

REACTION KINETICS, CATALYSIS AND.....

甲基丙烯酸-N, N-2-甲基乙胺酯原子转移自由基聚合动力学研究

江成发, 张允湘

Department of Chemical Engineering, Sichuan University, Chengdu 610065, China

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摘要 A kinetic model was developed to describe the atom transfer radical polymerization (ATRP) of 2-(N,N-dimethylamino) ethyl methacrylate (DMAEMA). The model was based on a polymerization mechanism, which included the atom transfer equilibrium for primary radical, the propagation of growing polymer radical, and the atom transfer equilibrium for the growing polymer radical. An experiment was carried out to measure the conversion of monomer, the number-average molecular weight of polymer and molecular weight distribution

for the ATRP process of DMAEMA. The experimental data were used to correlate the kinetic model and rate constants were obtained. The rate constants of activation and deactivation in the atom transfer equilibrium for primary radical are $1.0 \times 10^4 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$ and $0.04 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$, respectively. The rate constant of the propagation of growing polymer radical is $8.50 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$, and the rate constants of activation and deactivation in the atom transfer equilibrium for growing polymer radical are $0.045 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$ and $1.2 \times 10^5 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$, respectively. The values of the rate constants represent the features of the ATRP process. The kinetic model was used to calculate the ATRP process of DMAEMA. The results show that the calculations agree well with the measurements.

关键词 [二甲胺](#) [乙烷基](#) [异丁烯酸酯](#) [动力学](#) [原子传递](#)

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Kinetic Study of Atom Transfer Radical Polymerization of 2-(N,N-Dimethylamino) ethyl Methacrylate

JIANG Chengfa, ZHANG Yunxiang

Department of Chemical Engineering, Sichuan University, Chengdu 610065, China

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Abstract A kinetic model was developed to describe the atom transfer radical polymerization (ATRP) of 2-(N,N-dimethylamino) ethyl methacrylate (DMAEMA). The model was based on a polymerization mechanism, which included the atom transfer equilibrium for primary radical, the propagation of growing polymer radical, and the atom transfer equilibrium for the growing polymer radical. An experiment was carried out to measure the conversion of monomer, the number-average molecular weight of polymer and molecular weight distribution for the ATRP process of DMAEMA. The experimental data were used to correlate the kinetic model and rate constants were obtained. The rate constants of activation and deactivation in the atom transfer equilibrium for primary radical are $1.0 \times 10^4 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$ and $0.04 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$, respectively. The rate constant of the propagation of growing polymer radical is $8.50 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$, and the rate constants of activation and deactivation in the atom transfer equilibrium for growing polymer radical are $0.045 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$ and $1.2 \times 10^5 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$, respectively. The values of the rate constants represent the features of the ATRP process. The kinetic model was used to calculate the ATRP process of DMAEMA. The results show that the calculations agree well with the measurements.

Key words [kinetics](#); [modeling](#); [atom transfer radical polymerization](#); [moment method](#); [2-\(N,N-dimethylamino\)-ethyl methacrylate](#)

通讯作者:

江成发 jiangcf1@yahoo.com

作者个人主页: 江成发; 张允湘

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