Republic of Iraq
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University of Babylon
Collage of Material's
Department of Polymer
Engineering and
Petrochemical Industries .

{ Numerical Simulation of Natural Polymers Rheology in a Pipe }

A graduation project is submitted to the Material's Engineering College in partial fulfillment of the requirements for the degree of Bachelor of Science in Polymers and Petrochemicals Industries

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We are forever indebted to our parents, who have always kept us in their prayers

Dedication

To our family

To our friends

To our distinguished teachers

To all those who have trusted and documented our abilities and ambitions since childhood

Thank you from the deep of our heart

Contents :

Numerical simulation of natural polymers rheology in a pipe

Abstract

This project focuses on the numerical study of chitosan solution rheology in a pipe. Viscosity, density and shear rate of chitosan using as input data to the Ansys fluent program.

Govering equition such as quantity and momentum with non Newtonian viscosity models are used to simulate the flow behavior. The results show that the velocity of polymer is maximum at the center of pipe and then decreasing gradually towards the wall of pipe. This means that the shear rate and shear stress produce minimum value and viscosity produces maximum value at the center of pipe. Viscosity gives indication about molecular weight. There for it can controlling on the molecular weight and other polymer properties thought controlling on the velocity of polymer.

Chapter one
Introduction

Introduction

Recently, there have been attempts to switch from a synthetic polymer to a natural one. The rheological characteristics of natural polymeric materials such as viscosity and shear stress are studied for their importance in the pharmaceutical industries and it is suggested that rheology is the most sensitive method for material characterization because the flow behavior is sensitive to properties such as molecular weight and molecular weight distribution. This relationship is useful in the synthesis of polymers. The relationship between viscosity and molecular weight was also examined. According to the theses studies, different types of natural polymer have been used in different applications. The use of these polymers reduces the impact on health and the environment and achieves sustainability.

This study was carried out numerically by Ansys software based on basic equations and finite differences method.

Classificaton of polymers :-

Polymers are classified according to their sources into three categories, they are either (natural polymers) that arise from plant or animal products such as cellulose and natural rubber, or they are manufactured (Synthetic polymers). This type is prepared from simple chemical compounds such as synthetic fibers, dyes and various plastics. The third category is (Modified Natural Polymers) they are natural polymers that undergo some modifications by introducing new groups into the polymer, so a change in its chemical composition occurs, or it is created by grafting a natural polymer on an industrial one, for example, esters of cellulose .and cotton Grafted with acrylic fibers

Numerical simulation of polymer melts in a pipes is very common in polymer processing.

Ansys is an American company based in Canonsburg, Pennsylvania. It develops and markets multiphysics engineering simulation software for product design, testing and operation and offers its products and .services to customers worldwide

Ansys develops and markets engineering simulation software for use across the product life cycle [6]. Ansys Mechanical finite element analysis software is used to simulate computer models of fluid flow structures, electronics, or machine components for analyzing strength, toughness, elasticity, temperature distribution, electromagnetism, and other attributes [7]. Ansys is used to determine how a product will function with different specifications, without building test products or conducting crash tests . For example, Ansys software may simulate how a bridge will hold up after years of traffic, how to best process salmon in a cannery to reduce waste, or how to design a slide that uses less material without sacrificing safety [5].

Most Ansys simulations are performed using the Ansys Workbench system [8] , which is one of the company's main products. Typically Ansys users break down larger structures into small components that are each modeled and tested individually [5]. A user may start by defining the dimensions of an object, and then adding weight, pressure, temperature and other physical properties. Finally, the Ansys software simulates and analyzes movement, fatigue, fractures, fluid flow, temperature distribution, electromagnetic efficiency and other effects over time [9].

