Numerical Simulation of Sharkskin Phenomena in Polymer Melts

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Abstract:
A fluid dynamic analysis package, PolyFlow, based on the finite element method is used to study the sharkskin phenomenon. A stick-slip mechanism is used as the basis for the simulations. This study is aimed at illustrating how fluctuations in the stress at the exit from the die cause similar fluctuations in the extrudate swell ratio, resembling the sharkskin phenomenon. Such fluctuations in the stress at the exit from the die are produced by implementing a stick-slip boundary condition at the die wall, mimicking a mechanism of molecular entanglement/disentanglement at the wall. We use a superposition of stress relaxation/stress growth and a periodic change in extrudate swell governed by the die exit stress level to depict sharkskin. Three relatively monodisperse polybutadienes were used in this study. The simulated sharkskin time period was found to be in good agreement with experimental findings. We found that the simulated pictures of sharkskin are similar for all three molecular weight samples. A comparison between the simulated sharkskin and experimental results show qualitative resemblance. The main problems preventing us from generating more quantitative sharkskin results mainly reside in the model limitations in depicting stress singularity, limitations in mesh design refinement and the constitutive model employed. In spite of these limitations, the qualitative agreement between simulation results and experimental data is good.

Zusammenfassung:
Ein Softwarepaket für Fluiddynamik-Simulationen, das auf der Finite-Elemente-Methode beruht, PolyFlow, wird zur Untersuchung des Schmelzbruchverhaltens herangezogen. Ein Rückgleitmechanismus wird als Grundlage der Simulationen benutzt. Die Untersuchung zielt darauf ab, zu veranschaulichen, wie Fluktuationen in den Spannungen am Düsenausgang analoge Fluktuationen im Strangaufweitungsverhältnis verursachen, die Ähnlichkeit mit dem Schmelzbruchphänomen haben. Solche Spannungsfluktuationen am Düsenausgang werden durch Implementation einer Rückgleit-Randbedingung an der Düsenwand realisiert, welche einen molekularen Ver-/Entschlaufungsmechanismus an der Wand nachahmen. Zur Beschreibung des Schmelzbruchs benutzen wir eine Überlagerung von Spannungsrelaxation/Spannungsanstieg und eine periodische Variation der Strangaufweitung welche durch das Spannungsniveau am Düsenausgang bestimmt wird. Drei relativ monodisperse Polybutadiene wurden im Rahmen dieser Untersuchungen benutzt. Die simulierte Schmelzbruchfrequenz stimmte gut mit experimentellen Befunden überein. Wir sahen, dass die aus den Simulationen des Schmelzbruchs erhaltenen Bilder fuür die drei Proben mit unterschiedlichen Molekulargewichten ähnlich sind. Ein Vergleich des simulierten Schmelzbruchs und experimenteller Befunde zeigt qualitative Ähnlichkeit. Die Hauptprobleme, welche eine mehr quantitative Beschreibung des Schmelzbruchs verhindern, liegen in den Beschränkungen des Modells, Spannungssingularitäten vorherzusagen, Beschränkungen in der Verfeinerung der Gitterauflösung, und im konstitutiven Modell, welches benutzt wurde. Trotz dieser Beschränkungen ist die qualtitative Übereinstimmung von Simulationsergebnissen und experimentellen Daten gut.

Résumé:
Polyflow, un logiciel de calcul de dynamique des fluides basé sur la méthode d'éléments finis, est utilisé pour étudier le phénomène de défaut de peau de requin. Un mécanisme d'ancrage-glissement est utilisé comme point de départ des simulations. Cette étude a pour but d'illustrer comment les fluctuations de contrainte à la sortie de la chambre d'extrusion causent des fluctuations similaires dans le ratio de gonflement de l'extrudat, qui ressemblent au phénomène de peau de requin. De telles fluctuations de la contrainte à la sortie de la chambre d'extrusion sont générées en implémentant une condition d'ancrage-glissement à la paroi de la chambre, qui rend compte d'un mécanisme moléculaire d'enchevêtrement/désenchevêtrement à la paroi. Nous utilisons une superposition de relaxation de contrainte/augmentation de contrainte, ainsi qu'un changement périodique dans le gonflement de l'extrudat gouverné par le niveau de la contrainte en sortie de chambre d'extrusion, afin de décrire le défaut de peau de requin. Trois polybutadiènes, relativement monodisperses, ont été utilisés dans cette étude. La période temporelle du défaut de peau de requin simulé concorde bien avec les données expérimentales. Les images de défaut de peau de requin se révèlent être indépendantes du poids moléculaire des échantillons. Une comparaison entre les peaux de requin simulées et les résultats expérimentaux montre une similarité qualitative. Les principaux problèmes qui nous empêchent de générer des résultats plus quantitatifs résident principalement dans les limitations du modèle à décrire la singularité de la c ontrainte, les limitations dans les détails du dessin du maillage, et le modèle constitutif employé. En dépit de ces limitations, la concordance qualitative entre les résultats des simulations et les données expérimentales est bonne.

Key words: sharkskin, flow instabilities, extrudate swell, numerical simulations, finite element method, stress relaxation/stress growth

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A comparison of the numerical results in Fig. 9 and experimental data (for instance results in Fig. 4 of reference [3]) show qualitative resemblance. The main problem is reproducing accurately the sharkskin amplitude mainly due to the limitations in depicting stress singularities, problems associated with the constitutive model employed in the simulations, limitation in mesh design refinement over a certain limit. In spite of these limitations, the qualitative agreement between simulation results and experimental data is good.

7 CONCLUSIONS

We simulated the sharkskin phenomenon based on a stick-slip mechanism. Simulation results were obtained using a superposition of stress relaxation/stress growth and a periodic change in extrudate swell governed by the die exit stress level. We first simulated the stress relaxation at the die wall upon cessation of flow in a circular die. This information was then used to simulate the extrudate swell at different levels of die exit stress. The die exit stress level was modified by way of a special slip region and a slip coefficient.

The simulated sharkskin time periods were found to be in good agreement with experimental data. Moreover, the sharkskin time period scales with the molecular weight at a power of 3.48, which comes close to the expected value of 3.4. We found that the simulated appearances of sharkskin are similar for all three molecular weight samples. The rather small differences in sharkskin distance periods mark shorter periods for the higher molecular weight materials.

A comparison between simulated sharkskin and experiments show qualitative resemblance. The main problems preventing us from quantitatively reproducing the sharkskin amplitude are the model limitations in depicting stress singularity, limitations in mesh design refinement and the constitutive model employed. In spite of these limitations, the qualitative agreement between the simulation results and experimental data is good.

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