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Control of polymer network topology in semi-batch systems RUI WANG, BRADLEY OLSEN, Department of Chemical Engineering, Massachusetts Institute of Technology , JEREMIAH JOHNSON, Department of Chemistry, Massachusetts Institute of Technology — Polymer networks invariably possess topological defects: loops of different orders. Since small loops (primary loops and secondary loops) both lower the modulus of network and lead to stress concentration that causes material failure at low deformation, it is desirable to greatly reduce the loop fraction. We have shown that achieving loop fraction close to zero is extremely difficult in the batch process due to the slow decay of loop fraction with the polymer concentration and chain length. Here, we develop a modified kinetic graph theory that can model network formation reactions in semi-batch systems. We demonstrate that the loop fraction is not sensitive to the feeding policy if the reaction volume maintains constant during the network formation. However, if we initially put concentrated solution of small junction molecules in the reactor and continuously adding polymer solutions, the fractions of both primary loop and higher-order loops will be significantly reduced. There is a limiting value (nonzero) of loop fraction that can be achieved in the semi-batch system in condition of extremely slow feeding rate. This minimum loop fraction only depends on a single dimensionless variable, the product of concentration and with single chain pervaded volume, and defines an operating zone in which the loop fraction of polymer networks can be controlled through adjusting the feeding rate of the semi-batch process.

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