

MODEL-BASED DESIGN OF MADIX UNDER BULK AND SOLUTION CONDITIONS

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Macromolecular design by interchange of xanthates (MADIX) is a less studied controlled radical polymerization technique from a mechanistic and modeling point of view. In this contribution, MADIX of styrene and chain extension toward the synthesis of block copolymers is investigated, with azobisisobutyronitrile as conventional radical initiator and O-ethylxanthyl ethyl propionate as initial RAFT agent (R_0X). Degenerative transfer coefficients for both the exchange with R_0X and macro-RAFT agent are reported and their difference is highlighted to be relevant for the kinetic description. The model validity is supported by measurement of end-group functionality (EGF) data considering elemental analysis. Novel mechanistic insights are that in contrast to typical reversible addition fragmentation chain transfer (RAFT) polymerizations the macroradical CLD follows a Schulz-Flory distribution and that both during the homopolymerization and the chain extensions an exchange, so with monomer incorporation, only takes place once [1].

[1] D.J.G. Devlaminck, P.H.M. Van Steenberge, M.-F. Reyniers, D.R. D'hooge, *Polym Chem.* 2017, 8, 6948