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Conformation of a Single DNA Molecule in Slot Coating Flow

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Slot coating, one of pre-metered coatings, is an indispensable process in IT industries manufacturing flat panel displays, secondary batteries, etc. The final goal of this coating process, as in other coating processes, is to deposit thin uniform coating liquid layer on the web or the substrate with good mechanical and optical properties. Dynamics of this process has been elucidated by many experimenters and accounted for theoretically by analysts with the aid of appropriate approximations (Sartor, 1990; Gates, 1999; Chu et al., 2006). One of interesting topics is to incorporate polymeric coating liquids with non-Newtonian characteristics in this process. Then, it will be important to observe molecular orientation of polymer chains in coating liquids for the better quality control of coating products.

Thus, this paper examined the conformation of single polymer chain in coating bead regime of slot coating by combining Brownian dynamics (BD) with the conventional computational flow dynamics (CFD) simulations. Recent developments in direct visualization methods, coupled with Brownian dynamics simulations, have allowed the dynamics of single DNA molecules in flow fields to be studied with unprecedented details (Larson, 2005; Shaqfeh, 2005). Also, Duggal and Pasquali (2004) reported flow visualization of λ-DNA in roll coating equipment using fluorescence microscope and its conformation in various flow fields. Based on this background, we tried to investigate conformation of a polymer chain like DNA molecule in slot coating flow.

Coating bead flow in slot coating has been investigated by 1D and 2D models, as shown in Fig. 1. And coating operability windows can be established by determining the position of upstream meniscus. We have simulated the dynamic behavior λ-DNA in coating bead flow regime, employing the flow field obtained from Flow-3D. Brownian motion of λ-DNA can be estimated by the following equation, Eq. (1).

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

where, $\boldsymbol{Q}$ is the displacement vector, $\boldsymbol{\kappa}$ the flow gradient tensor in flow field and $\boldsymbol{W}$ the Wiener process for the random walk. $\boldsymbol{F}^S$ is spring force (worm-like chain (WLC) model is considered here). Computations have been performed for a number of springs N_s=9, with 17 Kuhn steps per spring which corresponds to λ–DNA at high salt concentration. First, BD simulations were carried out for free-draining for the simplicity.

In this abstract, we suggested the preliminary results of DNA extension in the homogenously converging channel as a simple case for the converging downstream coating bead region. When DNA molecules are subjected to hydrodynamic forces in a flow field, their conformational response depends on flow strength which is represented by the Weissenberg number, Wi, and the flow type parameter, α. Considering planar mixed flows, for example, the dimensionless velocity gradient is given by

$$\frac{\partial u_i^\infty}{\partial x_j} = \dot{\gamma}\begin{bmatrix} 0 & 1 & 0 \\ \alpha & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (2)$$

where $\dot{\gamma}$ is the strain rate. The Weissenberg number is then defined as Wi=$\dot{\gamma}\tau_0$, where τ_0 is the longest relaxation time of the molecule. The flow type parameter is defined by the magnitude of deformation and vorticity tensors, ranging from -1 (purely rotational flow) to 1 (purely extensional flow).

One important dimensionless parameter is denoted by the ratio between the residence time of fluid (t_p) and molecular relaxation time (τ_0). Even though the flow field shows the extensional flow characteristic (α=0.1), the λ-DNA does not fully extended until characteristic time (t_p/τ_0) less than 1 at the moderate Wi (Fig. 2). Therefore, it is very important to secure sufficient processing time in a slot coating process for making satisfactory coated film.

Moreover, the molecular orientation is also sensitive to the flow type. Under the shear flows like upstream and downstream coating bead flows, the average value of molecular extension, $<x>/L$ shows 0.5 at Wi=50 like previous results (Smith et al., 1999). Even if we increase the flow strength (or Wi), $<x>/L$ could not be raised due to tumbling motion. However, if the flow type slightly shifts to the extensional flow regime (α~0.01), the molecule remarkably aligns in the flow direction like Fig. 3. We will report more detailed results on the DNA extension onto streamlines in coating bead region in ECS2007.

References

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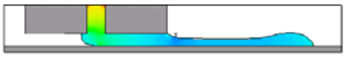

Fig.1. Flow behavior in coating coating bead region of slot coating.

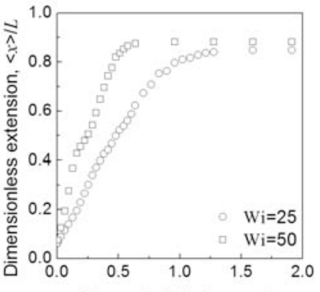

Fig.2. Effect of characteristic time on the molecular extension at α=0.1.

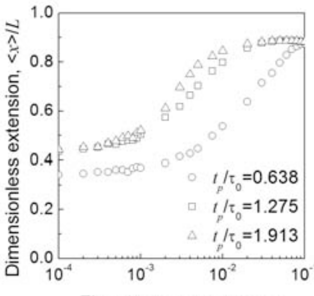

Fig.3. Effect of flow type parameter on the molecular extension at Wi=50.