공압출 유동에 대한 삼차원 수치모사와 실험결과의 비교

선우기병, 안경현, 이승종 서울대학교 응용화학부

Comparison of 3-D Numerical Simulation Results with Experimental Coextrusion Data

<u>Ki Byung Sunwoo</u>, Kyung Hyun Ahn, Seung Jong Lee School of Chemical Engineering, Seoul National University, Seoul 151-743, Korea

Introduction

Multicomponent coextrusion process has gained wide recognition as an approach to achieving unique product performance by combining the properties of different materials with lower expenses. Experimental investigations of stratified flow in a side-by-side coextrusion have so far identified the viscosity difference between the polymer melts to be the controlling factor of the encapsulation effect with the less viscous melt encapsulating the more viscous melt. Southern and Ballman [1] investigated the relative importance of viscosity and elasticity effects on interface shape. Karagiannis et al. [2] studied isothermal generalized Newtonian coextrusion process using a three-dimensional analysis and compared with the experimental results. Takase et al. [3] performed a three-dimensional numerical simulation with viscoelastic model and showed that the encapsulation phenomena were affected not only by viscous properties but also by elastic or non-linear properties. Sunwoo et al. [4] implemented the open boundary condition method to remove the ambiguity of outlet boundary conditions in three-dimensional numerical simulation of coextrusion process.

This work focuses on the effect of viscous heating of generalized Newtonian fluid and the viscoelastic property on the encapsulation phenomena in coextrusion flow of two immiscible fluids through a rectangular channel by three-dimensional finite element method. As viscoelastic constitutive equations, we used Gisekus model and two-mode Phan-Thien and Tanner model. We compared our numerical results with the experimental results reported in Karaginnis's study [2].

Governing equations and Numerical methods

In this study, the problem consists of the merging flow of two fluid streams and the interface shape development in the resulting bicomponent stratified flow inside the die.

Assuming incompressible, steady state, and creeping flow with no body forces, the three-dimensional forms of continuity, momentum, and energy equations for the flow of two generalized Newtonian fluids (I and II) are

$$\nabla \cdot \mathbf{v_k} = 0,$$
 $k=I, II$ (1)

$$\rho_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \cdot \nabla \mathbf{v}_{\mathbf{k}} = -\nabla p_{\mathbf{k}} + \nabla \cdot \mathbf{\tau}_{\mathbf{k}}, \qquad \qquad \mathbf{k} = \mathbf{I}, \mathbf{I} \mathbf{I}$$
 (2)

$$(\rho C_p)_k \mathbf{v}_k \cdot \nabla T_k = \kappa_k \nabla^2 T_k + \tau_k : \nabla \mathbf{v}_k, \qquad k=I, II$$
(3)

where,
$$\tau_k = \eta_k(T, II_{\Delta})\Delta_k = \eta_k(T, II_{\ddot{A}})(\nabla v_k + \nabla v_k^T)$$
 $k=I, II$ (4)

and the boundary conditions at the interface are expressed as followings.

kinematic conditions:

$$\mathbf{n} \cdot \mathbf{v}_{\mathrm{I}} = \mathbf{n} \cdot \mathbf{v}_{\mathrm{II}} = 0,\tag{3}$$

$$\mathbf{t}_{1} \cdot \mathbf{v}_{I} = \mathbf{t}_{1} \cdot \mathbf{v}_{II}, \tag{4}$$

$$\mathbf{t}_2 \cdot \mathbf{v}_{\mathrm{I}} = \mathbf{t}_2 \cdot \mathbf{v}_{\mathrm{II}} \tag{5}$$

dynamic conditions:

$$\mathbf{t}_1 \cdot \mathbf{\sigma}_1 = \mathbf{t}_1 \cdot \mathbf{\sigma}_{II}, \tag{6}$$

$$\mathbf{t}_2 \cdot \mathbf{\sigma}_{\mathrm{I}} = \mathbf{t}_2 \cdot \mathbf{\sigma}_{\mathrm{II}},\tag{7}$$

$$\mathbf{n}_2 \cdot \mathbf{\sigma}_1 - \mathbf{n}_2 \cdot \mathbf{\sigma}_{11} = 0 \tag{8}$$

As a viscoelastic constitutive equation, we used Giesekus model, which is written as,

$$\boldsymbol{\tau} = \boldsymbol{\tau}_{p} + 2\eta_{s} \boldsymbol{D}, \tag{5}$$

$$\boldsymbol{\tau}_{p} + \lambda_{1} \, \boldsymbol{\tau}_{p} + \alpha \, \frac{\lambda_{1}}{\eta_{p}} \, \boldsymbol{\tau}_{p}^{2} = 2\eta_{p} \mathbf{D} \,, \tag{6}$$

and also used two-mode Phan-Thien and Tanner model, which is written as,

$$\tau = \sum_{i=1}^{2} \tau_i \,, \tag{7}$$

$$(1 + \frac{\varepsilon_i \lambda_i}{\eta_{o,i}} \operatorname{tr} \tau_i) \tau_i + \lambda_i \left\{ (1 - \frac{\xi_i}{2}) \tau_i^{\nabla} + \frac{\lambda_i \xi_i}{2} \tau_i^{\Delta} \right\} = 2 \eta_{o,i} \mathbf{D}_i$$
 (8)

