OP-18-337

Thursday, May 12, 2011, 06:20-06:40 pm
Room: Karam 4

A NUMERICAL TREATMENT OF CRYSTALLIZATION IN TUBE FLOW

D. Lee Wo[a,*], R. I. Tanner.[a], D.F. Fletcher[b]

[a] *School of Aerospace, Mechanical and Mechatronic Engineering,* [b] *School of Chemical and Biomolecular Engineering, The University of Sydney, NSW 2006, Australia.*

**Corresponding author: duane.leewo@sydney.edu.au*

A viscosity-oriented, flow-induced crystallization model is used to predict the rate of crystal layer growth in a tube at high shear rates. A combined strain and strain-rate dependence on the enhancement of crystallization kinetics is proposed after showing excellent agreement with viscosity measurements at low deformation rates in simple shear and is therefore considered in a more complex Poiseuille flow at higher shear rates ($100s^{-1}$). Typically, a sharp increase in viscosity occurs with increasing crystallinity and suspension mechanics is used to link the relative volume fraction of crystallinity to the viscosity of the semi-crystalline polymer. The microstructure is also directly related to the simultaneous thermo-mechanical histories and this gives rise to geometric considerations, which can be accounted for in the total volume fraction using the Avrami-Kolmogorov model. The key characteristic of our model is to couple the flow history to induced crystallization of semi-crystalline polymers and link the flow-enhanced nucleation with viscosity and thermal gradients. In this way the flow can be described in terms of changes in crystallization due to changes in rheological behaviour.

Furthermore, a non-isothermal approach is needed as viscous shear heating occurs at the interface between recently formed layers of crystals and a molten amorphous core region. Since each fluid particle has its own unique shear deformation, temperature and viscosity histories, a finite volume numerical treatment was employed using the software CFX from Ansys to model the flow and layer growth. The problem now becomes one in which an unsteady, transient flow is governed by the development of crystallization layers where higher shear rates exist and viscosity changes due to the crystallization effect. In terms of the rheology, a generalized non-Newtonian model is employed with the governing equations for modelling tube flow. The model is further tested with the presence of nucleating agents and the sensitivity of the rheological properties of both organic and inorganic pigment-polymer blends to stress and temperature was evident.