Computer Simulation of Viscoelastic Flow in a Capillary Die for Rubber Compounds

Min-Young Lyu*, †, Dongmyung Park**, Hakjoo Kim**, and Jaeryong Yoon**

*Department of Die and Mould Design, Seoul National University of Technology,

172 Gongreung-Dong, Nowon-Gu, Seoul, 139-743, S. Korea

**Hankook Tire R&D Center, 23-1, Jang-Dong, Yusong-Gu, Daejon, 305-725, S. Korea

(Received August 26, 2006, Revised & Accepted November 14, 2006)

모세관 다이에서 고무 복합체의 점탄성 거둥에 대한 컴퓨터 모사

류 민 영*·박 동 명**·김 학 주**·윤 재 룡** *서울산업대학교 금형설계학과, **한국타이어 중앙연구소 (2006년 8월 26일 접수, 2006년 11월 14일 수정 및 채택)

ABSTRACT: Rubber compounds have a high viscoelastic property. One of the viscoelastic behaviors during profile extrusion is the swelling of extrudate, and the amount of swelling varies with operational conditions in extrusion. It is well recognized that the elastic portion in the viscoelastic property plays an important role in the extrudate swell. In this study computer simulation of the die swell at the capillary die for several rubber compounds has been performed using commercial CFD code, Polyflow. A non-linear differential viscoelastic model, Phan-Thien-Tanner (PTT) model, was used in the computer simulation. Non-isothermal behavior was considered in the calculation. Distribution of pressure, velocity and temperature in the reservoir and capillary die, and extrudate profiles were predicted through the simulation. The amount of the die swell for the different rubber compounds was investigated for various flow rates and three types of length to diameter of the capillary die. It is concluded that the PTT model successfully represented viscoelastic behavior of rubber compounds.

요 약: 고무복합체는 높은 점탄성 성질을 보이는데 압출성형 시 이 점탄성 성질 때문에 압출물이 팽창하게 된다. 그리고 팽윤양은 공정 조건에 따라서 변한다. 점탄성 성질에서 탄성 부분은 압출물의 팽창에 있어서 중요한 역할을 한다. 본 논문은 모세관 다이에서 여러 가지 고무복합체에 따른 다이팽윤을 알아 보기 위해 상용 CFD 프로그램인 Polyflow를 사용하여 해석을 수행하였다. 컴퓨터 모사에서는 비선형 미분 점탄성 모델인 Phan-Thien-Tanner(PTT) 모델을 사용하였고 온도를 고려하여 해석하였다. 해석을 통해서 레저버와 모세관 다이에서 압출물의 압력,속도, 그리고 온도 분포 등을 예측하였다. 여러 가지 고무 복합체의 다이 팽윤양을 알아보기위해서 유량과 모세관 다이의 지름을 변경하면서 연구하였다. 본 연구를 통해서 PPT 모델은고무 복합체에 대한 점탄성 거동을 잘 표현하고 있음을 확인할 수 있었다.

Keywords: Rubber compounds, Viscoelastic behavior, Extrudate swell, Phan-Thien-Tanner Model, Capillary Die

[†]대표저자(e-mail: mylyu@snut.ac.kr)

I. Introduction

Many kinds of rubber compounds are being used in tire industries. Automobile tires are consisted of rubber compounds and various reinforcing materials, such as textile and steel cords. Rubber compounds are mixed in the mixing equipments. Subsequently they are extruded through mostly single screw and pin barrel extruders to produce certain profiled sheets. Extruding rubber compounds to manufacturing flat shaped tread and side wall before curing involve multilayer co-extrusion. Rubbers are highly viscoelastic and this gives difficulties in dimensional accuracy during die extrusion. The final shape of extruded rubber distorts and swells because of high elastic nature of rubber. 1,2 Amount of die swell of rubber compound depends upon additives, shear rate, temperature of rubber compound, and etc.3.

Many researches dealing die swell and profile extrusion have been published. The influence of operating conditions for profile extrusions were studied experimentally and analytically. 4,5,6 The profile design of die and drawdown effect on the profile extrusion have been studied.^{7,8} In their papers the variables that affect profile of extrudate have been analyzed. Wall shear rate, die length, temperature, and drawing ratio were the most effective variables on the extrudate profile. Three different dies were analyzed for the die design in the reactive extrusion.9 Numerical simulation was also appeared in the paper. 10 However the material models were limited to Newtonian and power law fluids. The viscoelastic effect on the extrudate profile for rubber compounds is considered very high, and prediction of extrudate profile including viscoelastic effect is important.