Ansys also develops software for data management and backup, academic research and teaching. Ansys software is sold on an

.annual subscription basis

Other software that depend on finite element

1- Abaqus 2- mat lap 3- Comsol 4- Nastran

Computer specification :-

Processor : Intel (R) Celeron (R) CPU 1005M @1.90Hz 1.90 GHz

Installed memory (RAM) : 2.00 GB (1.62 GB usable) Hard

: 500

Material (Chitosan) :-

$C_{56}H_{103}N_9O_{39}$

Molecular Weight

1526.5 g/mol

Density (0.20-0.38) g/ml

Viscosity 4.72 Pa.s

Chitosan can be dissolved when added to a solution of 98% water and 2% acetic acid.

Numerical Method :-

Finite element (FEM)

The finite element method (FEM) is a widely used method for numerically solving differential equations arising in engineering and mathematical modeling. Typical problem areas of interest include the traditional fields of structural analysis, heat transfer, fluid flow, mass transport, and electromagnetic potential

The FEM is a general numerical method for solving partial differential equations in two or three space variables (i.e., some boundary value problems). To solve a problem, the FEM subdivides a large system into smaller, simpler parts that are called finite elements. This is achieved by a particular space discretization in the space dimensions, which is implemented by the construction of a mesh of the object: the numerical domain for the solution, which has a finite number of points. The finite element method formulation of a boundary value problem finally results in a system of algebraic equations. The method approximates the unknown function over the domain.[1] The simple equations that model these finite elements are then assembled into a larger system of equations that models the entire problem. The FEM then approximates a solution by minimizing an associated error function via .the calculus of variations

Studying or analyzing a phenomenon with FEM is often referred .to as finite element analysis (FEA)

A finite element method is characterized by a variational formulation, a discretization strategy, one or more solution .algorithms, and post-processing procedures

Examples of the variational formulation are the Galerkin method, the discontinuous Galerkin method, mixed methods, etc [1]

Finite difference (FDM)

In numerical analysis, finite-difference methods (FDM) are a class of numerical techniques for solving differential equations by approximating derivatives with finite differences. Both the spatial domain and time interval (if applicable) are discretized, or broken into a finite number of steps, and the value of the solution at these discrete points is approximated by solving algebraic equations containing finite differences and .values from nearby points

Finite difference methods convert ordinary differential equations (ODE) or partial differential equations (PDE), which may be nonlinear, into a system of linear equations that can be solved by matrix algebra techniques. Modern computers can perform these linear algebra computations efficiently which, along with their relative ease of implementation, has led to the widespread use of FDM in modern numerical analysis. Today, FDM are one of the most common approaches to the numerical solution of PDE, along with finite element methods.

The error in a method's solution is defined as the difference between the approximation and the exact analytical solution. The two sources of error in finite difference methods are roundoff error, the loss of precision due to computer rounding of decimal quantities, and truncation error or discretization error, the difference between the exact solution of the original differential equation and the exact quantity assuming perfect .arithmetic (that is, assuming no round-off) To use a finite difference method to approximate the solution to a problem, one must first discretize the problem's domain.

This is usually done by dividing the domain into a uniform grid (see image to the right). This means that finite-difference methods produce sets of discrete numerical approximations to the derivative, often in a "time-stepping" manner

Finite Difference Method for Solving a System of Third-Order Boundary Value Problems

We develop a new-two-stage finite difference method for computing approximate solutions of a system of third-order boundary value problems associated with odd-order obstacle problems. Such problems arise in physical oceanography, draining and coating flow problems and can be studied in the framework of variational inequalities. We show that the present method is of order three and give numerical results that are better than the other available results.

