점탄성 유체의 공압출 유동에 대한 삼차원 수치모사

선우기병, 박승준, 이성재*, 이승종
서울대학교 응용화학부
수원대학교 고분자공학과*

Three-Dimensional Numerical Simulation of Viscoelastic Coextrusion Flow

Ki Byung Sunwoo, Seung Joon Park, Seong Jae Lee*, Seung Jong Lee
School of Chemical Engineering, Seoul National University, Seoul 151-742, Korea
Department of Polymer Engineering, The University of Suwon, Suwon 445-743, Korea*

Introduction

In recent years coextrusion 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 phenomenon, i.e. the less viscous melt wraps around the more viscous melt [1-4]. Southern and Ballman [3] investigated the relative importance of viscosity and elasticity effects on interface shape. Takase et al. [5] performed a three-dimensional numerical simulation with viscoelastic model on the encapsulation phenomena. They showed that the encapsulation phenomena were affected not only by viscous properties but also by elastic or non-linear properties, but the fully developed boundary conditions imposed at the outlet of the analysis region were not correct.

This work focuses on the effects of the viscoelastic properties on the encapsulation phenomena in coextrusion flow of two immiscible fluids through a rectangular channel by three-dimensional finite element method. The viscosity and elasticity effects on the interface shape were investigated as regards the upper convected Maxwell model. For the Phan-Thien and Tanner model the effects of shear viscosity, elasticity, extensional viscosity, and the second normal stress difference were considered. In addition, the open boundary condition method [6] to viscoelastic simulations was implemented to remove the difficulty of imposition of outlet boundary condition.

Governing equations and Numerical methods

The three-dimensional continuity and momentum equations for the steady state flow of two viscoelastic fluids (I and II) are as follows,

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

$$\rho_k \mathbf{v}_k \cdot \nabla \mathbf{v}_k = -\nabla p_k + \nabla \cdot \boldsymbol{\tau}_k, \qquad k=I, II \qquad (2)$$

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

kinematic conditions :

$$\mathbf{n} \cdot \mathbf{v}_I = \mathbf{n} \cdot \mathbf{v}_{II} = 0, \qquad (3)$$

$$\mathbf{t}_1 \cdot \mathbf{v}_I = \mathbf{t}_1 \cdot \mathbf{v}_{II}, \qquad (4)$$

$$\mathbf{t}_2 \cdot \mathbf{v}_I = \mathbf{t}_2 \cdot \mathbf{v}_{II} \qquad (5)$$

dynamic conditions :

$$\mathbf{t}_1 \cdot \boldsymbol{\sigma}_I = \mathbf{t}_1 \cdot \boldsymbol{\sigma}_{II}, \qquad (6)$$

$$\mathbf{t}_2 \cdot \boldsymbol{\sigma}_I = \mathbf{t}_2 \cdot \boldsymbol{\sigma}_{II}, \qquad (7)$$

$$\mathbf{n}_2 \cdot \boldsymbol{\sigma}_I - \mathbf{n}_2 \cdot \boldsymbol{\sigma}_{II} = 0 \qquad (8)$$

The upper convected Maxwell model and the Phan-Thien and Tanner model as viscoelastic constitutive equations are used, which are written as,

$$\boldsymbol{\tau} + \lambda \overset{\nabla}{\boldsymbol{\tau}} = \eta(\nabla \mathbf{v} + \nabla \mathbf{v}^T) \qquad (9)$$

$$(1 + \frac{\varepsilon\lambda}{\eta_o} \mathrm{tr}\boldsymbol{\tau})\boldsymbol{\tau} + \lambda \left\{ (1 - \frac{\xi}{2}) \overset{\nabla}{\boldsymbol{\tau}} + \frac{\lambda\xi}{2} \overset{\Delta}{\boldsymbol{\tau}} \right\} = 2\eta_o \mathbf{D} \qquad (10)$$

The elastic viscous stress splitting method [7] was adopted to treat the viscoelastic stresses, and the streamline upwinding method [8-9] was applied to avoid the failure of convergence at high elasticity. If the accurate solution at the boundary is not known a priori, such as in the outflow boundary in the viscoelastic coextrusion flow, it is almost impossible to impose a proper boundary condition. In the open boundary condition method [6], boundary integral parts are treated as parts of unknown equations that have to be solved. Thus the imposition of boundary condition along the outflow is not required at all

The flow domain is discretized into 27-node hexahedron elements as shown in Fig.1, and the Galerkin finite element procedure is applied. The set of nonlinear algebraic equations is then finally solved by means of Newton's method and the frontal elimination technique.

Results and Discussion

The problem of adoption of ambiguous outlet boundary conditions in three-dimensional simulation of viscoelastic coextrusion flow was escaped by introducing the open boundary condition method. The abrupt changes of contact line positions near the outlet commonly occurred by using the fully developed outlet boundary conditions (fullybc) could be clearly removed by using the open boundary condition method (nobc) as shown in Fig.2.

From the results by using the upper convected Maxwell model as a constitutive equation, it was shown that the interface distortion increased as the elasticity ratio increased, although it was not so large and the first normal stress difference alone had no effect on the gradual increase of the degree of encapsulation along downstream direction.

From the results by using the Phan-Thien and Tanner model as a constitutive equation, it was found that the elasticity and the shear viscosity could not be treated separately in the flow simulations of viscoelastic fluid with shear thinning viscosity. When the elasticities of both layers increased while keeping the elasticity ratios constant, the degrees of encapsulation increased resulting from the increased viscosity ratios as shown in Figs. 3 and 4. The extensional viscosity had some effects on the interface curvature but little effects on the degree of encapsulation along downstream direction.

