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Polymer characterization and practical linear viscoelastic models by control theory

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Practical linear viscoelastic models of polymer flows, micro-macro relations, multiscale simulations and characterization of chain structures are discussed. We have applied control theory [1–4] to model the relationship between the relaxation modulus, dynamic viscosity, transient flow effects and molecular weight distribution (MWD). Similar way we have shown a direct simple linear micro-macro relation to molecular dynamics, explained Cox-Merz rules, power law, verified time–temperature superposition (TTS) for thermorheologically simple materials and used control theory for modelling temperature dependence for more complex polymers. We used a novel way to explain and sum all shear histories based on the respective effective viscosity using a new version of the classical Boltzmann superposition principle.

Shortly fundamentals of control theory and molecular dynamics are explained towards practical applications as industrial melt processing and polymer structure characterizations. The constitutive models for the viscoelasticity of polymers and computation algorithms are presented for determining molecular weight distributions (MWDs) from viscosity measurements. The results calculated from measured data confirmed that our model for determining the MWD from viscosity measurements works in practice, with the error being very small provided that the recorded data are accurate. Other properties and the influence of changes in the MWD on the behavior can be simulated using what-if analyses.

The developed models can simulate not only the pressure losses in capillaries and injection-moulding cavities, but also the molecular orientation and possible dimensional deviations of end products. Similar way can be modelled and understood many extrusion processes and behaviours of extrudates. As summary is connected chain dynamics to the different viscoelastic properties up to the macro scale in a linear manner.

References

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