Variational inequalities have had a great impact and influence in the development of almost all branches of pure and applied sciences. It has been shown that the variational inequalities provide a novel and general framework to study a wide class of problems arising in various branches of pure and applied sciences. The ideas and techniques of variational inequalities are being used in a variety of diverse fields and proved to be innovative and productive. In recent years, variational inequalities have been extended and generalized in several directions. A useful and important generalization of variational inequalities is called the general variational inequalities involving two continuous operators. It has been shown that a wide class of nonsymmetric and odd-order obstacle problems arising in industry, economics, optimization, mathematical and engineering sciences can be studied in the unified and general framework of the general variational inequalities [10]. Despite of their importance, little attention has been given to develop some efficient numerical technique of solving such type of problems. In principle, the finite difference techniques and other related methods cannot be applied directly to solve the obstacle-type problems. Using the technique of the penalty method, one rewrite the general variational inequalities as general variational equations. We note that, if the obstacle function is known, then one can use the idea and technique of Lewy and Stampacchia to express the general variational equations as a system of third-order boundary value problems. This resultant system of equations can be solved, which is the main advantage of this approach. The computational aspect of this method is its simple applicability for solving obstacle problems. Such type of penalty function method in conjunction with spline and finite difference techniques has been used quite effectively as a basis for solving system of third-order boundary value problems [11]. Our approach to these problems is to consider them in a general manner and specialize them later on. To convey an idea of the technique involved, we first introduce and develop a new two stage finite difference scheme for solving a third-order boundary value problems.

Chapter two

Newtonian and non-Newtonian fluids

Newtonian and non-Newtonian fluids, their equations, and their applications in polymers, especially the flow within the cylinder.

1- newtonian flow :- flow at constant viscosity with increasing of shear rate, such as (water, molten metal, and simple organic liquids).

$\tau = \mu\gamma$ τ is the shear stress (pa).

2-Non-Newtonian flow: flow with variable viscosity with increasing of shear rate, such as (polymer melts or solutions, paints, bloods, and some foods and drugs).

$\tau = \mu\gamma n$

The polymer melts and solutions are non-Newtonian flows ; because of polymer structures contain long chains macromolecules ,which produce non-Newtonian flow. **non-Newtonian fluid** is a fluid that does not follow Newton's law of viscosity, i.e., constant viscosity independent of stress. In non-Newtonian fluids, viscosity can change when under force to either more liquid or more solid. Ketchup, for example, becomes runnier when shaken and is thus a non-Newtonian fluid. Many salt solutions and molten polymers are nonNewtonian fluids, as are many commonly found substances such as custard, toothpaste, starch suspensions, corn starch, paint, blood, melted butter, and shampoo. [2]

The rheology and non-Newtonian flow are important in the flowing fields:

1-Polymer processing.
2- Paint industries.
3- Food industries.
4- Oil drilling.
5- Pharmacology.

The polymer material is a viscoelastic material their behavior between elastic solid and viscous fluid.

Advantages of finite element analysis :-

1- Models Bodies of Complex Shape

2- Can Handle General Loading/Boundary Conditions

3- Models Bodies Composed of Composite and Multiphase Materials

4- Model is Easily Refined for Improved Accuracy by Varying

5- Element Size and Type (Approximation Scheme)

6- Time Dependent and Dynamic Effects Can Be Included

7- Can Handle a Variety Nonlinear Effects Including Material Behaviour, Large Deformations, Boundary Conditions, Etc.

FINITE Any continuous object has infinite degrees of freedom and it's just not possible to solve the problem in this format. Finite Element Method reduces the degrees of freedom from infinite to finite with the help of discretization or meshing (nodes and elements).

ELEMENT under study into a finite number of pieces (sub domains) called The fundamental concept involves dividing the body elements.

A non-Newtonian fluid is a fluid that does not follow Newton's law of viscosity, i.e., constant viscosity independent of stress. In non-Newtonian fluids, viscosity can change when under force to either more liquid or more solid. Ketchup, for example, becomes runnier when shaken and is thus a non-Newtonian fluid. Many salt solutions and molten polymers are nonNewtonian fluids, as are many commonly found substances such as custard [4'2] Quantity equation

Momentum equqtion :

Power law Models:- The flow properties of polymer melts can be represented by log curves (τ) and (η) versus (γ)

Many models of varying compexity and form have been proposed.

Some of these models are direct curve fitting of shear stress vs. shear rate experimental data.

