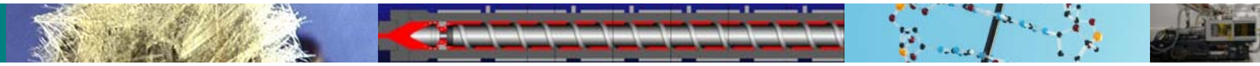

Simulation of Injection Molding Thermoplastic Reinforced with Micro and Nano-Particles

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ABSTRACT

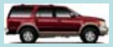
The redefinitions of the energy policy of the US have multiple fronts. One objective of the DOE is to enforce the development of new lightweight materials with identical or better properties than existing materials. The goal is to reduce the weight of vehicles by 33% (in comparison to 2002) by 2010. One of the promising alternatives under consideration is injection molded parts made of polymers reinforced with large aspect ratio particles (i.e. long fibers or nanoparticles). However, these types of parts have not been successfully manufactured because of the unknown molecular behavior of the materials during processing. In this research we are trying to extend the Doi's theory for rod-like systems to simulate the rheological behavior of these composites.

A numerical code is being written to simulate the flow of fiber suspensions in injection molding flow geometries. The preliminary results of the simulation for shear flow shows that the model can reproduce the experimental data under stress growth conditions. The code has been validated in shear and extensional flow which are used to determine material parameters.

BACKGROUND

High Strength Weight Reduction Materials

Office of FreedomCAR and Vehicle Technologies



To identify and develop materials and materials processing technologies which can contribute to weight reduction without sacrificing strength and functionality:

- Increase the fuel efficiency
- Reduce emissions of class 1-8 trucks

GOAL

To combine numerical simulation and experimental programs to confirm the pre-diction of microstructure in both glass and nano-particle reinforced thermoplastics

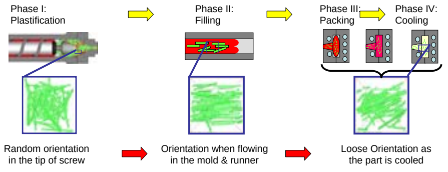
OBJECTIVES

- To simulate the mold filling process for thermoplastic melts reinforced with short fibers, long fibers and nano-particles of high aspect ratio using constitutive relations (i.e. stress tensors coupled with a generation expression) which allow coupling between the flow and particle orientation.
- A key aspect of this work will be an experimental evaluation of the predicted fiber or particle orientation distribution throughout an injection molded part.

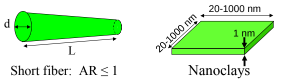
INNOVATION

Use of constitutive relations, which contain the micro-structural aspects of the reinforced melts and viscoelastic effects.

ORIENTATION DURING INJECTION MOLDING



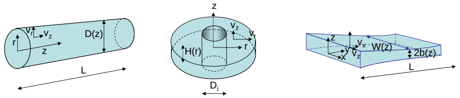
$$\text{Aspect Ratio} = \frac{Length}{Diameter}$$



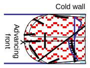
Short fiber: AR $\leq$ 1
Long fiber: AR > 1

Nanoclays
(i.e. Montmorillenite)

Geometric elements commonly found in injection molding tooling



- Mechanism of flow
  Shear and Elongational flow



CHALLENGES

- **Predict fiber orientation correctly:**
  - **Should Doi Model be improved?**
  - **Do results strongly depend on initial orientation?**
- **Develop a stable and accurate numerical scheme**
- **To measure fiber orientation**
- **Is the final flow induced orientation governed by the Brownian motion effects or by the relaxation process of the system, *i.e. elastic recoiling of non-Newtonian matrix*?**

MODELLING

- Behavior polymer – glass fibers
  - Actual model: Doi's Theory: LCP assuming Newtonian solvent

Evolution tensor of orientation

$$\frac{\partial \underline{\underline{S}}}{\partial t} = \underline{\underline{F}}(\underline{\underline{S}}) + \underline{\underline{G}}(\underline{\underline{S}})$$

Brownian contribution

$$\underline{\underline{F}}\left(\underline{\underline{S}}\right) = -6\overline{D_r}\left(\underline{\underline{S}} - \frac{1}{3}\underline{\underline{I}}\right) + 6\overline{D_r}U\left(\underline{\underline{S}} \bullet \underline{\underline{S}} - \underline{\underline{S}} \bullet \underline{\underline{\underline{\underline{SS}}}}\right)$$

Kinematics contribution

$$\underline{\underline{G}}\left(\underline{\underline{S}}\right) = \underline{\nabla}\underline{v}^T \bullet \underline{\underline{S}} + \underline{\underline{S}} \bullet \underline{\nabla}\underline{v} - 2\left(\underline{\nabla}\underline{v} + \underline{\nabla}\underline{v}^T\right) : \underline{\underline{\underline{\underline{SS}}}}$$

Stress due oriented fiber

$$\underline{\underline{\tau}} = \underbrace{G\left[\underline{\underline{S}} - \frac{1}{3}\underline{\underline{I}} - U\,\underline{\underline{S}} \bullet \underline{\underline{S}} + U\,\underline{\underline{S}} : \underline{\underline{\underline{\underline{SS}}}}\right] + \frac{AG}{6D_r}\left[\underline{\nabla}\underline{v} + \underline{\nabla}\underline{v}^T\right]}_{\text{Original Doi Theory stress equation}} + \underbrace{\eta_r\eta_s\left(\underline{\nabla}\underline{v} + \underline{\nabla}\underline{v}^T\right)}_{\text{High }\dot{\gamma}}$$