In this study, flow behaviors of rubber compounds in the capilary die have been analyzed. And also die swell of several rubber compounds have been investigated through computer simulation. The rubber compounds used in this study were natural rubber (NR), blend of natural rubber (NR) and butadiene rubber (BR), and blend of butadiene rubber (BR) and styrene butadiene rubber (SBR). For the computer simulation of die swell commercial code, Polyflow was used. Flow rate and L/D were variables of computer simulations to predict extrudate swell

II. Materials and simulation

1. Materials and model

The rubber compounds used in this study were NR (denoted by C1), NR with BR (denoted by C2), and BR with SBR (denoted by C3). All compounds were compounded with carbon black for the extrusion of tire tread. Figure 1 shows viscosity and moduli for three rubber compounds.

A non-linear differential viscoelastic model, Phan-Thien-Tanner (PTT) model¹¹ was used in the simulation of flow behaviors of those compounds in the capillary die. Equation (1) shows PTT model.

$$\exp\left[\frac{\varepsilon\lambda}{\eta_1}tr(T_1)\right]T_1 + \lambda\left[\left(1 - \frac{\xi}{2}\right)^{\nabla}T_1 + \frac{\xi}{2}^{\Delta}T_1\right] = 2\eta_1 D \tag{1}$$

where T_1 is a viscoelastic component of extra stress, ε and ξ are control parameters for shear viscosity and elongational behavior of material, respectively. λ is a relaxation time and η_1 is a shear viscosity factor for viscoelastic component. Viscoelastic curve fitting for PTT model was performed using Polyflow (Version 3.9, Fluent Co.). Relaxation time λ

Table 1. Parameters in the Phan-Thien-Tanner Model after Curve Fitting for Compound C3

Relaxation Time λ	Parameter ε , ξ
$\lambda = 0.05$	$\varepsilon = 0.5774643E-03$
	$\xi = 0.9921486E+00$
$\lambda = 0.5$	$\varepsilon = 0.1011817E-02$
	$\xi = 0.1011051E+01$
λ = 5	$\varepsilon = 0.4578574E-03$
	$\xi = 0.1003347E+01$

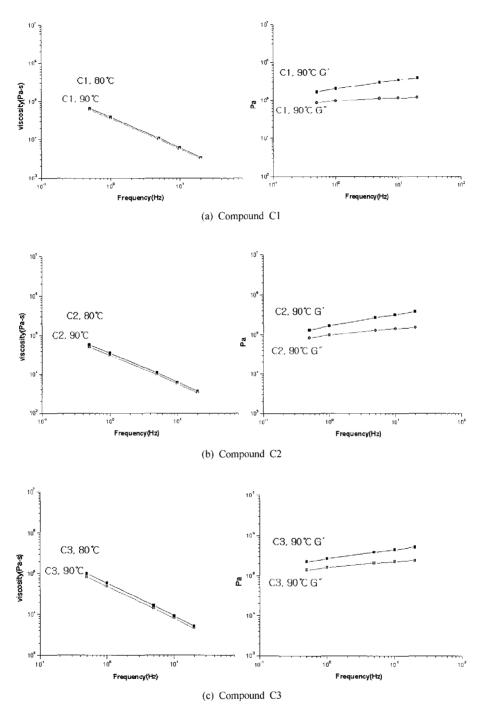


Figure 1. Viscosities and moduli for various rubber compounds.

was assigned to the range between 0.05 to 5 sec. The parameters after curve fitting for compound C1 are listed in Table 1.

2. Simulation

Die swell phenomena of rubber compounds have been investigated through capillary die. The die diameter was 2.5 mm and L/Ds were 1, 3 and 5. Polyflow was used in the simulations considering non-linear viscoelastic and non-isothermal behaviors. Arrhenius law was used in predicting non-isothermal material property as shown in equations (2a) and (2b).

$$\eta(\dot{\gamma}, T) = F(\dot{\gamma})H(T) \tag{2a}$$

and

$$H(T) = \exp\left[\alpha \left(\frac{1}{T - T_0} - \frac{1}{T_\alpha - T_0}\right)\right]$$
 (2b)

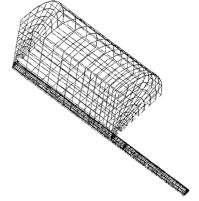
Where α is 3735.4, T_{α} is 90, T_0 is -273.15 for compound C1.

Figure 2 shows mesh in the quarter of domain for the simulation and also side views of the meshes. Figure 3 shows the boundary conditions for the simulation. Inlet and die temperatures were set 100 °C, and several flow rates were imposed at the inlet boundary. Heat convection was imposed at the material after exiting from the die. To calculate extrudate profiles 'Optimesh' technique was adopted. 12

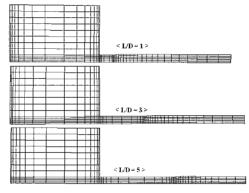
III. Results and discussion

1. Pressure drop

Figure 4 shows pressure drops in the capillary die for different L/D according to the volume flow rate. Pressure increases drastically for the range of small flow rate. However the increment of pressure falls and linearly increases as flow rate increases. The largest L/D in all compounds shows the highest pressure. Compound C3 shows higher pressure drop



(a) Mesh in quarter of domain



(b) Side view of mesh for different L/D

Figure 2. Mesh for computation.

