No. EAR1-001-03 First registration:1999/11/25 New:2001/11/ 2

Title	Prediction of rheological properties of linear polymers.
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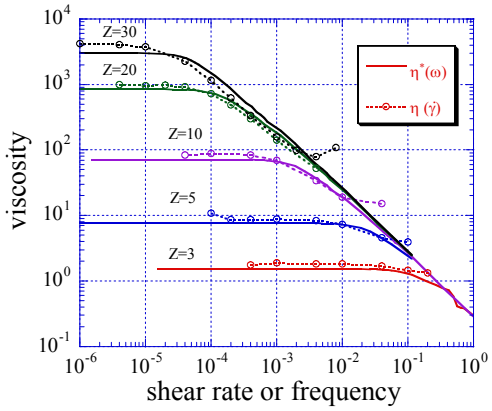
Purpose of this study	Development and research of a new simulation method for the prediction of the rheological properties of linear polymers with arbitrary molecular weight distributions.
System (Material)	Linear monodisperse or polydisperse polymer system （PS, PE, ... etc.）
Program (including analysis)	PASTA
Method & Some important input parameters	(Method) Stochastic simulation based on the slip-link model, takes account of contour length fluctuation, reptation 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.
Advance & Problem	(Advance) - Applications to the linear polymers have shown good agreement with experiments(shear flow, uniaxial elongational flow, stress relaxation in step strain shear experiment, ...etc.) (Problem) - Prediction of the rheological properties of polymers with extremely broad molecular weight distributions and long chain branching structures.
References	[Manuscript] [Presentation at conferences (Meetings)] 47th Rheology tohronkai, p.263 (1999)
KeyWords (in English)	Rheology, tube model, entanglement, contour length fluctuation, constraint release, viscosity, viscoelasticity, Cox-Merz rule, Doi-Edwards, linear, monodisperse, binary blend, shear modulus, shear flow, elongational flow

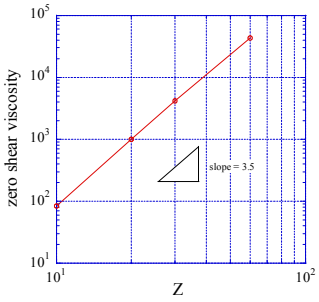
Results (Remarks)

Output : Stress
Shear viscosity, uniaxial elongational viscosity,
relaxation modulus and linear viscoelastic functions(G'(ω),G''(ω),
η*(ω)) ... etc.

[Example of analysis]

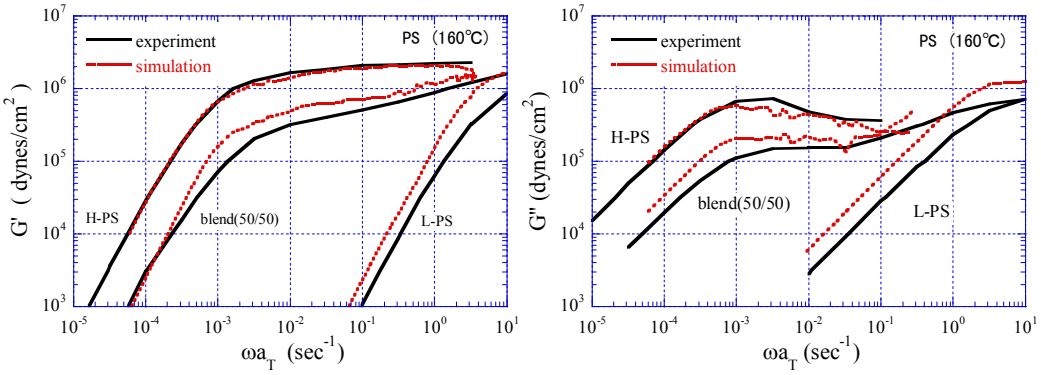


Cox-Merz rule



Molecular weight dependency of
zero shear viscosity (3.5th power of Z)

	Experiment	Simulation
H-PS	Mw 581,000	Z32
L-PS	Mw 58,700	Z 3 (=Mw/Me)



Comparison of simulation to experiment
in storage moduli(G') and loss moduli