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Citation for published version (APA):

Document status and date:
Published: 01/01/2017

Document Version:
Publisher’s PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:
• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher’s website.
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Modelling of Flow Induced Crystallization: Multiple Phases and Multiple Morphologies


Motivation
In products made of stereo-regular isotactic polypropylene four different crystal phases can be found: the α-, the β-, the γ- and the mesomorphic phase. Moreover these phases show cross-hedging, i.e. lamella nucleating on lamella (parents and daughters). The formation of these phases strongly depends on processing conditions, like flow, pressure and temperature history. Being able to properly model the final polymer structure, as a function of the local thermal and mechanical history, is essential for predicting the final properties of polymeric products. For this reason, this project aims at developing a numerical model able to reproduce processing dynamics and directly simulate the crystalline structure formation.

Methods
The present model consists of a non-isothermal, non-linear viscoelastic flow solver, including flow induced crystallization1, implemented in an in-house finite element code.

The flow equations for a slightly compressible fluid are

\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f} \]

The constitutive model for a non-linear viscoelastic fluid is

\[ \sigma = 2\mu\varepsilon^\text{dev} \]

Energy Equation
Shear heating and crystallization heat release

\[ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \nabla \cdot (\kappa \nabla T) + Q_{\text{crystallization}} \]

Crystallization Equations
- different crystal phases \( \alpha, \beta, \gamma \) and meso
- various crystalline morphologies \( \alpha, \alpha', \alpha'' \)
- spherical and hexagonal crystals

As a test case, a piston driven channel flow with varying initial pressure level is taken (see Figure 1). A flow pulse is applied for 0.25 s, after which the crystallization evolution is evaluated for 20 minutes. The build up and relaxation of the pressure difference and the molecular stretch of the longest molecules during and after flow are accounted for.

Figure 1: geometry of the piston driven channel flow.

Preliminary Results
Numerical simulations have been run for different average pressures and flow rates. The results are compared with experimental results of morphological and structural development during flow and during subsequent crystallization (see Figure 2 and 3). Experimental data was collected using wide-angle diffraction at the beamline BM62B of the ESFR (Grenoble, France)².

Figure 2: Experimental and model results for the pressure difference, (a) and (c), and for the crystalline space filling, (b) and (d), for different piston speeds (20, 40, 60 and 80 mm/s) at average pressures of 100 bar (top panels) and 400 bar (bottom panels).

Figure 3: Space filling ratio between \( \alpha \)-parents and \( \gamma \)-parents and daughters (a) and between \( \alpha \)-daughters and \( \gamma \)-parents and daughters (b) for different average pressures and piston speeds.

Outlook and Conclusions
Results look already very promising and the model is being tuned to better capture the complex rheological and morphological behaviour of IPP during processing. The model will be used in future to simulate different processing conditions like fiber spinning and film blowing.
