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Introduction

A well-known method for producing polymer materials with specific properties is blending multiple existing polymers. Our aim is to quantitatively model the evolution of the morphology of immiscible disperse polymer blends (see Figure 1) during processing and implement this in a finite element framework.

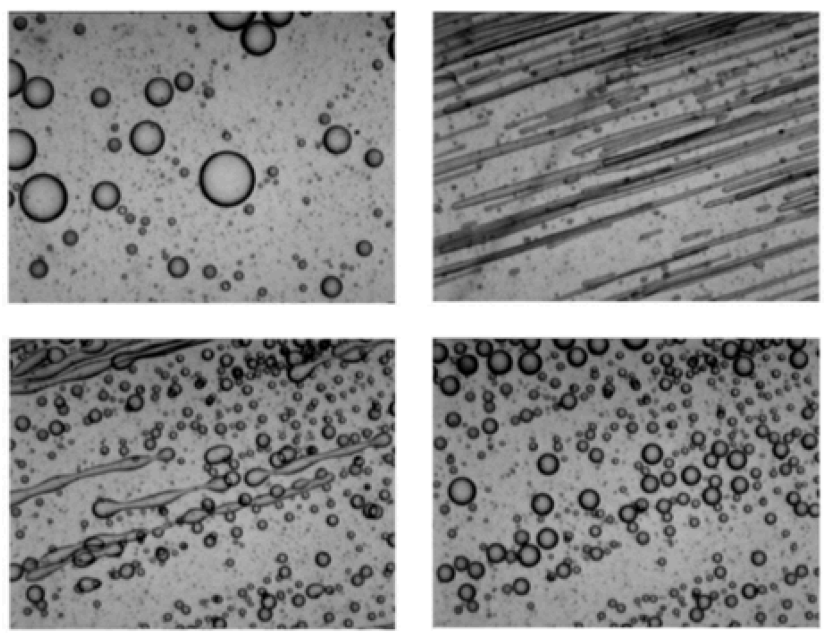

Figure 1. *Drops of PIB inside a matrix of PDMS [1]. Deformation, break-up and coalescence of the drops occur during processing.*

Constitutive model

Based on [2], we model the morphology as fields of polydisperse macroscopic droplet populations. Every population is described by an average unstretched droplet radius (defined as R_0), stretch ratio, orientation vector and the number of droplets, which undergo changes based on the background flow field (see Figure 2). We calculate the flow field according to the Stokes equations.

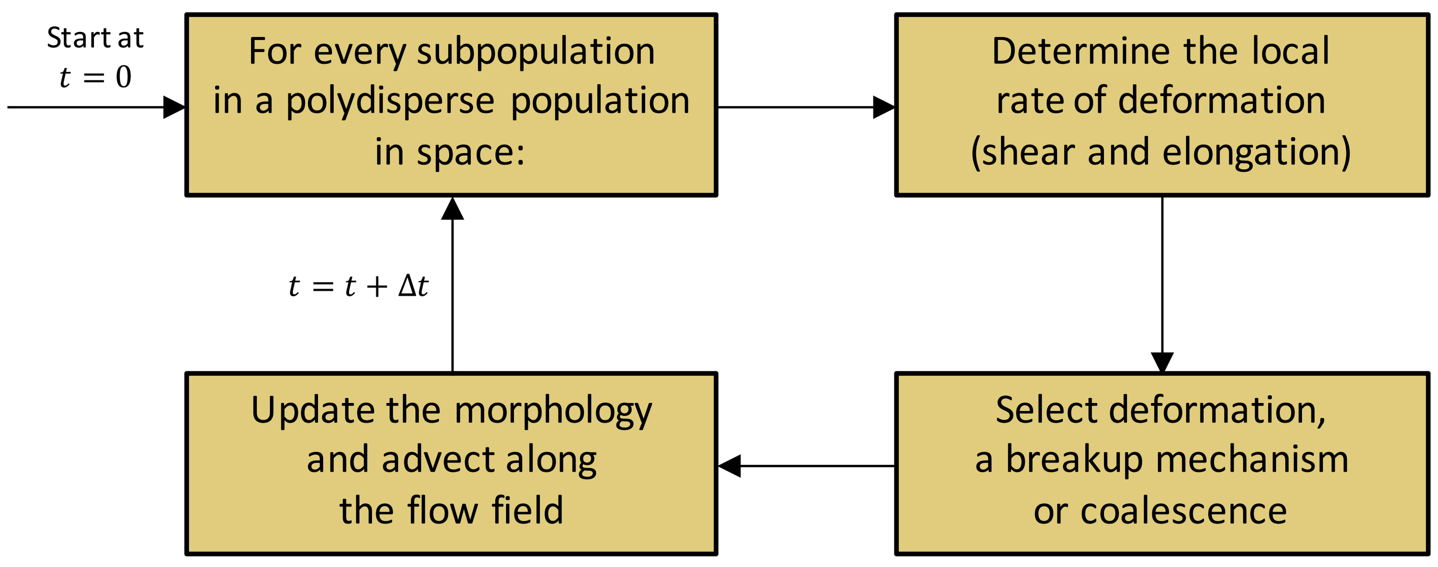

Figure 2. *Schematic overview of the time-stepping procedure.*

Numerical simulation

In this example (see Figure 3), we investigated the morphology development of a 10% PIB - 90% PDMS blend in an eccentric cylinder flow, where the outer cylinder rotates anticlockwise with an angular velocity of $1\ \mathrm{rad/s}$. The initial droplet radius distribution consists of 100 populations distributed logarithmically between $10^{-7}\ \mathrm{m}$ and $10^{-4}\ \mathrm{m}$. The histograms were extracted from a sample point located halfway in the gap below the inner cylinder.