Power law or ostwald de waale model :- Non-linear shear stress vs. shear rate curve of shear thinning fluids can be represented by power law models as give bellow :

$$\tau_{yx} = m(\gamma)^n$$

m and n are two empirical curve fitting parameters. n

is power law fluid behavior index (dimensionless)

n<1 indicate shear-thinning behaviour of fluid (0<n<1)

n=1 indicate Newtonian fluid behaviour m is powerlaw

fluid consistency index (Pa.s)

At low shear, the randomizing effect of the thermal motion of the chain segments overcomes any tendency towards molecular alignment in the shear field -random state- greatest resistance to flow

As the shear increased, the molecules will begin to untangle and align in the shear field, reducing their resistance to slippage past one another.

Under severe shear, they will be completely untangled and aligned and reach a minimum state of resistance to flow. Further intense shearing eventually leads to extensive hreakage of main-main bonds mechanical degradation.

Most commercial polymer processing is done in regions of the viscosity versus shear rate curve where the viscosity is decreasing with shear rate.

Such flow behavior is pseudoplastic (shear thinning) and can be can be described by the power law equation

$\tau = K(\gamma)^n$ where K= consistency index [Pa.sn] - Typical values 1,000-

100,000 Pa.sn n= power-law index (dimensionless] - Typical values 0.2-0.8.

For a shear thinning fluid is between zero and 1. The more shear thinning the product the closer is to zero.

In logarithmic form the power law equation may be written as When

log(τ) = log k +n log(γ)

n=1 , the fluid is Newtonian n<1 implies that the fluid is pseudoplastic n>1 implies that the fluid is dilatant [3]

Equation relating viscosity to shear rate for apower law fluid is given - :bellow

$$\tau = \eta(\dot{\gamma})\dot{\gamma} \qquad (1)$$

$$\eta(\dot{\gamma}) = \frac{\tau}{\dot{\gamma}} \qquad (2)$$

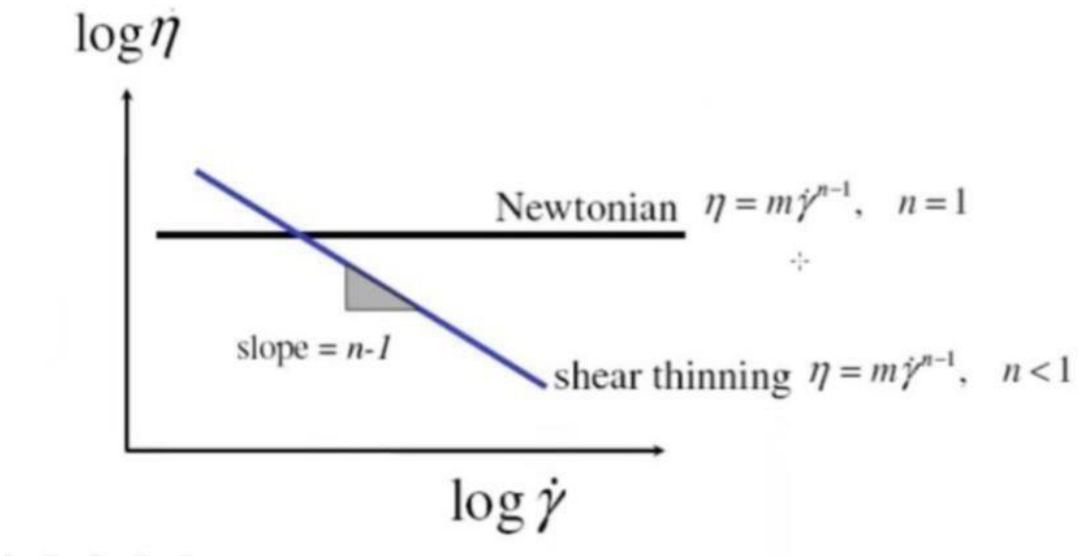
$$\tau = K(\dot{\gamma})^n \qquad (3)$$

$$\eta(\dot{\gamma}) = \frac{K(\dot{\gamma})^n}{\dot{\gamma}} \qquad (3) \text{ in } (2)$$

$$\eta(\dot{\gamma}) = K(\dot{\gamma})^{n-1} \quad \text{Viscosity function}$$

$$\log \eta(\dot{\gamma}) = \log K + (n-1)\log \dot{\gamma}$$

Thus alog - log plot of n vs. γ for apower law fluid is linear with aslope of n-1 therefore n=slop +1



Although the power law model accurately represents the pseudoplastic region, it neglects the Newtonian plateau at small and large strain rates. The viscosity goes to infinity at low strain rates and zero at high strain rates.

