Dynamics of Single Polymer Molecule in Slot Coating Flow

Jeong Yong Lee[*], Joo Sung Lee[**], Myung-Suk Chun[***], Hyun Wook Jung[*] and Jae Chun Hyun[*]

[*]Department of Chemical and Biological Engineering, Applied Rheology Center,
Korea University, Seoul, 136-713, Korea

[**]Information Technology and Electronic Materials R&D,
LG Chem/Research Park, Daejeon, 350-380, Korea

[***]Complex Fluids Research Lab., Korea Institute of Science and Technology (KIST),
39-1 Hawolgok-dong, Seongbuk-gu, Seoul, 136-791, Korea

Presented at the 14th International Coating Science and Technology Symposium,
September 7-10, 2008, Marina del Rey, California[1]

Introduction

Slot coating process, as one of pre-metered coatings, plays an important role in manufacturing IT products such as flat panel displays, secondary batteries, etc. The final purpose of this coating process is to coat thin uniform liquid layer on the web or the substrate. Many researchers have studied dynamics and stability of slot coating system with the aid of appropriate approximations (Ruschak, 1976; Higgins and Scriven, 1980). One of recent interesting issues is to incorporate polymeric coating liquids with non-Newtonian characteristic nature in the coating system. Therefore, it will be important to analyze the molecular orientation of polymer chains in coating liquids for the better quality control of coating products.

Recently, development in direct visualization methods (Smith and Chu, 1998; Smith *et al*., 1999), coupled with Brownian dynamics simulations (Larson, 2005; Shaqfeh, 2005), has allowed the dynamics of polymer molecule in simple flows to be studied with unprecedented details. Also, Duggal and Pasquali (2004) reported the flow visualization of λ-DNA in a micro roll coating equipment. In this study, we have investigated the conformation of a single polymer chain in the slot coating flow which can be regarded as

---

[1] Unpublished. ISCST shall not be responsible for statements or opinions contained in papers or printed in its publications.

a kind of microfluidic channels, by combining Brownian dynamics with the conventional computational flow dynamics simulations.

Brownian dynamics and slot coating simulation

Coating bead flow for Newtonian liquids in slot coating system has been calculated by two-dimensional model using the commercial CFD package Flow-3D under the various operating conditions, as depicted in Fig. 1(a). We applied bead pressure condition between upstream and downstream menisci for stabilizing the coating bead flow (Gates, 1999). Flow field inside coating bead regime can be represented from the flow type parameter (α) defined as

$$\alpha = \frac{\|\boldsymbol{D}\| - \|\boldsymbol{\Omega}\|}{\|\boldsymbol{D}\| + \|\boldsymbol{\Omega}\|} \tag{1}$$

where, $\|\boldsymbol{D}\|$ and $\|\boldsymbol{\Omega}\|$ are the magnitudes of the deformation and vorticity tensors, respectively. Flow type parameter (α) varies from -1 (purely rotational flow), 0 (purely shear flow), to 1 (purely extensional flow). Brownian motion has been estimated by the following stochastic equation, Eq. (2), based on the fact that external forces on each bead sum to zero (Shaqfeh, 2005). It was assumed here that coating liquid is theta solvent, and thus molecule is a phantom chain. Moreover, it is noted that the microstructural change of polymer molecules is not significantly affected by the flow field in the Newtonian system (*Suen et al*., 2002). In Eq. (2), spring force of worm-like chain model is chosen, which is good for stiff polymers.

$$d\boldsymbol{Q}_i = \left[\boldsymbol{\kappa} \cdot \boldsymbol{Q}_i + \frac{\boldsymbol{F}_{i+1}^S - 2\boldsymbol{F}_i^S + \boldsymbol{F}_{i-1}^S}{4} \right] dt + \sqrt{\frac{1}{2}} \left(d\boldsymbol{W}_{i+1} - d\boldsymbol{W}_i \right) \tag{2}$$

The velocity components in slot coating flow regime have been evaluated from two dimensional simulations with rectangular meshes. A steady profile in slot coating bead region with the velocity magnitude contour is portrayed in Fig. 1(a). To effectively characterize the flow field, a flow strength (∇v) as well as flow type parameter (α) has been considered (Lee et al., 2007). The temporal pictures of a

single molecule were plotted along its streamlines on Fig. 1(b). The molecule entered at x_0= +50μm from the slit centerline was strongly stretched at the downstream, because of the extensional-like flow generated by the free surface curvature. Another molecule started at x_0=-50μm was slightly extended in the upstream region when it turns below upstream die lip, however, it will eventually be recoiled by the plug flow acting on the downstream region (Lee et al., 2008).

