CFD – Polymer Stretching by Turbulent Flow Field

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1. Introduction

A polymer is a substance composed of molecules characterized by the multiple repetition of one or more species of atoms or group of atoms (called monomers) linked to each other in amounts sufficient to provide a set of properties that do not vary markedly with the addition of one or a few constitutional repeating units. The polymeric (visco-elastic) fluid have several properties that makes its studies important in different sectors of industry. One of the most interesting properties regards the so called *"Toms effect"*: that is the property to reduce a flow's drag force by introducing a very small amount (one part per milion) of polymers in the fluid. This properties allows to drastically reduce the energy required to pump a fluid into pipe or channel, with a notable decrease of the costs.
The study of polymer liquids it is very relevant for Chemical Enginnering, since in chemical plant this property is largely used. Even though this property is known from the 1940s it is still not well understood, and so the research of polymeric liquids is very interesting for the science and industry. Particular intersest is given to the polymer stretching phenomena, that take place more often in the near wall flow, but experimental studies [1] have demonstrated that this happens also under certain conditions in the turbulent flow homogeneous and isotropic regime. In this first part of the research project we are study the stretching phenomena studing a realistic case, studied experimentally, in which the polymers show stretching phenomena under turbulent flow.

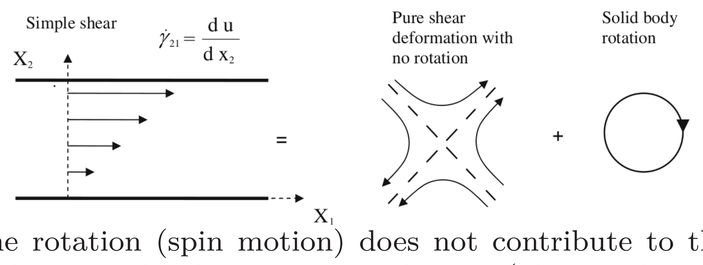
2. Polymer Stretching

Polymer chain in turbulent flow can be stretched under certain condition. The basic idea of polymer stretching is that this take place when the eigen vector of the strain rate align with the polymer [2, 3]

$$\underline{\underline{\sigma}} + \underline{\underline{I}}P = 2\eta\underline{\underline{\dot{\varepsilon}}}$$

Where σ is the symmetric stress tensor, P the hydrostatic pressure, η the viscosity and $\dot{\varepsilon}$ the symmetric component of the general strain rate (velocity gradient) tensor $\dot{\gamma}$. The strain rate can be divided into two components, a symmetric deformation component $\dot{\varepsilon}_{ij}$ and an antisymmetric rotation component ω_{ij}:

$$\dot{\varepsilon}_{ij} = \frac{1}{2}(\dot{\gamma}_{ij} + \dot{\gamma}_{ji}) \quad ; \quad \omega_{ij} = \frac{1}{2}(\dot{\gamma}_{ij} - \dot{\gamma}_{ji})$$



The rotation (spin motion) does not contribute to the chain stretching indeed the strain rate (high strain rate at lower turbulent scale)

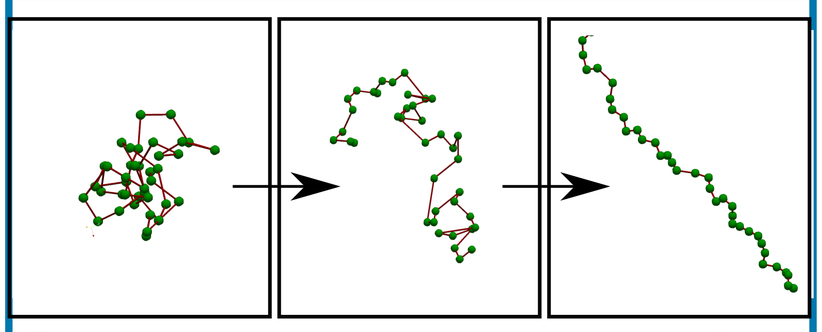
$$\varepsilon_{ij}\vec{\lambda} = \lambda_i\vec{\lambda_i} \qquad i = 1, 2, 3$$

