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Title	Prediction of the uniaxial elongational viscosity of polydisperse Polystyrene(PS) melt.
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Purpose of this study	Prediction of the uniaxial elongational viscosities of polymers.
System (Material)	-PS(Mw =2.85 x 10^5, Mw/Mn = 2.0) -PS + 1.5wt.% high molecular weight PS(HMW-PS, Mw =3.2 x 10^6)
Program (including analysis)	PASTA (Smoothing and 2D-plottting programs)
Method & Some important input parameters	(Method) Stochastic simulation based on the Slip-link model, which takes account of the reptation, contour length fluctuation and constraint renewal (constraint release or constraint creation). (Inputs) Molecular Weight : Z = M / Me (M : Molecular weight, Me : Entanglement molecular weight) Numbers of polymer : n *Some set of Z and n is available. MaxStretchRatio : Extended chain length / Equilibrium chain length (or 0 for Gauss chain)
Advance & Problem	(Advance) - The strain hardening of elongational viscosities, which has strong effect on the processability of polymer, is very sensitive to the existence of very high molecular weight components. Our simulation method can predict the effects of molecular weight distribution and high molecular weight component on the strain hardening quantitatively. (Problem) - Prediction of the rheological properties of polymers with extremely broad molecular weight distributions and branching structures, such as pom-pom and comb.
References	[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)] - 47th Rheology tohronkai, p.263 (1999) - J. Takimoto, H. Tasaki and M. Doi, Proceeding of XIIIth International Congress on Rheology, Cambridge, UK, 2, 97 (2000) - H. Tasaki, J. Takimoto, M. Doi, Proceeding of Materials Science for the 21st Century, Osaka, Japan, **B**, 15 (2001)
KeyWords (in English)	Rheology, slip-link model, entanglement, constraint release, constraint renewal, contour length fluctuation, polystyrene, elongational viscoelasticity, strain hardening, PASTA

Results (Remarks)

(1)We prepared 10^4 chains in a computer to mimic the GPC data.

Input :

Z	n	MaxStretchRatio
3.1	354	4.4
3.5	394	4.4
....		
107.4	2	4.4

(2)First, we calculated the dynamic moduli, and determined two model parameters(the time scale and the stress scale) by fitting the simulation results to the experiment.

(3)Then we calculated the elongational viscosities at the same strain rates as experiments. Uniaxial elongational stress(σ_E) is calculated by following equation.

$$\sigma_E = N_1 + \frac{1}{2} N_2$$

N1: First normal stress difference
N2: Second normal stress difference

[Example of analysis]

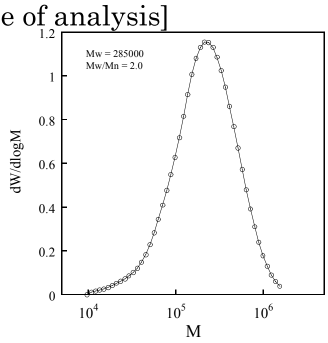

Fig.1 GPC profile

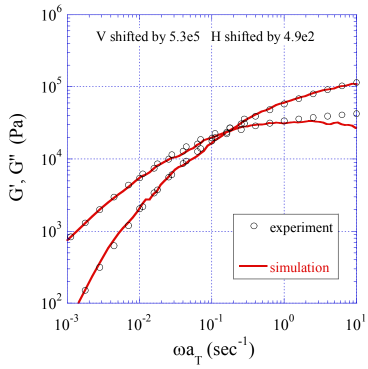

Fig.2 Storage modulus(G') and Loss modulus(G")

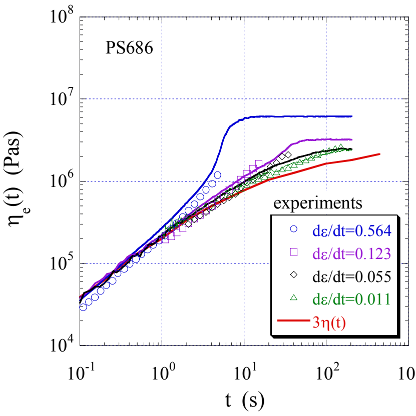

Fig.3 Elongational viscosity of polydisperse system. Symbols and lines represent the experiments and simulations, respectively

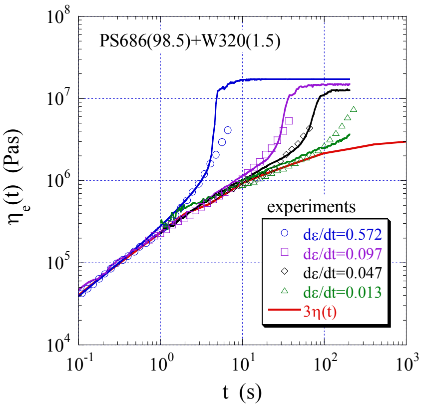

Fig.4 Elongational viscosity of polydisperse system containing 1.5wt.% HMW-PS