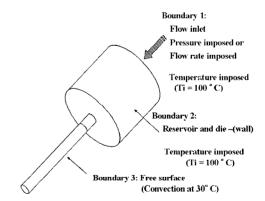
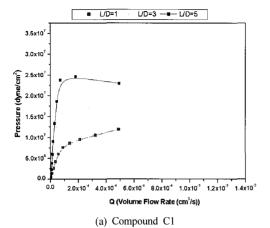
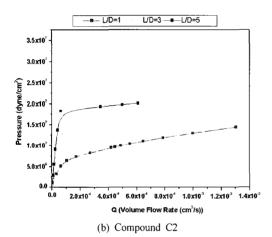


Figure 3. Boundary conditions for computation.

compared with the compound C1 and C2 since compound C3 has higher viscosity than compounds C1 and C2.





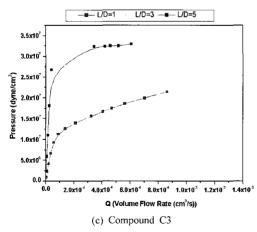


Figure 4. Pressure drops in the capillary die.

2. Pressure distribution

Pressure distributions in the capillary dies are shown in Figure 5 for the Compound C1. No pressure drops are observed in the reservoir. However the pressure in the reservoir increases as L/D of capillary die increases since high pressure is needed for long length of the die or small diameter of the die. Pressure decreases as material passes through capillary die. Large pressure drops are observed in the capillary die. Pressure drop in the capillary die increases as L/D increases from 1 to 5.

3. Temperature distribution

Temperature distributions are shown in Figure 6 for the Compound C2. The temperatures are all the same in reservoir and capillary die except at the end of die. Inlet material and die wall temperatures were set to 100~%. Thus the calculated temperature of material was 100~% in the reservoir and die. However the temperature decreases abruptly at the end of the die because the die end is exposed to room temperature. The Compounds C1 and C3 have similar temperature distributions.

4. Velocity distribution

Velocity distributions in the capillary die are shown in Figure 7 for the Compound C3. The velocity in the reservoir is very slow because cross section is very large for given flow rate. As the material approaches to the entrance of capillary die velocity increases because the cross section of the die is very small compared with the reservoir. Maximum velocity occurs at the center of the capillary die. The wall velocity was set to zero because no slip at wall was being assumed. The velocity becomes uniform after the material is extruded from the die.

5. Circulation flow

Circulation flows at the corner of reservoir are shown in Figure 8. The circulation flow indicates viscoelastic characteristics. It increases as Debora

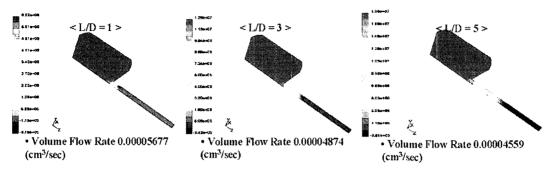


Figure 5. Pressure distributions of compound C1.

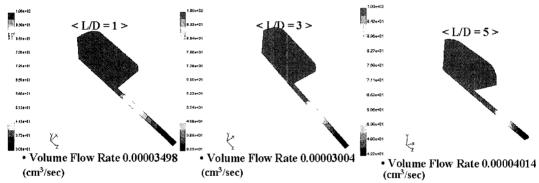


Figure 6. Temperature distributions of compound C2.

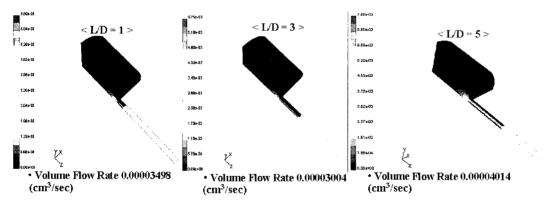


Figure 7. Velocity distributions of the Compound C3.

number and Weissenberg number that means increasing the elastic behavior in the viscoelastic characteristic. 13.14 The circulation flow at the corner increases as elastic portion in the viscoelastic property increases. Generally it increases as flow rate increases. It was well known that the circulation

flow increases as shear rate increases because elastic behavior highly depends upon shear rate. 13,14

6. Die swell

Die swells of extrudates for flow rate and L/D are shown in Figures 9 and 10, respectively. Die swell

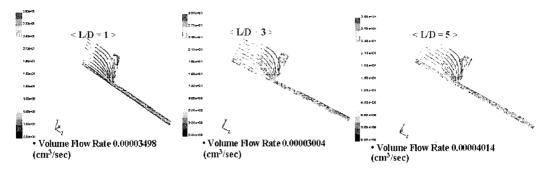


Figure 8. Circulation flows of compound C3 at the corner of reservoir.

