Numerical modelling of dispersive polymer blends

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.
• The final author version and the galley proof are versions of the publication after peer review.
• The final published version features the final layout of the paper including the volume, issue and page numbers.

Link to publication

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
• You may not further distribute the material or use it for any profit-making activity or commercial gain
• You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the “Taverne” license above, please follow below link for the End User Agreement:
www.tue.nl/taverne

Take down policy
If you believe that this document breaches copyright please contact us at:
openaccess@tue.nl
providing details and we will investigate your claim.

Download date: 10. Jan. 2021
Numerical modelling of dispersive polymer blends

Wing-Hin B. Wong, Martien A. Hulsen, Patrick D. Anderson

Introduction
A well-known method for obtaining polymer materials with specific properties is blending multiple existing polymers. In this project, the evolution of the droplet morphology of immiscible dispersive polymer blends (See Figure 1) is studied using TFEM, an in-house developed FEM code.

Constitutive model
Based on [2], the morphology is described with mono-disperse macroscopic droplet populations using the following morphology field variables: the deformation gradient tensor \( \mathbf{F} \), the stretch ratio \( \beta \) and the unstretched droplet radius \( R_0 \). These variables are described using convection-type equations, which evolve over a Stokes velocity field:

\[
\nabla \cdot \mathbf{u} = 0, \quad -\nabla p + \nabla \cdot (2\mu_e \mathbf{D}) = 0, \\
\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f = g,
\]

where \( \mu_e \) is the effective blend dynamic viscosity (currently assumed constant), \( f \) is (a component of) a morphology variable and \( g \) is a nonlinear function that depends on the flow and morphological state.

Numerical simulation
In the example below (See Figure 2), the morphology development of a 10% PIB-90% PDMS mixture has been simulated in a channel with a cylindrical obstacle.

Results
The simulation was run until \( t = 30 \) with initially uniform \( \beta = 1 \) and \( R_0 = 10^{-2} \). Three illustrative frames have been plotted (See Figures 3 and 4):

![Figure 1. Drops of PIB inside a matrix of PDMS. Deformation, break-up and coalescence of the droplets occur during processing [1].](image1)

![Figure 3. Three frames of the stretch ratio \( \beta \). The scale is logarithmic. At \( t = 3 \), the droplets rapidly stretch near the cylinder due to the high extension rate there. At \( t = 16 \), the highly stretched droplets near the cylinder have broken up and high \( \beta \) has developed near the top wall. At \( t = 30 \), the highly stretched droplets near the top wall have broken up and some stretch remains behind the cylinder.](image3)

![Figure 4. Three frames of the unstretched droplet radius \( R_0 \). The scale is logarithmic. At \( t = 3 \), the droplets are still stretching, so \( R_0 \) does not change. At \( t = 16 \), the highly stretched droplets near the cylinder have broken up and a wide range of droplet sizes can now be observed. At \( t = 30 \), the remaining highly stretched droplets have broken up, but also some of the previously small droplets near the symmetry axis have coalesced into slightly larger droplets.](image4)

Future work
The model yields qualitatively good results but needs to be experimentally validated. Points for future work are: (i) extending the model with polydisperse droplet populations, (ii) following the morphology evolution along a 3D particle path in complex flows and (iii) extending the model with viscoelasticity of the blend constituents.

References