MWD COMPUTATIONS FROM VISCOSITY AND VICE VERSA BY NEW LINEAR MODEL

Tommi Borg *
TomCoat Oy, Koskisenkuja 11, 62510 Kuoppa-aho, Finland
E-mail: tommi.borg@tomcoat.com

Esko J. Pääkkönen
Laboratory of Plastics Technology, Tampere University of Technology, P.O. Box 589, 33101 Tampere, Finland

* To whom all correspondence should be addressed.

A new assertion to model viscoelasticity of polymers starting from their real molecular structure is presented. The theory is based on the principle of electrostatic energy on electric fields and it gives, as used relatively, a simple linear differential constitutive formula. The solutions of the formula join viscosity, modulus and other flow properties to the molecular structure. Viscoelasticity and properties of polymers are described by means of the active and passive structure components. The concept also helps to overcome major ill-pose inverse problems of the field. Some results for determining molecular weight distribution (MWD) of polyethylene (PE) and polystyrene (PS) starting from viscosity measurements and vice versa are presented. The error of the viscosity fit is small compared to the procedures published earlier.

The principle of our model starts from real structure of polymer and gives relations to the properties. The main formula is partitioned to the two tools which are introduced: *an active P' and a passive P" component function* related to structure. These functions are needed to describe the behaviour of polymer during flow. The component functions P' and P" are related to dynamic modulus components G' and G". In the case of some polymers when storage modulus and loss modulus were computed from P' and P" , the resulted G' and G" were equal to measured modulus values.

The main features of the principle are:

1. Viscoelastic properties are modelled by active and passive component functions influenced to the properties and related from structure.
2. Passive component detects the deformation of flow and active component the deformation of molecules.
3. Particular solutions of linear differential formula generated from molecular relations give properties at different states.
4. Relaxation time spectra procedures are not used.

The basic criteria mentioned above gives the procedure, by which MWD and other structures from rheological measurements can be achieved. The model gives also normalized time-dependent relaxation modulus, which have been used for determinations of spectrum by well-known formulas.

The theory is based on the principle of electrostatic energy on electric fields. This fundamental well-known definition explains the electrostatic potential energy for a particle, which is used to join external properties and internal molecular structure.

On the standpoint of inversion problems the relation between properties and structure to construct by energy concept without direct use of time procedures has been managed. Also inversion problems have been partitioned to the smaller components with real relations to the molecular structure. Some general lines of coordinate systems generating problems will be discussed.

For these analyses, the RheoPower software package have been developed. RheoPower enables to make modelling and real time computations.