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Diffuse interface modelling of the rheology of immiscible polymer blends

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Objective

Predict macroscopic properties of polymer blends, such as the first normal stress difference \((N_1)\), based on the information obtained with simulations of morphology development on a microstructural level [1].

Methods

The Cahn-Hilliard (CH) equations, based on a diffuse interface model, are used to describe non-uniform systems:

\[
\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \frac{1}{P_e} \nabla \cdot \mathbf{q} ,
\]

\[
P_e = \frac{\rho \xi^2 L V}{M c} ,
\]

\[
\mu = c^N - c - C \cdot \nabla^2 c ,
\]

\[
C = \frac{\xi}{L} ,
\]

in which the chemical potential \(\mu\) is the driving force for the topological changes \((\partial c/\partial t)\). Besides \(\mu\) and the concentration \(c\) the velocity \(\mathbf{v}\) is unknown in these two equations and has to be calculated using the momentum balance (eq. 5) with prescribed simple shear via the boundary conditions:

\[
\nabla \mathbf{g} = \rho \mu \nabla c + \nabla \cdot (2\eta \mathbf{D}) .
\]

In 2D a stream function \(\psi\), which is defined by \(\mathbf{v} = (\partial \psi/\partial y, -\partial \psi/\partial x)\) can be used to govern balance of mass and by taking the rotation \(\nabla \psi\) is eliminated. Scaling of this equation then yields:

\[
\nabla^4 \psi = \frac{1}{C_a C} \nabla \times \mu \nabla c ,
\]

\[
C_a = \frac{\xi \eta V}{\rho c \xi B} = \frac{\eta V}{\gamma} ,
\]

In all subsequent simulations \(N = 7\) in eq. 4 to create a more immiscible behaviour between the two components, which corresponds to a higher \(\chi\) parameter.

Results

The simulations, depicted in figure 1 and 2 are carried out with \(P_e = 5\), \(C = 0.02\) and \(C_{\alpha} = 10\). Except for the red curves in figure 3 (right), in which the scaling of the interface is tested with \(C = 0.04\) (doubled) and \(P_{en} = (C/C_{\alpha}) \cdot Pe\) (\(\times\)), \(P_{en} = (C_{\alpha}/C) \cdot Pe\) (\(\div\)) and \(P_{en} = (C_{\alpha}/C)^2 \cdot Pe\) (\(\div\))

Conclusions

- The method describes breakup and coalescence without additional decision criteria.
- Scaling of the interface to more realistic domains looks promising, but requires additional work.
- The relation between microscopic and macroscopic parameters can be established.

References:


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