Fig. 2 represents the relationship between flow characteristics and polymer chain extensions in downstream region, following three different streamlines entered at x_0= -50, 0, and +50μm from the slit centerline, respectively. Dimensionless mean extension ($\langle x \rangle / L$) of polymer chains has been influenced by variation of flow characteristics such as ∇v or α. As exhibited in Fig. 2, the flow type plays a key role in the molecular conformational change of polymer chains. Even though α could not evolve to purely extensional flow (i.e., $\alpha<0.2$ under the operating conditions involved in this study), molecule conformation has changed from the coiled state to the stretched state (Graham, 2003). It has been found that a small change of flow type from pure shear to extensional flow can remarkably extend flexible polymer chains, and their conformation can be controlled by further drying strep. The hybridization method between computational fluid dynamics and Brownian dynamics simulations used in this study can be a useful tool to qualitatively estimate conformations of polymeric molecules in coated films.

Acknowledgments

This study was supported by research grants from the Seoul R&BD program and the Korea Science and Engineering Foundation (KOSEF) through the applied Rheology Center (ARC). Also, the support of the KOSEF(R01-2008-000-11701-0) is gratefully acknowledged.

References

1. K. J. Ruschak, *Chem. Eng. Sci.* **31**, 1057 (1976).

2. B. G. Higgins and L. E. Scriven, *Chem. Eng. Sci.* **35**, 673 (1980).

3.D. E. Smith and S. Chu, *Science*, **281**, 1335 (1998)

4. D. E. Smith, H. P. Babcock and S. Chu, *Science*, **283**, 1724 (1999).

5. R. G. Larson, *J. Rheol.* **49**, 1 (2005).

6. E. S. G. Shaqfeh, *J. Non-Newtonian Fluid Mech.* **130**, 1 (2005).

7. R. Duggal, and M. Pasquali, *J. Rheol.* **48**, 745 (2004).

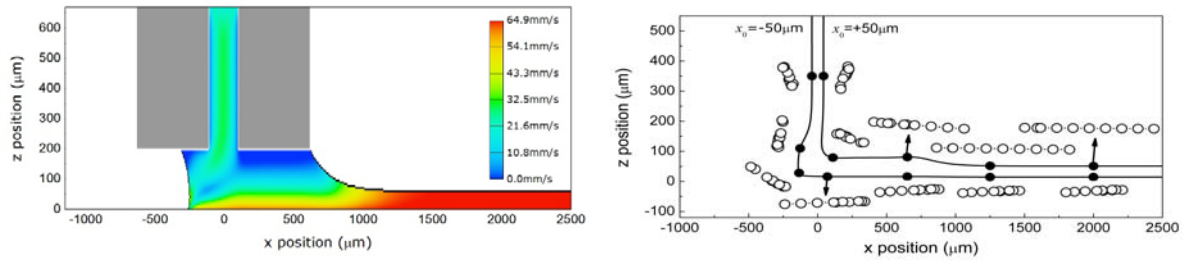
8. I. A. Gates, *Slot coating flows: Feasibility, Quality,* PhD Thesis, University of Minnesota (1999).

9. J. K. C. Suen, Y. L. Joo and R. C. Armstrong, *Ann. Rev. Fluid Mech*., **34**, 417 (2002).

10. J. S. Lee, E. S. G. Shaqfeh and S. J. Muller, *Phys. Rev. E* **75**, 030802 (2007).

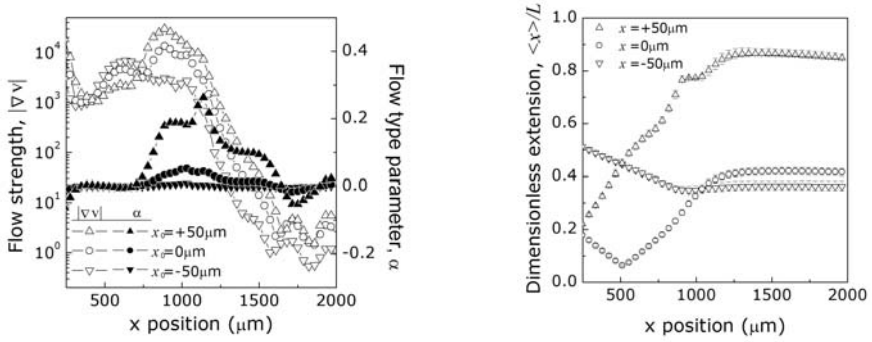
11. J. Y. Lee, B. K. Ryu, J. S. Lee, H. W. Jung and J. C. Hyun, *KARJ*, **20**, 89 (2008)

12. M. D. Graham, *Phys. Fluids*, **15**, 1702 (2003).



(a) (b)

Figure 1. (a) Velocity magnitude contour under the operating conditions considered in this study. (b) Conformational change of around polymer molecule along different streamlines in the slot coating flow.



(a) (b)

Figure 2. (a) The changes of flow strength (∇v) and flow type parameter (α) around polymer chains entered at three different positions and (b) the change of extension (<*x*>/*L*) of each molecule along the flow directions (*x*).