This limits the use of the power law model in predicting the flow .behavior of polymeric materials

Direct numerical simulation of the weakly turbulent flow of non-Newtonian fluids with shear-thinning rheology are undertaken. Results agree reasonably well with the experimentally determined logarithmic layer correlation presented by Clapp (1961) and with other previously published experimental work. As the power law index becomes smaller for the same Reynolds number, the flow deviates further from the Newtonian profile and the results suggest that transition is delayed. Use of this technique shows promise in understanding transition and turbulence in non-Newtonian fluids. [4]

Chapter three

Results and Discussion

Results and Discussion:

Fig. 1. Show the geometry of the three dimensions pipe used in this study . The length of pipe is ( ) and the diameter is ( ).

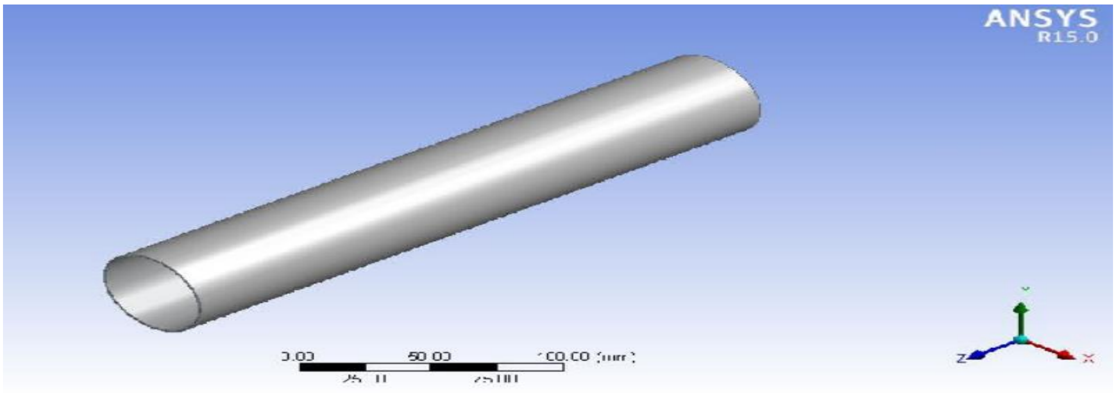
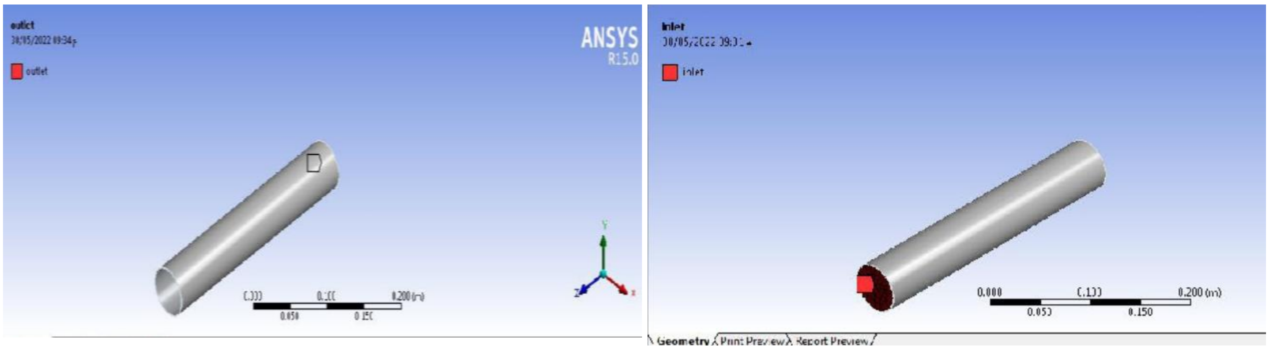


Fig. 1: The geometry of three dimensions used in this study.



