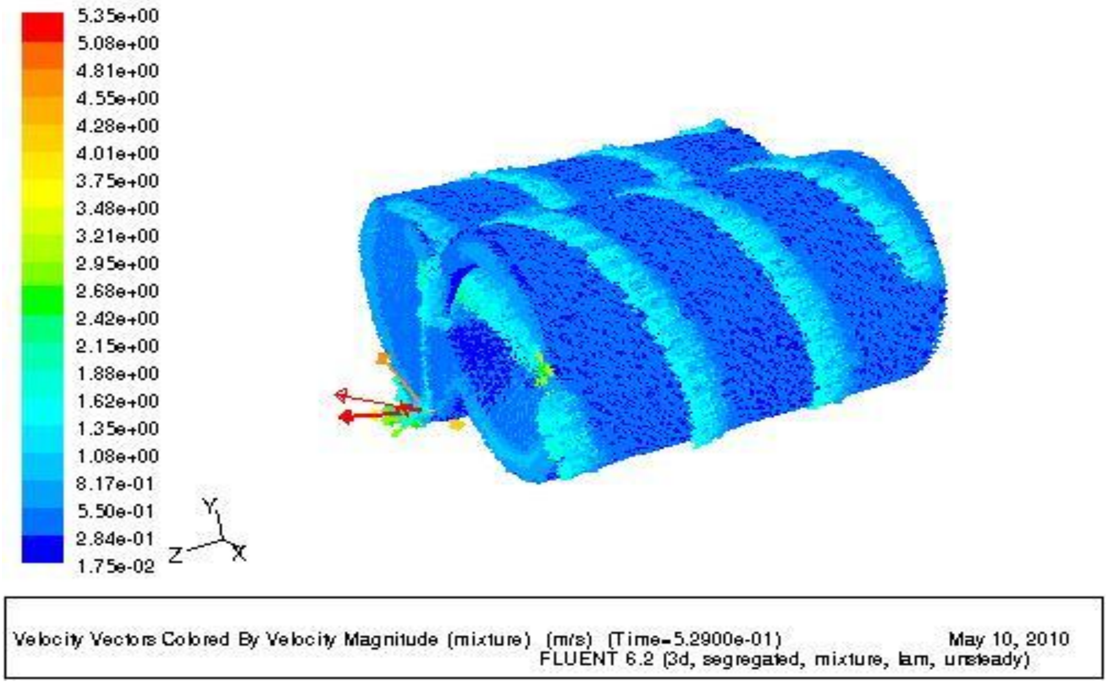

Fig 5.12 Contours of velocity vector of twin screw extruder

5.8 Volume Fraction

Mixture model tracks the volume fraction of secondary phase which is EG in this case. The contours of volume fraction at the inlet and outlet face of single and twin screw extruder are shown in Fig 5.13 & 5.14 respectively.

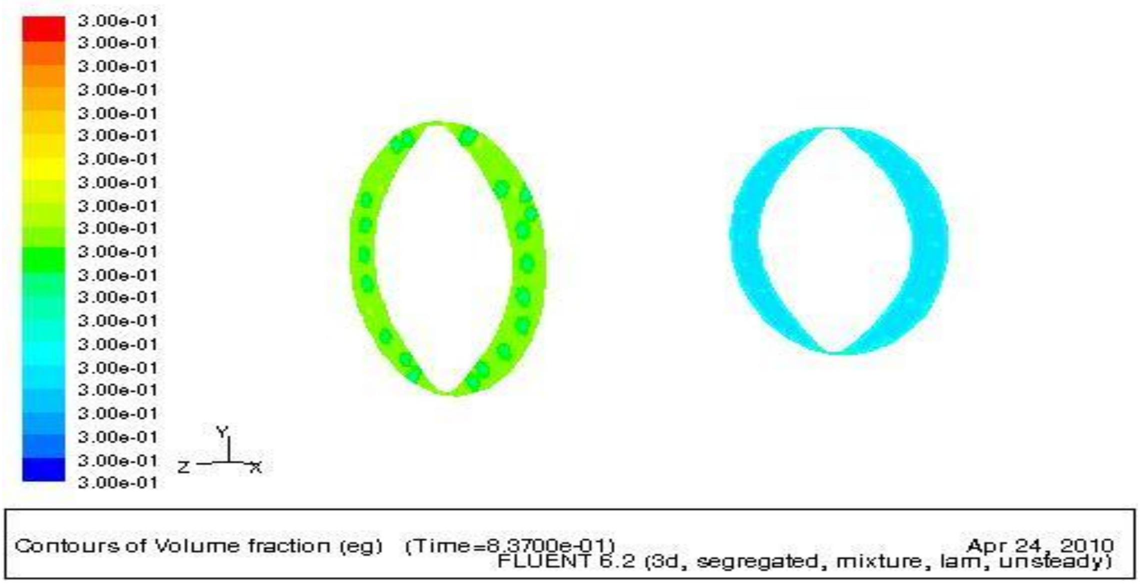

Fig 5.13 Contours of volume fraction of EG at the inlet and outlet of single screw extruder