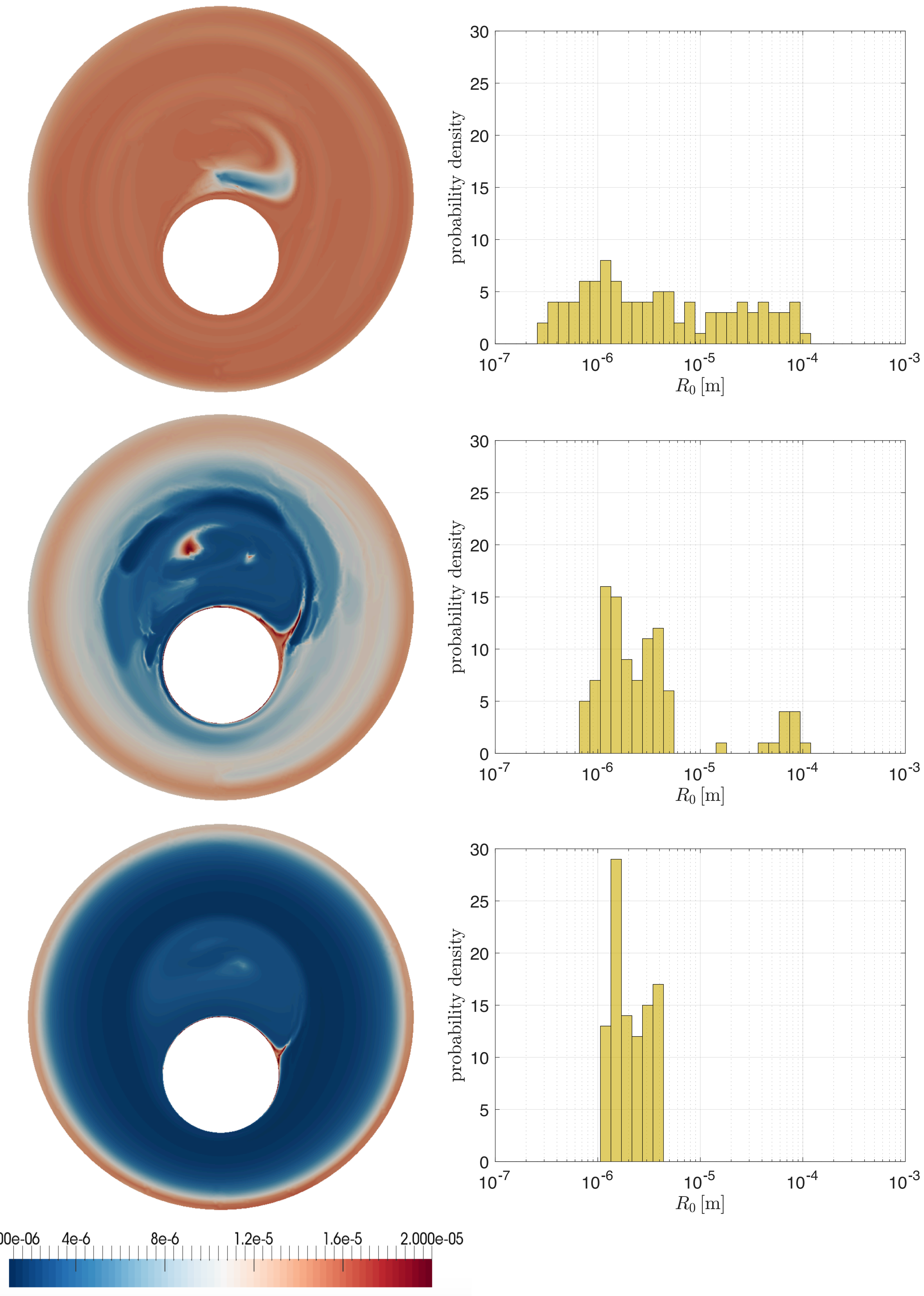

Figure 3. *Mean R_0 in the flow geometry and the distribution of R_0 in the sample point. Top row: after 4 rotations. Middle row: after 8 rotations. Bottom row: after 12 rotations. At the early stages, the distribution is relatively wide. Over time, the distribution narrows, but larger droplets still need more time to break up. The final value is determined by the material properties and local rate of deformation.*

Conclusions

We have developed a predictive tool for the morphology development of polydisperse blends under the influence of processing flow conditions and material properties. Points for future work are: (i) studying the morphology evolution in a three-dimensional industrial mixer flow and (ii) extending the model with viscoelasticity of the blend constituents.

References

[1] M. Iza, M. Bousmina, *Journal of Rheology*, **44**, 1363-1384 (2000)

[2] G.W.M. Peters et al., *Journal of Rheology*, **45**(3), 659–689 (2001)