Molecular Architecture of Non-Linear Polymers: Kinetic Modeling and Experimental Characterization of the System Methyl Methacrylate + Ethylene Glycol Dimethacrylate

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A general kinetic approach[1-4] allowing the prediction of the molecular architecture of non-linear polymers is applied to the study of the copolymerization of methyl methacrylate (MMA) with ethylene glycol dimethacrylate (EGDMA). Dynamic predictions of molecular weight distributions, sequence length distributions and mean square radius of gyration are possible before and after gelation.

A set of experiences concerning the copolymerization of MMA and EGDMA was carried out in toluene solution at 60 °C for which classic radical kinetics is a good approximation. The time evolution of some polymers properties was done using a GPC system with a refractive index detector coupled with MALLS. With this combination it is possible the determination of absolute weight average molecular weight and distributions for non-linear polymers, as well as the *z*-average radius of gyration of the products. Therefore some experimental information about the architecture of the networks can be obtained. The influence of the initial amount of cross-linker on the dynamics of the non-linear structure of these products was investigated.

A complex kinetic scheme comprising 23 different chemical species and 59 chemical reactions was applied in the modeling studies of this chemical system. Most of the kinetic parameters used in the simulations were collected from previous studies and a good agreement between predictions and experimental measurements is observed for molecular weights and z-average radius of gyration (see Figures 1 and 2).

These studies can be used to improve the properties of crosslinked/branched polymers which nowadays have important applications in biomedicine or separation processes useful in biotechnology and pharmaceutical industries.

[1] Dias R.C.S., Costa M.R.P.F.N, Macromol. React. Eng., 1, 440, 2007
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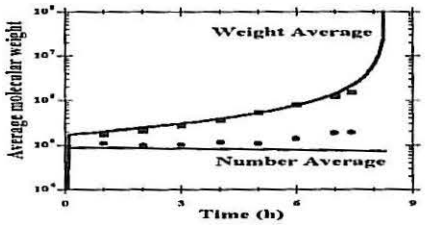

Fig.1: Experimental and predicted $\overline{M}_n$ and $\overline{M}_w$ in the copolymerization MMA/EGDMA

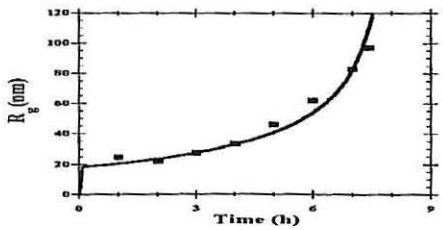

Fig. 2: Experimental and predicted R_g in the copolymerization MMA/EGDMA