(a) (b)

Fig. 2: The boundary conditions used in this study (a) outlet flow. (b) inlet flow..

Fig.2: indicates the boundary conditions in the inlet and outlet of pipe, while Fig 3. Shows the mesh of the pipe which contains of 2964 elements and 3240

nodes.The mesh number can be change according to the accuracy requiredment.

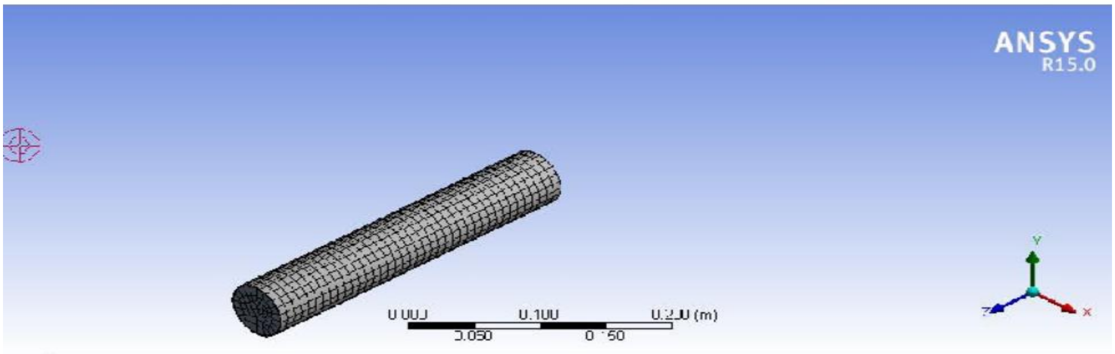


Fig.3: Show the mesh of the pipe, which contains 2964 elements and 3240 nodes.

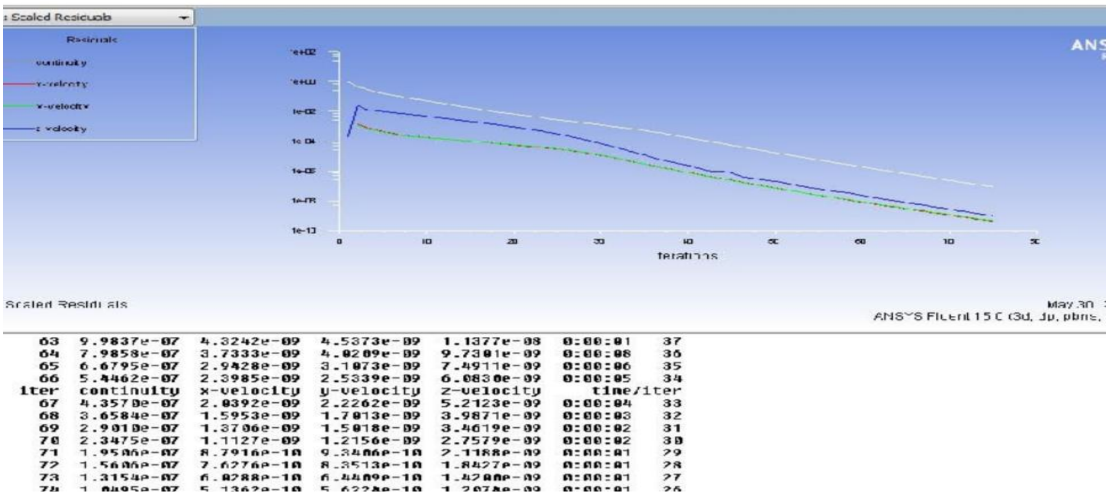


Fig.4: Shows the convergence of solution.

