## The relevance of the termination rate coefficient model to accurately describe the chain length distribution in the industrial production of expandable polystyrene

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An advanced kinetic model is presented for the bulk/suspension polymerization kinetics of vinylic monomers [1] and is successfully applied to improve the industrial production of expandable polystyrene (EPS), an important material in the packaging and construction industry due to its attractive insulation properties. For a broad range of conditions, the reported set of model parameters allows an excellent description of the experimental data on monomer conversion and molar mass distribution (MMD). It is demonstrated that the more recently developed composite  $k_t$  model [2] is the most suited one to accurately account for diffusional limitations on termination. A unique characteristic of the kinetic model is its ability to describe the complete chain length distribution, in particular its multimodality. For low temperatures and DCP amounts (< 403 K; < 0.20 m% DCP), a bimodal log-MMD is obtained, which is explained by the inability of chain transfer reactions to compensate for the gel-effect (see figure). For the opposite conditions, only the composite  $k_t$  model provides an excellent description of the termination rate of the short chains formed via chain transfer to monomer, allowing to predict the experimentally observed unimodal log-MMD. These unimodal log-MMDs can also be obtained by adding a sufficiently high amount of the blowing agent *n*-pentane. The impact of degradation reactions on the EPS product is demonstrated to be irrelevant.



## References:

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