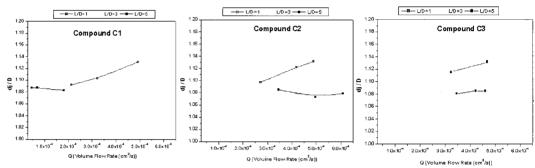


Figure 9. Die swells for flow rate.

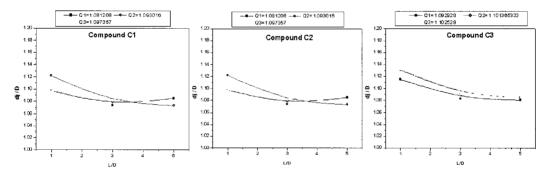


Figure 10. Die swells for L/D.

increases as flow rate increases for all dies and three compounds except 5 of L/D for the Compounds C1 and C2. Die swell should increase as flow rate increases regardless of the die length.³ However, some inconsistent points are observed and this comes from the computational error for calculating pressure drop for the Compounds C1 and C2 at L/D = 5 as shown in Figure 4. Swelling of extruded material is the

recovering of elastic strain and it increases as shear rate increases. However recoverable elastic strain decreases as L/D increases because elastic strain is relaxed while material flows in long die.³ The Compounds C1, and C2 show similar die swell because they have similar viscoelastic property. The Compound C3 has higher viscoelastic property and shows higher die swell than the Compounds C1 and C2.

W. Conclusion

Flow and viscoelastic behaviors in the capillary die for the three different rubber compounds have been simulated using PTT model through Polyflow. This study contains computer simulation of flow behaviors and die swell characteristics in the capillary die. Rubber compounds of C1 (NR) and C2 (NR+BR) had similar viscosity, storage and loss moduli, thus their flow and die swell behaviors were quite similar. The Compound C3 had high viscosity and high elastic property compare with the Compounds of C1 and C2. Subsequently it showed large die swell. Die swell increased as flow rate increases while it decreased as die length was increased. Pressure drop increased with the increased die length. and the Compound C3 showed higher pressure drop. Compared with the Compounds C1 and C2, circulation flows at the corner of the reservoir were observed. Through this study it is concluded that the PTT model successfully represents viscoelastic flow behaviors of rubber compounds.

References

- N. Sombatsompop and R. Dangtangee, "Effects of the Actual Diameters and Diameter Ratios of Barrels and Dies on the Elastic Swell and Entrance Pressure Drop of Natural Rubber in Capillary Die Flow", J. Appl. polym. Sci., 86, 1762 (2002).
- N. Sombatsompop and R. Dangtangee, "Flow Visualization and Extrudate Swell of Natural Rubber in a Capillary Rheometer: Effect of Die/Barrel

- System", J. Appl. Polym. Sci., 82, 2525 (2001).
- C. D. Han, "Rheology in Polymer Processing", Academic Press, NY (1976).
- B. Yang and L. J. Lee, "Process Control of Profile Extrusion Using Thermal Method.
 Part I: Mathematical Modeling and System Analysis", *Polym. Eng. Sci.*, 28, 697 (1988).
- B. Yang and L. J. Lee, "Process Control of Profile Extrusion Using Thermal Method.
 Part II: Closed Loop Control", Polym. Eng. Sci.,
 28, 708 (1988).
- E. B. Rabinovitch and J. G. Quisenberry, "Shrinkage in Rigid PVC Profile Extrusion", *Vinyl Tech.*, 10, 200 (1988).
- 7. P. Hurez and P.A Tanguy, "A New Design Procedure for Profile Extrusion Dies", *Polym. Eng. Sci.*, **36**, 626 (1996).
- 8. M. A. Huneault, P. G. Lafleur, and P. J. Carreau, "Extrudate Swell and Drawdown Effects on Extruded Profile Dimensions and Shape", *Polym. Eng. Sci.*, **30**, 1544 (1990).
- J.-P. Pan, P.-Y. Wu, and T.-J. Liu, "Extrusion Die Design for Slowly Reacting Materials", *Polym. Eng. Sci.*, 37, 856 (1997).
- P. Hurez and P.A Tanguy, "Numerical Simulation of Profile Extrusion Dies without Flow Separation", *Polym. Eng. Sci.*, 33, 971 (1993).
- Polyflow V. 3.9, Polymat manual, Fluent Co. (2002).
- 12. Polyflow V. 3.9, User's manual, Fluent Co. (2002).
- 13. J. L. White, "Principles of Polymer Engineering Rheology", John Wiley & Sons, NY (1990).
- R. B. Bird, R. C. Armstrong, and O. Hassager, "Dynamics of Polymeric Liquids", Vol. 1, 2nd Ed., John Wiley & Sons, NY (1987).