Where $\vec{\lambda}$ and λ are the eigenvector and eigen value respectly. $\lambda_1 > 0$ always, considering a polymer of length $= l$ we can say that the stretching phenomena happens when:

$$\vec{\lambda_1} \cdot \vec{l} \neq 0 \qquad \frac{\vec{\lambda_1} \cdot \vec{l}}{|\lambda||l|} = \cos\theta \neq 0$$

It is very important to know the eigenvectors and the $\cos\theta$. When we have $\cos\theta \pm 1$, the polymer stretching is maximum.

6. Polymer Result



The above picture shown polymer in three different configuration from equilibrium configuration to stretch configuration, This behavior is due to the interaction with the turbulent smaller eddies.

8. References

[1] Richard Vonlanthen and Peter A. Monkewitz. Grid turbulence in dilute polymer solutions: Peo in water. *Journal of Fluid Mechanics*, 730:76–98, 2013.

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[3] Fred. T. Trouton. On the coefficient of viscous traction and its relation to that of viscosity. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 77(519):426–440, 1906.

[4] Theo G. Theofanous Demosthenes Kivotides, S. Louise Wilkin. Stretching of polymer chains by fluctuating flow fields. *Physics Letters A*, 375(Issue 1):48–52.

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3. Mathematical Model

Hydrodynamic interactions (Polymer-Water) take place at smaller scales then the turbulence eddies cascade [4]. In order to study this scale we have to fully resolve the turbulence spectrum (DNS) using an in-House Fortran90 code. We solved a coupling system of Navier-Stokes *(fluid)* and Langevin equation *(Polymer)* [5].

$$\frac{\partial\bar{u}_i}{\partial t} = 0; \qquad \rho\frac{\partial\bar{u}_i}{\partial t} + \rho\frac{\partial(\bar{u}_i\bar{u}_j)}{\partial x_j} + \frac{\partial\bar{p}}{\partial x_i} + \rho\frac{\partial(\overline{u_i'u_j'})}{\partial x_j} = \mu\frac{\partial^2\bar{u}_i}{\partial^2 x_j} + {}^dF_i^k\, G_\xi(\mathbf{x} - \mathbf{r}^k) = 0 \tag{1}$$

$${}^iF_i^k + {}^eF_i^k + {}^mF_i^k + {}^dF_i^k + {}^tF_i^k = 0 \tag{2}$$

$$\frac{\partial u_i^{\mathcal{S}}}{\partial x_i} = 0; \qquad \frac{\partial p^{\mathcal{S}}}{\partial x_i} - \mu\frac{\partial^2 u_i^{\mathcal{S}}}{\partial^2 x_j} - {}^dF_i^k\delta(\mathbf{x} - \mathbf{r}^k) = 0 \tag{3}$$

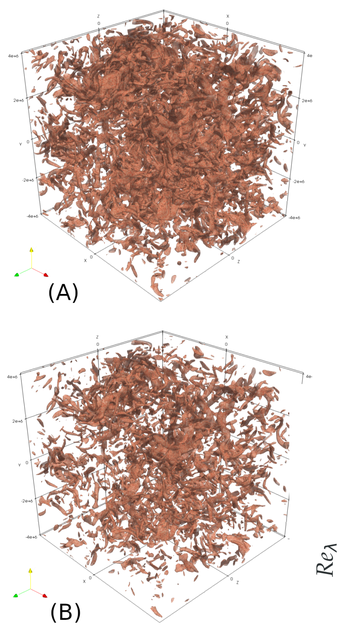
$$\overline{u_i'u_j'}(\mathbf{x}) = \overline{(u_l^{\mathcal{S}})_i(u_l^{\mathcal{S}})_j}(\mathbf{x}) = \int_V (u_l^{\mathcal{S}})_i(\mathbf{x} - \mathbf{x}')(u_l^{\mathcal{S}})_j(\mathbf{x} - \mathbf{x}')G_\xi(\mathbf{x}')d\mathbf{x}' \tag{4}$$

Where Eq 1 is the Navier Stokes equtions, Eq. 2 is the stochastic Langevin equation, Eq. 3 are the creeping flow (Stokes equations), and Eq. 4 describe the residual stress in 1 in terms of local a local field $u_l^{\mathcal{S}}$
We deal with Homogeneous and Isotropic Turbulence, that is the flow condition present in the center of a channel in the turbulent "wake" regime (y^+ curve).