Fig.4: Indicates the behavior of solution after drawing the geometry , meshing, and applying the boundary conditions.

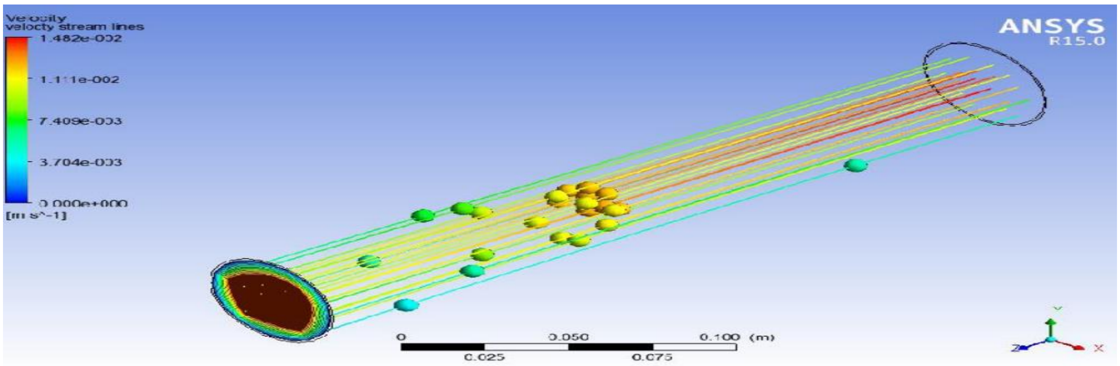


Fig.5: Shows the velocity streamlines of polymer according to the particles movements

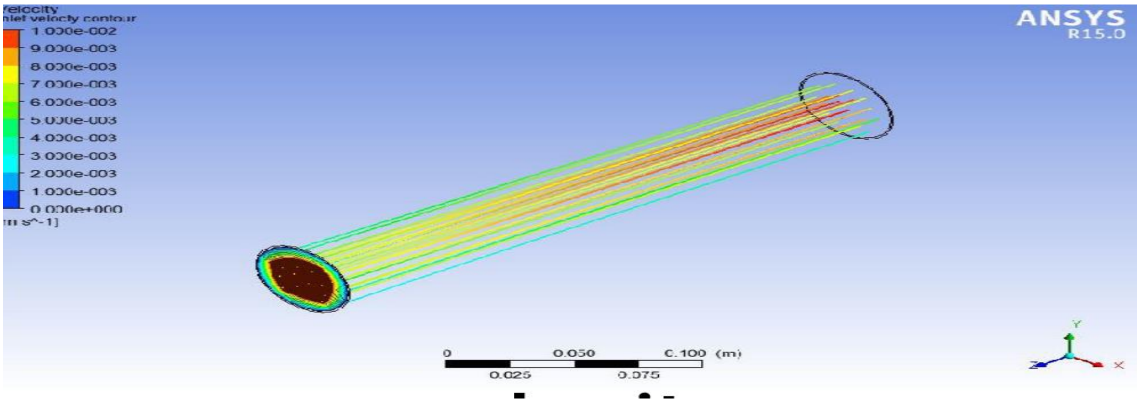


Fig.6: Shows the velocity streamlines of polymer .

Figs 5 and 6: Show the velocity of polymer according to the solution of quantity and momentum equations. The velocity is maximum at the center of pipe and then decreases gradually towards the pipe wall. This behavior produce the low shear rate and shear stress and high viscosity at the center of pipe. The high viscosity in the center of pipe produce high molecular weight.

According to that results it can be control on the velocity of polymer to control on the viscosity and then molecular weight. The controlling on the molecular weight can be modify and improve the mechanical and thermal properties of the final polymer product.

Chapter four

Conclusions

Conclusions:

From this study can be conclude the following:

1- Numerical simulation is a powerful tool to check the polymer viscosity and then the molecular weight.

2- Finite difference is suitable numerical method to simulate the rheology of polymer.

3- The numerical simulation reduce time, cost, and effort to study the polymer behavior.

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