Numerical Studies of the Effect of Constitutive Model Parameters as Reflecting Polymer Molecular Structure on Extrudate Swell

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Abstract:
PolyFlow, a software package based on the finite element method was employed to simulate the extrudate swell for polybutadiene of various molecular weight (M_w) and molecular weight distribution (MWD). We calculated the relaxation spectra for the different samples and then inserted the spectra into a standard K-BKZ constitutive model used in the numerical simulations. Accurate predictions of MWD confirm the completeness of frequency range in the oscillatory shear experimental data. In turn, the wholeness of relaxation spectra as substantiated by MWD predictions, sustain the level of confidence when using constitutive models based on these spectra. We demonstrate the importance of using the full range of relaxation spectrum rather than a short range around typical shear rates for the accuracy of the numerical predictions. We found extrudate swell ratio (ESR) to be strongly dependent on MWD and stress conditions at the die exit.

Zusammenfassung:
Das auf der Finite-Element-Methode basierende Softwarepaket PolyFlow wird hier eingesetzt, um das Schwellen von Polybutadien bei verschiedenen Molekulargewichten (M_w) und Molekulargewichtverteilungen (MWD) im Austritt aus einer Röhre zu simulieren. Wir errechnen die Relaxationsspektren für unterschiedliche Proben und setzten dann die Spektren in ein Standard K-BKZ-konstitutives Modell ein, das in den numerischen Simulationen benutzt wurde. Genaue Vorhersagen der MWD bestätigen die Vollständigkeit des Frequenzbereichs in den experimentellen Daten. Umgekehrt unterstützt die Gesamtheit der Relaxationsspektren, wie durch MWD Vorhersagen bestätigt, das Vertrauen in die konstitutiven Modelle. Wir demonstrieren auch, wie wichtig es ist, den vollen Frequenzbereich des Spektrums zu nutzen, um genaue numerische Voraussagen zu erhalten. Wir finden eine starke Abhängigkeit der Austrittsschwellung (ESR) von der MWD und dem Spannungszustand am Röhrenausgang.

Résumé:
Polyflow, un logiciel basé sur la méthode d'élément fini, a été utilisé pour simuler le gonflement d'extrudats dans le cas de polybutadiènes de masses moléculaires variées (M_w) et de distributions en masses moléculaires variées (MWD). Nous avons calculé les spectres de relaxation pour les différents échantillons, puis nous avons insérer ces spectres dans un modèle constitutif standard de type K-BKZ utilisé dans les simulations numériques. Les prédictions précises des MWD sont en accord avec la gamme entière de fréquences des données expérimentales de cisaillement dynamique oscillatoire. De manière réciproque, les spectres de relaxation, qui ont été validés par les prédictions de MWD, supportent le niveau de précision dans toute la gamme de fréquence lorsque des modèles constitutifs basés sur ces spectres sont utilisés. Nous démontrons l'importance d'utiliser la totalité du spectre de relaxation plutôt que une courte plage de fréquences autour des vitesses de cisaillement typiques, afin que les prédictions numériques soient précises. Nous trouvons que les rapports de gonflement d'extrudats (ESR) dépendent fortement des MWD et des conditions de contrainte en sortie d'extrusion.

Key Words: K-BKZ constitutive model; Extrudate swell; Numerical simulation; Finite element method; Relaxation time spectrum; Molecular weight distribution

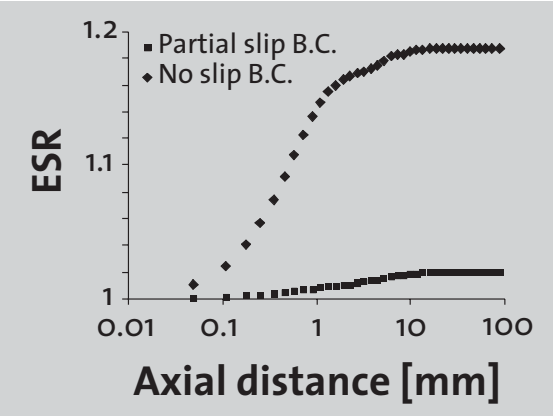

Figure 12: ESR comparison between no-slip and partial slip boundary condition at the die exit.

shows ESR results obtained using the same polybutadiene sample and identical flow rate conditions. The difference is in the boundary condition at die exit. This result illustrates that the stress singularity at the die exit region highly influences the extrudate swell. Partial slip conditions at exit region reduce extrudate swell significantly. Similar findings have been reported before [8, 40].

5 CONCLUSIONS

In this work we analyzed the effect of constitutive equation parameters as linked to sample molecular weight and molecular weight distribution on the extrudate swell simulation results. Molecular parameters affect the relaxation spectra for the different samples used in this study, which in turn alter the extrudate swell results.

Accuracy in the calculated MWD strengthens our level of confidence in the frequency range completeness for the oscillatory shear experimental data used in the calculation. On the other hand, the breadth of relaxation spectra as substantiated by MWD calculations, augment our level of confidence in using constitutive models based on such spectra.

We found the extrudate swell ratio to be strongly affected by the sample polydispersity. The major limitations in our current numerical results are primarily related to mesh refinement in the region of stress singularity at die exit and the number of relaxation modes in relaxation spectra especially for high molecular weight samples. In spite of these limitations, the results clearly illustrate the strong dependence of extrudate swell ratio on the sample molecular weight distribution. The results also reiterate the importance of using the full spectrum of relaxation times for a given sample rather than a limited spectrum around a characteristic shear rate for the experiment.

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