PREDDICTING AVERAGE MOLECULAR WEIGHTS AND BRANCHING LEVEL FOR SELF-CONDENSING VINYL COPOLYMERIZATION IN A CSTR

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A continuous stirred-tank reactor (CSTR) model is developed for production of arborescent polyisobutylene (arbPIB, shown in Figure 1), using multidimensional method of moments. ArbPIB is a promising biomaterial, suitable for human implantation, especially for breast reconstruction after cancer surgery.[1,2] To our knowledge, arbPIB has only been produced via carbocationic polymerization in batch and semi-batch reactors, never in a CSTR. ArbPIB is made by copolymerizing IB monomer with an inimer, which is a molecule that contains an initiating group and vinyl group. As such, inimers act both as initiators and monomers, forming T-shaped branching points in the polymer. The CSTR model is used to predict dynamic changes in average branching level and number-average and weight-average molecular weights ($\bar{M}_n$ and $\bar{M}_w$). Simulations of this self-condensing vinyl copolymerization (SCVCP) show a tendency toward higher polydispersity and higher branching level compared to batch reactor simulations conducted using the same recipes and residence times.[3] At high inimer feed concentrations and/or long residence times, the model predicts that a CSTR will not reach steady-state operation due to $\bar{M}_w$ increasing toward infinity. As a result, there is a narrow operating range in which inimer feed concentrations can be adjusted to achieve a desired steady-state $\bar{M}_w$. If SCVCP is to be conducted in a CSTR, it will be important to ensure that residence times and inimer feed concentrations are selected within the stable operating window (Figure 2).