AUTO-GENERATED CHEMICAL REACTION NETWORKS FOR POLYMERIZATION PROCESSES

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In this paper we consider the application of automatic reaction network generation on a polymerization process. Such networks characterize transformations that molecules undergo until they turn into final, stable products using a graphical representation of reactions and chemical compounds. The automatic generation of such networks allows treating complex reaction systems like biological pathways or pyrolysis of hydrocarbons in an elegant manner. Complex polymerization problems like the drying of oils with high unsaturation content offer a challenge for the application of reaction network generation for polymers. A major problem arises considering polymerization processes, as the molecular species grow to the infinite size, which makes explicit representation of such molecular species prohibitive. Therefore, we introduce the so-called "monomer approach" into the field of reaction networks and adjust a methodology so that it allows us to work with polymers [1].
The monomer approach is illustrated as following: when two molecules connect to each other, we do not consider them as a new unit, but view them as two different monomer species and indicate that each of them has one crosslink. Thus, we count the number and type of crosslinks per monomer species assuming that it is a part of bigger connected component. Such monomer species is represented as a molecular graph with nodes represented as atoms and edges as bonds between atoms. Further, we define reaction rules as transformations on the reactive sites of the monomer species. Every time reaction rule is applied, it is recorded in the reaction network. The reaction network captures how all-possible configurations of monomer species in the system are connected to each other through the reaction rules. The reaction network is automatically transformed into the kinetic balance equations. From this result we extract the concentrations of monomer species having various numbers and types of crosslinks and apply configuration model for random graph to obtain the global properties of the polymer network. For instance, the component size distribution from the random graph model corresponds to the molecular weight distribution in polymer reaction engineering. To illustrate this, we modeled copolymerization of inimer and isobutylene and verified the results by data obtained by means of Monte Carlo simulation from Ref. [2]. Figure 1 shows the correspondence between results coming from these completely different modeling techniques. Furthermore, the methodology is generic and can be applied for other polymerization processes.

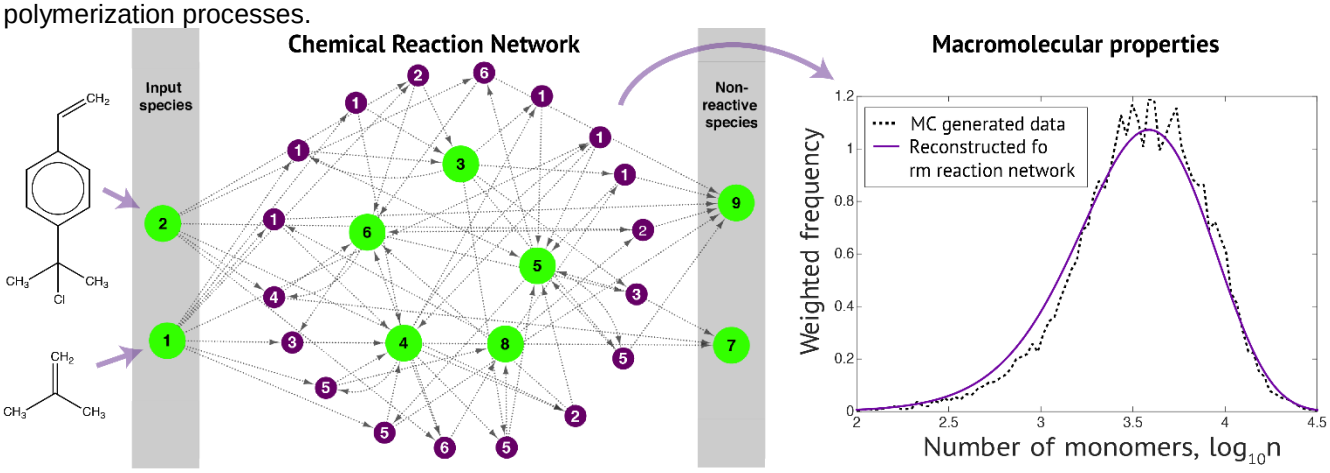

Figure 1 - Reaction network for copolymerization of inimer and isobutylene (left); molecular weight distribution from configuration model for random graph compared to data from Monte Carlo simulation (right).

References:
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[2] Y. R. Zhao, K. B. McAuley, P. D. Iedema, and J. E. Puskas, Advanced Monte Carlo modeling using weight-based selection of arborescent polyisobutylene molecules in a batch reactor. *Macromolecular Theory and Simulations*, 25:134–154, 2016.