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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].
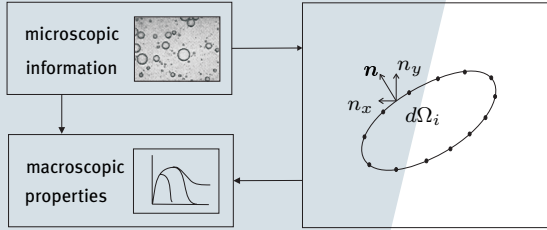
$$q = \frac{1}{V} \int (\boldsymbol{n} \cdot \boldsymbol{n} - \frac{1}{3}\boldsymbol{I}) d\Omega . \quad (1)$$

$$\frac{N_1 V}{\gamma} = q_{yy} - q_{xx} = \sum (n_{yy,i} - n_{xx,i}) d\Omega_i . \quad (2)$$

The major advantage with respect to the work of Peters [2] is that the model requires no additional critical criteria for breakup and coalescence phenomena.
Numerical discretization limits the maximum domainsize (~ 50 times the interface thickness ξ). Rescaling of the interface is therefore an important issue in diffuse interface modelling.

Methods

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

$$\frac{\partial c}{\partial t} + \boldsymbol{v} \cdot \nabla c = \frac{1}{Pe}\nabla^2 \mu , \qquad Pe = \frac{\rho \xi^2 LV}{M\epsilon} , \quad (3)$$

$$\mu = c^N - c - C^2 \nabla^2 c , \qquad C = \frac{\xi}{L} , \quad (4)$$

in which the chemical potential μ is the driving force for the topological changes ($\partial c/\partial t$). Besides μ and the concentration c the velocity $\boldsymbol{v}$ 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:

$$\nabla g = \rho\mu\nabla c + \nabla \cdot (2\eta \boldsymbol{D}) . \quad (5)$$

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

$$\nabla^4 \psi = \frac{1}{Ca}\frac{1}{C}\nabla \times \mu\nabla c , \qquad Ca = \frac{\xi\eta V}{\rho\epsilon c_B^2} = \frac{\eta V}{\gamma} , \quad (6)$$

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

/department of mechanical engineering

Results

The simulations, depicted in figure 1 and 2 are carried out with $Pe = 5$, $C = 0.02$ and $Ca = 10$. Except for the red curves in figure 3 (right), in which the scaling of the interface is tested with $C = 0.04$ (doubled) and $Pe_n = (C/C_n)Pe$ (○), $Pe_n = (C_n/C)Pe$ (◁) and $Pe_n = (C_n/C)^2 Pe$ (+)
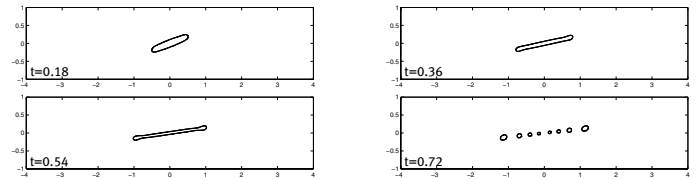

Figure 1 *Break up of one single droplet as a result of prescribed shear on the top and bottom boundary.*
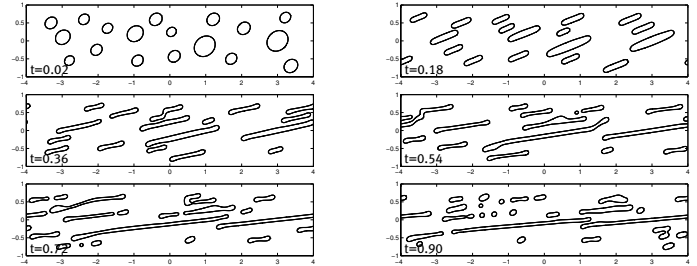

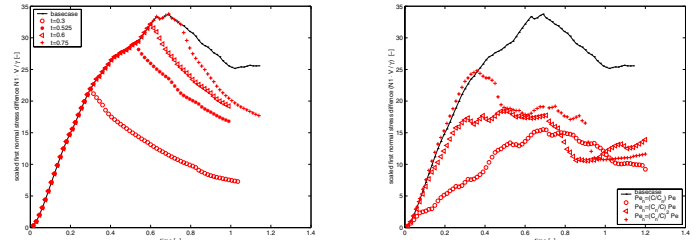**Figure 2** *Breakup and coalescence in a multi-droplet domain subjected to a start up flow.*

Figure 3 *Left: first normal stress difference (N_1) scaled with the interfacial tension (γ). Right: Scaling results of Peclet for thicker interfaces.*

In figure 1 the stretching and breakup is observed. In figure 2 more droplets are used to introduce the possibility of coalescence. The red curves in figure 3 (left) show the relaxation of droplets after cessation of shear at various time-steps.

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:

[1] TUCKER III, C.L., MOLDENAERS, P.: *Microstructural evolution in polymer blends*, Ann. Rev. Fluid Mech, 34:177-210,2002

[2] PETERS, G.W.M., HANSEN, S., MEIJER,H.E.H.: *Constitutive modeling of dispersive mixtures*, J. of Rheol., 45:3,659-689, 2001