When the ratio of the second normal stress differences (ξ_{II}/ξ_{I}) increased, the curvature of outlet interface increased resulting from the increased protruding effect of the upper fluid with the higher second normal stress difference into the lower fluid with the lower second normal stress difference in magnitude. The second normal stress difference was shown to have a great influence on the gradual increase of the degree of encapsulation along downstream direction.

References

1. C. D. Han, *J. Appl. Polym. Sci.*, **17**, 1289 (1973).
2. B. L. Lee and J. L. White, *Trans. Soc. Rheol.*, **18**, 467 (1974).
3. J. H. Southern and R. L. Ballman, *J. Polym. Sci.*, **13**, 863 (1975).
4. C. D. Han and Y. W. Kim, *J. Appl. Polym. Sci.*, **20**, 2609 (1976).
5. M. Takase, S. Kihara and K. Funatsu, *Rheol. Acta*, **37**, 624 (1998).
6. S. J. Park and S. J. Lee, *J. Non-Newtonian Fluid Mech.*, **87**, 197 (1999).
7. D. Rajagopalan, R. C. Armstrong and R. A. Brown, *J. Non-Newtonian Fluid Mech.*, **36**, 159 (1990).
8. F. Debae, V. Legat and M. J. Crochet, *J. Rheol.*, **38**(2), 421 (1994).
9. J. M. Marchal, M. J. Crochet, *J. Non-Newtonian Fluid Mech.*, **26**, 77 (1987).

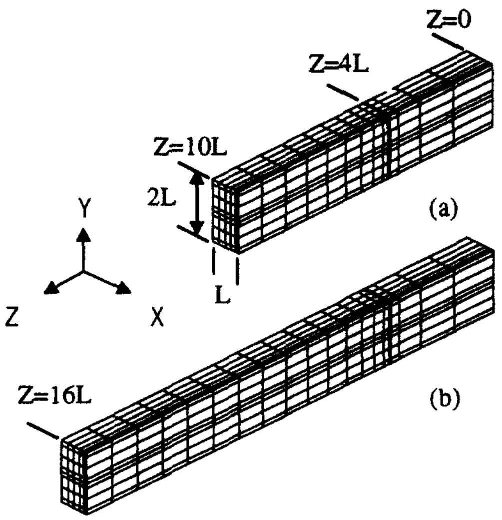

Fig.1. Finite element meshes
(a) Mesh1, (b) Mesh2.

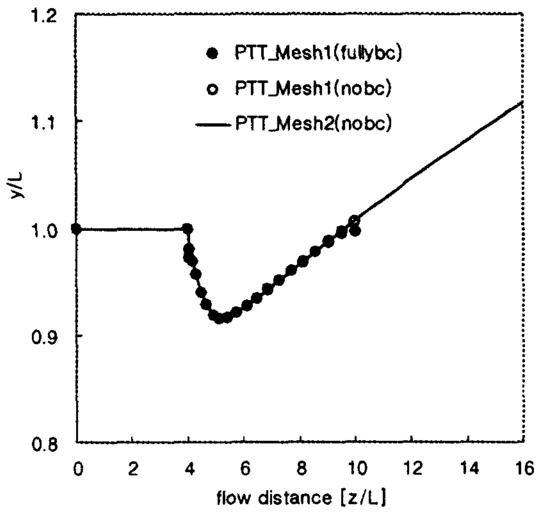

Fig.2. Contact line position along downstream direction with different boundary conditions and meshes.

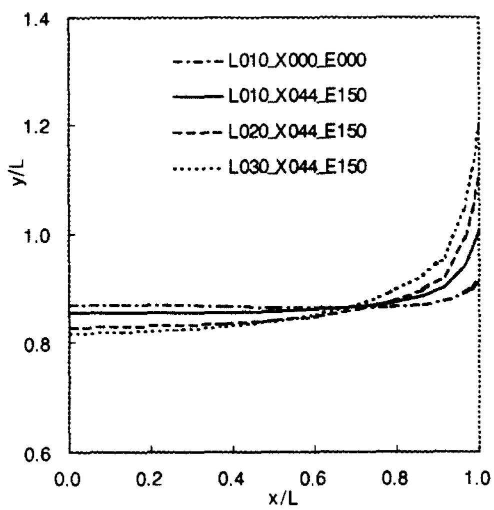

Fig.3. Outlet interface curves with different elasticities at Mesh1. Symbols L, X and E represent λ, ξ and ε, respectively.

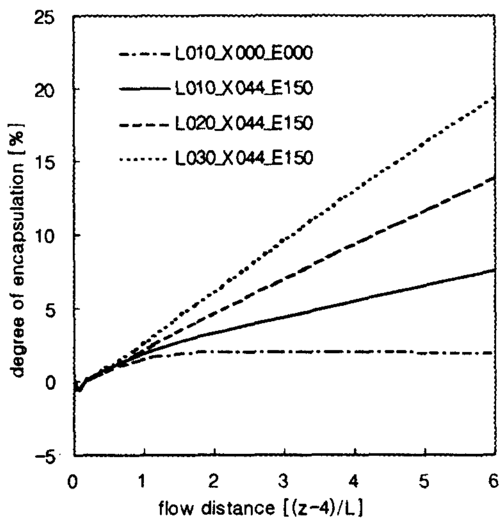

Fig.4. Degree of encapsulation along downstream direction with different elasticities at Mesh1.