Parameters adjusted for optimal rheological data:

$$\overline{D_r} = D_r\frac{4}{9}\left(1 - \underline{\underline{S}} : \underline{\underline{S}}\right)^{-2} \qquad U = v_2 c d L^2$$

η_r = relative viscosity
η_s = solvent/matrix viscosity

- Behavior of polymer melt
  - Introduce modifications: Extend to non-Newtonian solvents (polymer melts)
    - Shear-thinning (viscous) model: Carreau -Yasuda Model

$$\frac{\eta_s - \eta_{s,\infty}}{\eta_{s,0} - \eta_{s,\infty}} = \left[1 + \left(\lambda I_2\right)^a\right]^{\frac{n-1}{a}}$$

    - Memory effects (Viscoelastic) : Upper Convected Maxwell

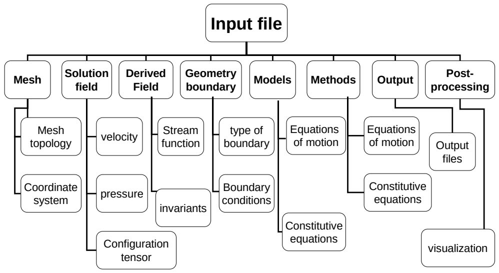
$$\underline{\underline{\tau}} + \lambda\left[\frac{\partial \underline{\underline{\tau}}}{\partial t} + \left(\underline{v} \bullet \underline{\nabla}\,\underline{\underline{\tau}}\right) - \left[\left(\underline{\nabla}\underline{v}\right)^T \bullet \underline{\underline{\tau}} + \underline{\underline{\tau}} \bullet \underline{\nabla}\underline{v}\right]\right] = \eta\left(\underline{\nabla}\underline{v} + \underline{\nabla}\underline{v}^T\right)$$

- Equations of Transport

$$\underline{\nabla} \bullet \underline{v} = 0 \qquad \underline{\underline{\sigma}} = \underline{\underline{\tau}} - p\underline{\underline{I}} \qquad \rho C_p \frac{DT}{Dt} = \underline{\nabla} \bullet (k\underline{\nabla}T) + \underline{\underline{\tau}} : \left(\underline{\nabla}\underline{v} + \underline{\nabla}\underline{v}^T\right)$$

(Mass) (Momentum) (Energy)

STRUCTURE OF THE PROGRAM



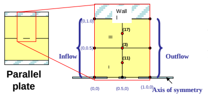
Input file
- Mesh
  - Mesh topology
  - Coordinate system
- Solution field
  - velocity
  - pressure
  - Configuration tensor
- Derived Field
  - Stream function
  - invariants
- Geometry boundary
  - type of boundary
  - Boundary conditions
- Models
  - Equations of motion
  - Constitutive equations
- Methods
  - Equations of motion
  - Constitutive equations
- Output
  - Output files
- Post-processing
  - visualization

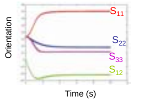
SIMULATION SCHEME

- Determine the free surface shape
  - Mavridis technique
- Orientation tensor of fiber suspensions
  - Discontinuous Galerkin (DG) finite element methods have been successful for the discretization of the equations of motion when additionally a discrete elastic viscous stress splitting technique is used
  - The discretized equations can be solved element by element
- Configuration tensor of viscoelastic fluids
  - Galerkin finite element methods have been successful for the discretization of the equations of motion when additionally a discrete elastic viscous stress splitting technique is used
  - A frontal solver will be used to solve the matrix-vector equation resulting from the Galerkin method
- Use of two techniques recently developed to ensure positive definiteness of the configuration tensor at the discrete level
- A typical iteration step consists of three stages

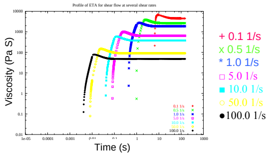
1. Update the velocity using the stresses from the previous time step
2. Update the orientation tensor and the stress using the velocity computed in 1
3. Update the free boundary coordinates and mesh using the velocity computed in stage 1

NUMERICAL RESULTS





Preliminary results on model predictions of the orientation for S_{11}, S_{22} ,S_{33} S_{12} components using Backward-tracking Lagrangian Mehtod (BLPM). The model predicted orientation components, at an Node 3, for 0 ≤ t ≤ 10 s in a fluid moving between parallel plates. Similar results were obtained using a rheometrical simulation method.



The rheometrical simulations are able to predict some important viscoelastic quantities. Here is shown a representative result of the prediction of the transient viscosity at several shear rates. The constants used for the model were: A=0, G=30,000, Dr=3.0, U=0.1.

EXPERIMENTAL DETERMINATION OF FIBER ORIENTATION

Long glass fiber
Pultruded in PP

Short shots progression

Top view

Side view

Short shots progression

Front view

A method to determine the fiber orientation in Injection Molded part will be tried to develop during this summer in collaboration with:

ornl

FINDINGS

- Preliminary orientations of fibers have been determined using two simulation methods: complex flow and rheometrical flow.
- The interaction of the long fibers with each other seems to require that an additional modification of the theory be used Initial experiments indicate that additional modification of the theory may be necessary to simulate long fiber orientations.

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