Design of polymer configuration and flow

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1 Problem Description

Polymer melts are entangled macromolecules that exhibit time-dependent viscoelastic behavior. It is important to analyze and quantify this behavior in order to control the rheology of polymeric materials within a certain range so as to guarantee smooth processing. Dynamic mechanical analysis (DMA) measures the complete rheological response of polymer melts. This process applies a sinusoidal stress at different frequencies to a polymer melt and results in deformation, after which the material relaxes in response to the external stimuli. The resulting strain is measured during the relaxation response. Two rheological response variables are obtained: G', the shear storage modulus that measures the stored energy due to elasticity, and G'', the loss modulus that measures the dissipated energy due to viscosity.

The rheology of polymers melts is very sensitive to polymeric configuration and structure. For example, heavier polymers (higher molecular weight) have higher viscosity, and branching structures affect the elasticity of the polymer melt. We are interested in the following problem:

Given a target rheological behavior and a simulator that predicts rheological behavior from polymer architecture, identify all polymer architectures whose rheological time-behavior resembles that of the target melt.

In the oscillatory test, the motion of a polymer molecule is assumed to follow a tube model which restricts the movement of a polymer within a virtual tube formed by the surrounding entangled polymers. We use a black-box simulator to calculate the rheological responses of the polymer melts using the extended tube model [2, 1].

In the polymer melt, we focus on binary polymer blends with star structure and lognormal arm length distribution. We consider the following design variables for each component in the polymer blends: mole fraction, weight-averaged mass and polydispersity index (PDI). A total of six input variables are fed into the simulator to calculate the transient response in strong shear and extension of the input test materials.

Computational experiments with this problem are published in [3].

2 Simulator

Download and unzip the archive for Linux or Windows. Make sure that bob simulator is saved under the same directory. Input values of the design variables must be provided in the file `myin`.

The executable `PD-exe` sends input values to bob and returns the output objective value in `myout`. Run the executable as follows.

Linux: [user@server lin_exe]$ `bash PD-exe`

Win: C:\Users\Desktop\win_exe> `bash PD-exe`

The executable requires a python 3 environment and the following python packages: `numpy, pandas, os, matplotlib.pyplot, csv, math, sys, operator, random`.

2.1 Create the target rheological responses using bob

The extended tube model can be downloaded at `https://sourceforge.net/projects/bob-rheology/files/`. We recommend using bob version 2.5 for more accurate simulation results. An input file needs to be created for bob to generate the target rheological responses. This input file should specify the following configuration parameters as shown in Figure 1 The configuration file is saved under name `bob_target.dat`. Go in the bob directory and run bob simulator as follows.

Linux: [user@server lin_exe]$ `./bob2p5 -b -i bob_target.dat`

Win: C:\Users\Desktop\win_exe> `bob2p5.exe -b -i bob_target.dat`

The viscoelastic responses will be generated under the same directory. Relaxation modulus G(t) is stored under `gt.dat`, and dynamic modulus G'(t) is stored under `gtp.dat`. Under the current directory, create a new folder by doing `mkdir target` and move both response files to the `target` directory.

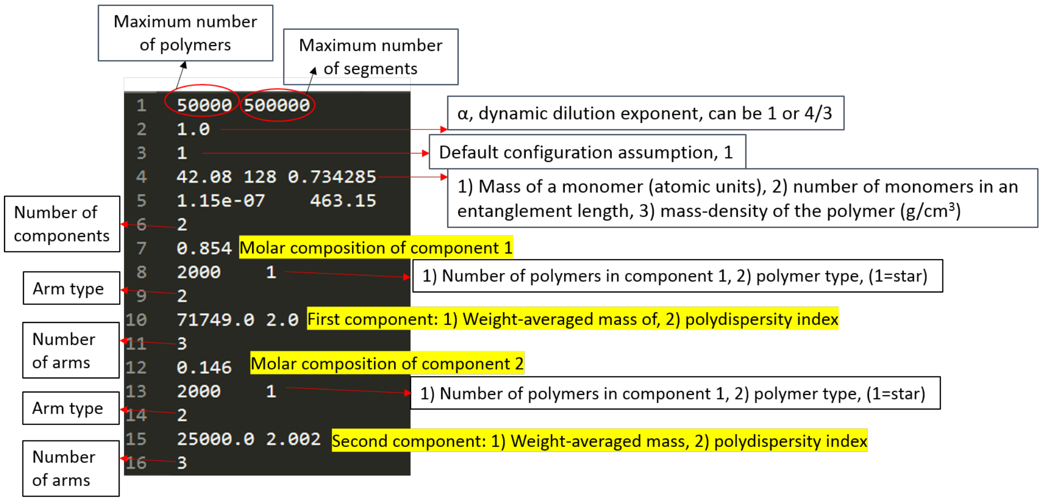

Figure 1: Text in box represents fixed parameters. Text in highlight represents variables we are going to solve for using DFO.

3 Reference

References

[1] C. Das et al. "Computational linear rheology of general branch-on-branch polymers". In: *Journal of Rheology* 50 (2006), pp. 207–234.

[2] D. J. Read et al. "Linking Models of Polymerization and Dynamics to Predict Branched Polymer Structure and Flow". In: *Science* 333 (2011), pp. 1871–1874.

[3] Yijia Sun et al. "Derivative-free optimization for chemical product design". In: *Current Opinion in Chemical Engineering* 27 (2020), pp. 98–106.