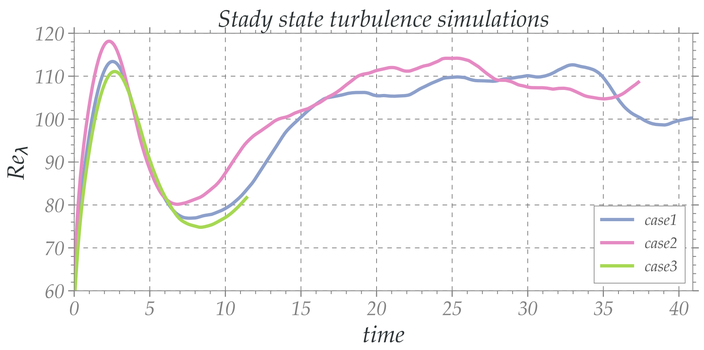
4. Method of Solution

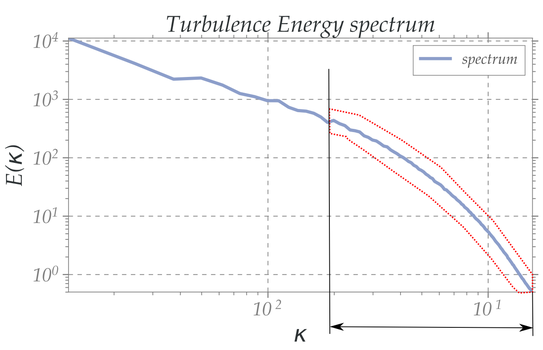
We solve the system of equations using a in-House Fortran code, that uses a FVM (Finite Volume Method) approach for discretizing the system in a staggered cubic grid with 256^3 computational cell, the accuracy of the solver is first order for the time-marching and second order semi-Implicit method for space. Brownian Stochastic Dynamics is used for the Polymer, that interacts with the flow by computing the Langevin Equation. The Flow is Homogeneous Isotropic Turbulent, and we forced the flow to be in a steady state compute a previous purely Fluid dynamic simulation in order to reach suitable Reynolds number (based on a Taylor microscale) and then using this condition of flow to initialize the fluid-polymer computations, in this way, we obtain a steady state homogeneous isotropic turbulence which allows us to study the hydrodynamic interaction between polymer and solvent.

5. Result



Results for the Turbulent iso-surface of Vorticity 30% of the maximum value (A), and Vorticity 70% of the maximum value (B) have been reported in figure. It is possible to observe that also using a Re_λ relatively small (≈ 100) the vorticity is increased, this is due to the fact that we are resolving all the turbulent spectrum starting from the smaller scale, called the "Kolmogorov scale η" (upper turbulence spectrum of frequency) to the largest called "Large Eddy Turn over". The plot below reports the steady state turbulent flow with which we initialize the Polymer-Fluid simulations (left). It is possible to observe that the flow reaches the steady state after a certain period of time, this period of time is almost equal to thirty times the Large eddy turnover. The plot on the right is the turbulence spectrum, highlighting the viscous cut-off regime it is the area in which we would that the polymer chain reside in order to be stretched as also reported in the study of Vonlanthen et al [1]





7. Conclusions

The aims of this project is to better understand the Polymer dynamics in a Turbulent homogeneous and isotropic flow. We now have concluded that:

- We had calculated all the quantities that represent the experiments condition [1]
- We have computed a Turbulence statistically steady state Flow
- We now are moving on perform a simulations including polymers.
- We have the software facility to show the behaviour of polymer under the influence of the surrounding flow (Demonstrate using movie of the polymer evolution).