8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

Numerical Simulation on Nanotube

*** Mathieu Colin[1], Thierry Colin[2], Kevin Santugini[3]**

[1] Université Bordeaux 1
IMB - Inria Futurs,
351 Cours de la Libération
Talence 33405, FRANCE
mcolin@math.u-bordeaux1.fr,
http://www.math.u-bordeaux1.fr/~mcolin/

[2] Université Bordeaux 1
IMB - Inria Futurs,
351 Cours de la Libération
Talence 33405, FRANCE
colin@math.u-bordeaux1.fr,
http://www.math.u-bordeaux1.fr/~colin/

[3] Université Bordeaux 1
IMB - Inria Futurs,
351 Cours de la Libération
Talence 33405, FRANCE
kevin.santugini@math.u-bordeaux1.fr,
http://www.math.u-bordeaux1.fr/~santugini/

Key Words: Nanotube, Penalization Method

ABSTRACT

Carbon nanotubes have remarkable mechanical properties. Fibers made with carbon nanotubes are of great interest from the industrial point of view. The experimental situation that we want to model in this paper is the following one [2]. A solution of nanotubes is injected as a jet in a cylindrical channel inside a solution of polymers.

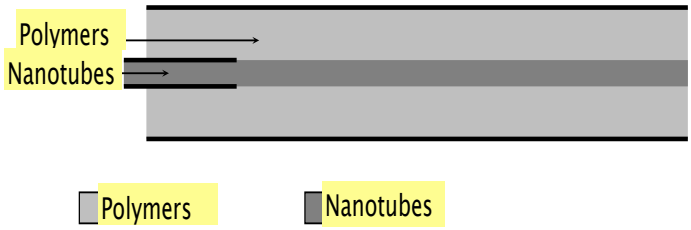

FIG. 1 - Injection of nanotubes inside a polymer flow

The diameter of the internal jet is approximatively 0.3 mm. The diameter of the external channel is 20 mm and its lenght is of order 1 meter. In the small one, the nanotube solution is injected at a the speed of $5m.s^{-1}$ and the velocity of the polymer solution is $2.5m.s^{-1}$. At the interface of both solutions, a chemical reaction takes place and creates a visco-elastic gel which is convected by the outflow. The polymer solution diffuses through the gel aloung the channel and the chemical reaction keeps on going.

The aim of this talk is to present a model which discribes the production of nanotube gel and to present some numerical simulations. The model has to described in each points of the channel the fraction of volume of the different component of the mixing as well as the diffusion process.

We assume that each specie is transported by the flow at the speed v and has its own diffusion coefficient. The concentration of nanotube, gel and polymer which will denote respectively by c_N, c_g and c_p satisfy

$$\frac{\partial}{\partial t}\begin{bmatrix} c_p \\ c_N \\ c_g \end{bmatrix} + (\boldsymbol{v}\cdot\nabla)\begin{bmatrix} c_p \\ c_N \\ c_g \end{bmatrix} = K\begin{bmatrix} -\alpha_p c_p c_N \\ -\alpha_N c_p c_N \\ c_p c_N \end{bmatrix} + \nabla\cdot\begin{bmatrix} D_p(c_p,c_N,c_g)\nabla c_p \\ D_N(c_p,c_N,c_g)\nabla c_N \\ D_g(c_p,c_N,c_g)\nabla c_g \end{bmatrix} \tag{1}$$

where the diffusion coefficient are given by

$$D_p = \frac{RT}{6\pi\eta r_p \mathcal{N}_A} \qquad\qquad D_N = \frac{RT}{6\pi\eta r_N \mathcal{N}_A}$$

with $\eta = c_g\nu_g + c_p\nu_p + c_N\nu_N$. The diffusion of the gel will be neglected. Here ν_g, ν_p and ν_N denote respectively the viscosity coefficient of the gel, the polymer and the the nanotube. One has that $\nu_N = 10\nu_{water}$ while the viscosity of the polymer solution is $\nu_P = 200\nu_{water}$.

More details o n K, D_p, D_N and D_g will be discussed during the talk.

The result of the mixing and and the gel will be considered as an incompressible non-Newtonian fluid. The equation satisfied by v which express the conservation of the motion is then a Navier-Stokes equation of the type

$$\rho\left(\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right) = -\nabla p + \nabla\cdot\sigma + \nabla\cdot(2\nu(c_N,c_p,c_g)D(\boldsymbol{v})). \tag{2}$$

where σ denotes the visco-elastic constraint tensor. Finally, we will introduce an equation for the tensor σ:

$$\frac{\partial\sigma}{\partial t} + (\boldsymbol{v}\cdot\nabla)\sigma - \nabla\boldsymbol{v}^{\mathrm{T}}\sigma - \sigma\nabla\boldsymbol{v} + (1-a)(\sigma D(\boldsymbol{v}) + D(\boldsymbol{v})\sigma) = 2GD(\boldsymbol{v}) - \omega\sigma \tag{3}$$

with a in interval $[0,1]$.

Parameter G describes the elasticity properties of the gel. One takes $\omega = \frac{1}{c_g}\frac{1}{\tau}$.

We discretize this model on a cartesian mesh. The Navier-Stokes equation is discretized on a staggered mesh and the divergence-free condition is handled by an artificial compressibility method. In time, we use a splitting scheme. Since the characteristic time of the chemical reaction is small compare to that of the flow, we consider it as being locally instantaneous. For the equation on the stress tensor σ, we use an exponential scheme in the spirit of [1].

During the talk, we will discuss the influence of the physics on the different coefficients and the physical law that we have to take into account in order to close the system, we will provide a parametric study of the formation of the fibers.

REFERENCES

[1] F. Boyer, L. Chupin and P. Fabrie. *Numerical study of viscoelastic mixtures through a Cahn-Hilliard flow model.* European Journal of Mechanics - B Fluids, vol. 23, 5 pp. 759-780 (2004).

[2] P. Poulin, B. Vigolo, P. Launois. *Films and fibers of oriented single wall nanotubes*, Carbon, 40, 1741-1749, (2002).