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**Predicting Polymer Properties Directly from Processing Conditions**

\*Han E. H. Meijer, Leon E. Govaert, Tom A. P. Engels

*MaTe, DPI, TU/e, P.O. Box 513, 5600 MB Eindhoven, The Netherlands.*

It took our group more than 15 years to arrive at a validated 3D constitutive equation for amorphous solid polymers, like PC, PMMA, PVC, PS or PS/PPO blends, that is not only quantitative, but is also able to predict the mechanical performance of products made of these polymers on the short term (impact loading) and long term (creep and fatigue failure, including the prediction of an endurance limit) without even performing one mechanical test.

The model is based on solid state rheology and uses a compressible form of the Leonov model as a starting point to describe the fluid character of the secondary interactions. They determine on one hand the polymers (non-linear) elastic response (modulus of the order of 1 GPa) up to yield (at a stress of the order of 0.1 GPa) and on the other hand the rate dependence of the flow that starts at yield: stress-induced melting of these secondary interactions or passage of the glass transition temperature. Key point is the extreme stress dependence of the non-linear viscosity in this remarkable fluid, contained in the Maxwell part of the model, changing viscosity with 20 decades in the stress range of 0-0.1 GPa. During flow, the network formed by the primary molecular interactions, starts to be stretched. Its contribution is a hardening stress, represented by a (rather weak with modulus of the order of 0.01 GPa) neo-Hookean spring put parallel to the Maxwell element (in the one-mode version of the model). It gives the strain hardening, necessary for the important delocalization of strain which is the key to understand a polymer response.

The basic model was first extended by incorporating the stress dependence of the viscosity specifically necessary to describe arbitrary 3D loading situations. Most time in the development of the model took, however, next the incorporation of the aging process, finally captured by a single stress- and temperature-activated parameter  $S$  that uniquely describes the state of the material. An increase in  $S$  shifts yield on a semi-log scale to lower deformation rates. Alternatively, at a given deformation rate it increases the yield stress. Upon flow after yield, the influence of  $S$  is erased by mechanical rejuvenation, captured by a simple function  $R$ . (Once mechanically rejuvenated, all polymers are completely ductile, including the brittle PS that does not show crazing anymore and even allows to become knotted at room temperature). Most important is that the development of the state parameter  $S$  in time, which introduces the strain softening of polymers that leads to more or less severe localization of strain, is independent of the molecular weight and molecular weight distribution of the material, as it should be since this rate is determined by local changes in secondary interactions only without major flow.

If we start to compute the development of the state parameter  $S$  already during processing, e.g. the injection moulding process, the state of the polymer is completely known and no mechanical tests after moulding are necessary anymore. Here the break-through of the quality of the model is easily manifested, since for the first time we can predict properties on beforehand and consequently we can optimize product design given the process conditions necessary to make the product.