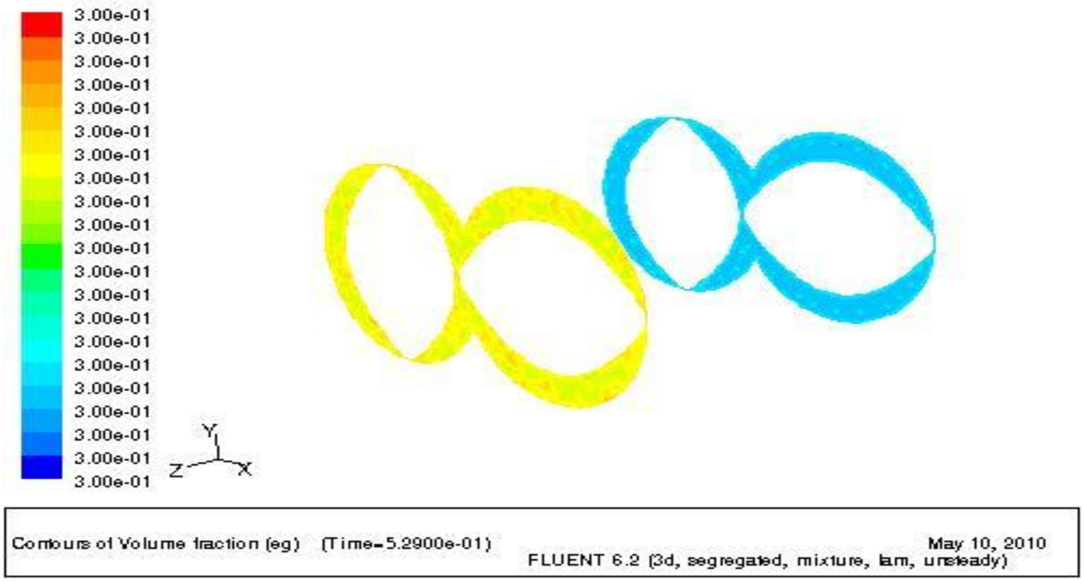

Fig 5.14 Contours of volume fraction of EG at the inlet and outlet of twin screw extruder

The results indicate that there is minor change in the volume fraction of EG throughout the flow domain. The minimum and maximum values of volume fraction comes out to be 0.2999~ 0.30002. There is slight increase in volume fraction of EG and slight decrease of EVA at the outlet is indicative of mixing of component.

5.9 Conclusion

CFD software FLUENT 6.2 is utilized for the modeling of mixing of two immiscible fluids i.e Ethylene Vinyl acetate (EVA) and Ethylene Glycol (EG). EVA of type EVA28420 (28% Ethylene and melt index of 420gm/10 minutes) is selected at its melting temperature of 140 ^{0}C .The zero shear stress viscosity of EVA is 80 Pa.s while EG possess viscosity of 0.0157 Pa.s. Study is conducted on mixing section of single and twin screw extruder. The viscosity ratio between continuous phase to dispersed phase i.e EVA and EG is in the range of 5.095e-03 requiring very high shear stresses and shear rate for the breaking of dispersed phase droplets. The results are indicative of that concept. High shear stresses and and shear rates are observed close to the barrel and falls to minimum at the centre of the channel due to presence of large volume of fluid. This shear stress and strain rate gradients are indications of deformation in the fluid necessary for the dispersive mixing. More elongational stretching is observed in twin screw extruder due to high axial velocity in the intermeshing (nip) region. Mixing index range varies from 0~1.0 with 0.5 being pure shear flow and 1.0 is elongational flow. Mixing index from 0.6~0.7 indicates very good dispersive mixing. The mixing index in single screw extruder varies from 0.51~0.64 showing very good shear and elongational stretching, a very good indication of dispersive mixing. Mixing index in twin screw extruder ranges from 0.55~0.61 indicating more elongational stretching hence better dispersive mixing.

5.10 Future recommendations

1) Modifications in screw geometry by incorporating mixing enhancer for better distributive mixing.
2) Mesh refinement for better refined simulation results
3) Study of Viscous energy dissipations by adding energy equation in the solver algorithm.
4) Non Newtonian model can be included in the simulation model to study the effect of viscosity changes during the mixing.

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