The flow domain is discretized into 27-node hexahedron elements as shown in Fig.1, and the Galerkin finite element procedure is applied. Zero shear viscosity ratio ($\eta_{o,11}/\eta_{o,1}$) and flow rate ratio (Q_{11}/Q_1) are 2.5 and 13.2, respectively. We set the flow conditions to agree as much as possible and made a comparison with the interface shape and degree of encapsulation along the downstream direction observed experimentally by Karagiannis et al. [2]. In addition, the open boundary condition method [5] was implemented to remove the difficulty of imposition of outlet boundary condition.

Results and Discussion

From the nonisothermal results by using the generalized Newtonian fluids, it was shown that the degree of encapsulation along the downstream direction deviated a little from one of isothermal results and decreased gradually along the downstream direction even though it is not so large, due to the decreased viscosity ratio caused by the continuous viscous heating near the side wall of the higher viscosity lower layer. The difference of degree of encapsulation ($DE(\%) = (y_w - y_c)/L \times 100$) with the one observed experimentally cannot be explained by the viscous heating effect alone but should be interpreted by the effect of viscoelastic property.

For Giesekus model as a viscoelastic constitutive equation, firstly we fitted the shear viscosity data by nonlinear fitting algorithm (Marquardt-Levenberg algorithm) after fixing α to 0.15 or 0.30. Fitted viscosity curves using α value as 0.15 or 0.30 nearly coincide with the experimental shear viscosity curves as shown in Fig. 3. For two Phan-Thien and Tanner model, we did the similar procedure as Giesekus mode, but the fitted viscosity curves are not as smooth as that of Giesekus model. If we use multimode more than two, we may get the smooth viscosity curves, but the analysis time for numerical simulation of coextrusion process will increase greatly.

As α increases from 0.15 to 0.30, the degree of encapsulation increased and approached the experimental results as represented in Fig. 4. The α represents the second normal stress difference as ξ of Phan-Thien and Tanner model does, so we can guess that the second normal stress difference has a great influence on the gradual increase of the degree of encapsulation along the downstream direction.

We have fitted parameters of viscoelastic constitutive equations using the shear viscosity data only because it is very difficult to measure the second normal stress difference accurately. So, if we can get the accurate second normal stress difference data, we can evaluate the accuracy of our numerical results more precisely.

We removed the ambiguity of outlet boundary conditions by using the open boundary condition method as shown in Figures 2 and 4, where no abrupt change of curves of degree of encapsulation near the outlet was shown.

References

- 1. Southern, J.H. and R. L. Ballman, J. Polym. Sci., 13, 863 (1975).
- 2. Karagiannis, A., A. N. Hrymak, and J. Vlachopoulos, Rheol. Acta, 29, 71 (1990).

- 3. Takase, M., S. Kihara, and K. Funatsu, Rheol. Acta, 37, 624 (1998).
- 4. Sunwoo, K.B., S. J. Park, S. J. Lee, K. H. Ahn, and S. J. Lee, J. Non-Newtonian Fluid Mech., (submitted).
- 5. Park, S.J. and S. J. Lee, J. Non-Newtonian Fluid Mech., 87, 197 (1999).

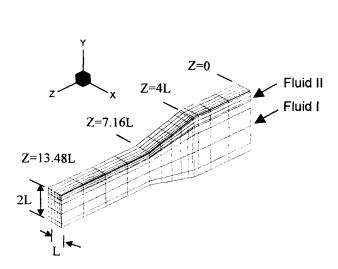


Fig. 1. Finite element mesh (Mesh1).

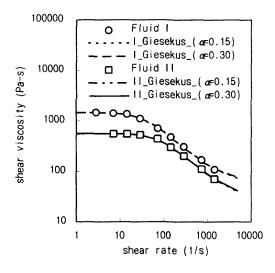


Fig.3. Fitting of shear viscosity with Giesekus model using different α values.

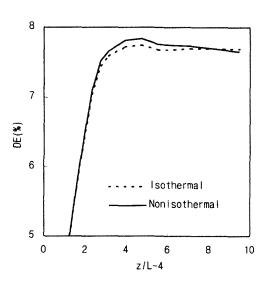


Fig.2. Degree of encapsulation alon downstream direction with generalize Newtonian fluid.

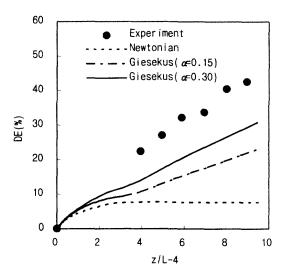


Fig.4. Degree of encapsulation alon downstream direction with Gieseku model using different α values.