A DETAILED CHARACTERIZATION AND DESIGN OF COPOLYMERIZATION

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Many industrial polymerizations are copolymerizations in which two or more comonomers are copolymerized together to obtain a final product with a wide variety of properties originating from the related homopolymers. Crucial is the identification of the correct comonomer types and the reaction conditions so that the suited connectivity of monomer units is ensured in the copolymer chains. In view of this challenge a detailed characterization tool is indispensable. A sole focus on experimental tools is insufficient as they only allow the assessment of copolymer properties through relative properties and/or are limited to average properties [1-4]. The latter implies the lack of validation of intermolecular homogeneities, inhibiting process control on the polymer property level. To solve this issue and thanks to the advance in recent computer technologies, simulation tools have been developed which allow a characterization of copolymerization processes at the molecular level (see Figure 1; [3]). Monomer sequences of individual chains can be visualized allowing an unambiguous product qualification. In this contribution, the potential of these simulation tools is highlighted through several case studies. Focus in on both bulk/solution radical and cationic polymerizations and the interplay of chemistry and diffusional limitations [5-7].

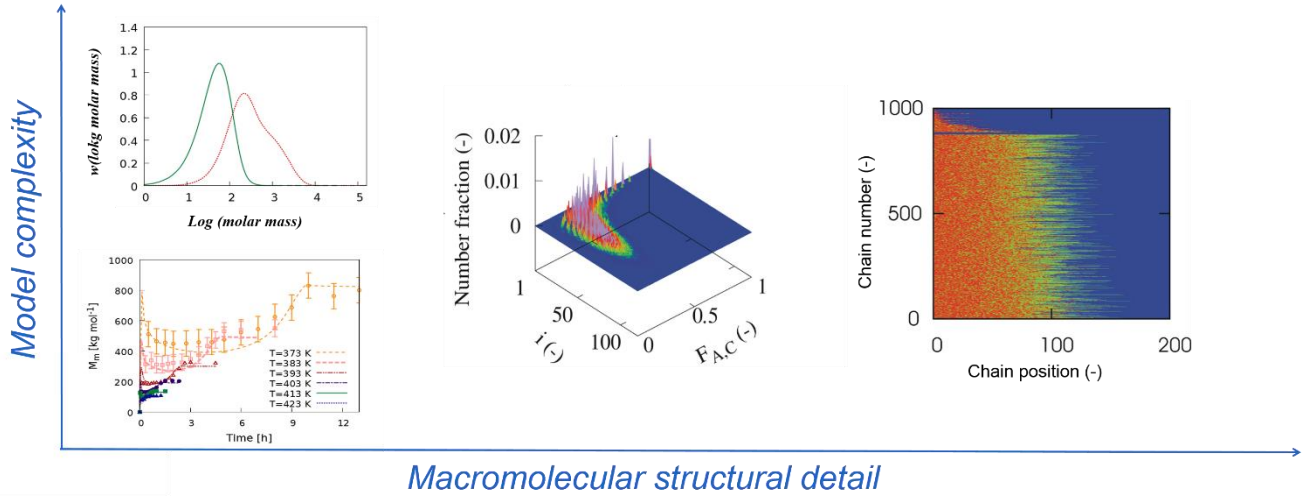

Figure 7 – Modeling platform to support the design of copolymerization processes ([3]*)*

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