

Extensional Rheology of Bimodal Blends Studied with Primitive Chain Network Simulation

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1. Introduction

The extensional flow characteristics of a polymer material are relevant for many polymer processing operations. For instance, strain hardening acts to stabilize the flow in fiber spinning. Recently Minegishi et al. [ref.1] found that adding a small fraction of higher molecular weight component to Polystyrene significantly enhanced strain hardening of the sample. We are interested in obtaining a molecular understanding of these results and the extensional rheology of bimodal blends in general, especially in terms of the deformation of the chain molecules themselves. Therefore, we performed extensive simulations of several chain molecular weights blended at different concentrations using the Primitive Chain Network (PCN) model of Masubuchi et al. [ref.2]. Further, we also investigate systems that can be directly compared with the experimental results mentioned above.

2. Investigated Systems

We considered chains of about five entanglement segments on average ($\langle Z \rangle = 5$) blended with chain molecular weights, $\langle Z \rangle = 10, 20, 40$ and 80 . For each of these blend systems, the critical volume fraction (ϕ^*) where the long chain begins to self entangle was calculated and at least three concentrations were studied ($\phi^*/2, \phi^*, 2\phi^*$). We also investigated blend systems appropriate for direct comparison with experimental data of Minegishi et al. [ref.1]. We studied the start-up extensional viscosity of the blends systems over a range of strain rates $\dot{\epsilon}$ that included ($1/\tau_d < \dot{\epsilon} < 1/\tau_R$) and $\dot{\epsilon} > 1/\tau_R$ where τ_d and τ_R are respectively the disentanglement time and the Rouse time of the long chain.

3. Extensional viscosities of monodisperse samples

The τ_d was determined from the linear rheology of the long chain. The Rouse time of the long chain was calculated using [ref.3]. Figure 1 shows the start-up transient extensional viscosities of polystyrene sample, $\langle Z \rangle = 5$ blended with 2.5% $\langle Z \rangle = 40$. Figure 2 shows the start-up transient extensional viscosities of polystyrene sample, $\langle Z \rangle = 5$. It is clear from these figures that this fraction of long chains is sufficient to induce extension hardening in this sample. The result is consistent with that obtained by Minegishi et al. [ref.1] and suggests that the PCN model can be used to study the extensional rheology of these systems. Further, we calculated the variation of the chain end-to-end distance with extension ratio and investigated the relationship between the chain deformation and extensional hardening. These and other results will be discussed in detail during the presentation.

4. References:

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- [2] Y. Masubuchi, J. Takimoto, K. Koyama, G. Ianniruberto, G. Marrucci, and F. Greco, *J. Chem. Phys.*, **115**, 4387 (2001)
- [3] K. Furuichi, C. Nonomura, Y. Masubuchi, H. Watanabe, G. Ianniruberto, F. Greco and G. Marrucci, *Rheol. Acta*, **47**, 591 (2008)

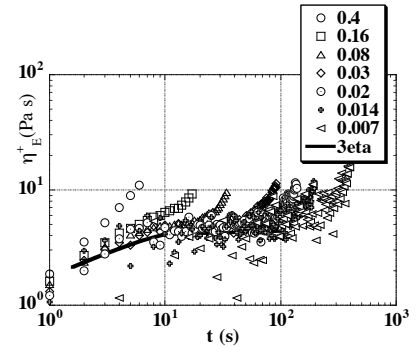


Fig.1 Start-up extensional viscosities of Z5 blended with 2.5% Z40 at different strain rates.

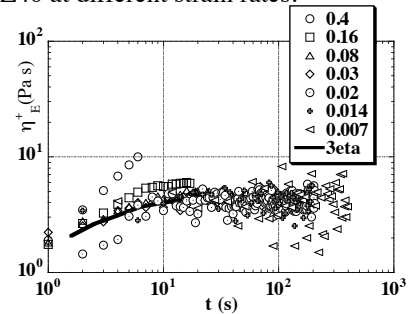


Fig.2 Start-up extensional viscosities of Z5 at different strain rates.