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POSTER

Nitroxide - Mediated Radical Copolymerization of Styrene and Divinylbenzene: Predictions in the Pre- and Post-Gelation Periods using Different Modeling Approaches

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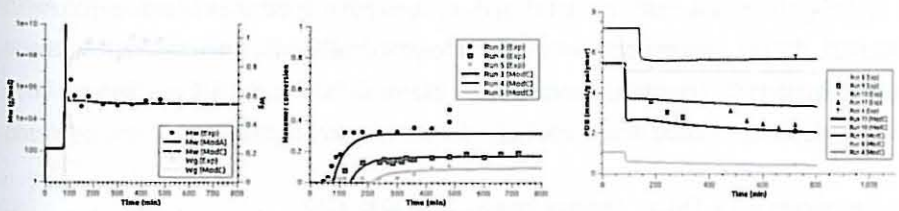
Three modeling approaches for the NMRP of styrene-divinylbenzene were used for describing experiments performed at different initial conditions: a rigorous approach (model A) based on balance of species and method of characteristics in terms of generating functions and two simplified approaches based upon mass and moment balances, numerical fractionation and pseudo-kinetic method (models B and C). Balances of paths connecting groups were used for tackling loop formation reactions. A critical comparison of the effect of underlying assumptions of the three approaches was carried out. Simulations making use of the concept of path balances presented good results for the predictions of pendant double bonds (PDB) concentration. Numerical fractionation can easily allow for empirical reactivity changes with average molecular size (through the generation index). Thus, simultaneous agreement for predictions of sol weight-average molecular weight (M_w) and gel fraction (W_g) could be found with experiments at 90 °C. Experiments at 130 °C implied a higher crosslinking reactivity, which might be related to a higher mobility of polymer chains.



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