Reactor Dynamics, Control, Optimization

Exothermic polymerization reactions in continuous flow reactors may cause complex nonlinear steady state and transient behaviors. The topic of reactor dynamics has been the subject of research by many researchers in the past, notably by Prof. W. H. Ray at Univ. of Wisconsin and his research group. Understanding the nonlinear reactor dynamics is not only interesting from academic point of view but also important in operating industrial polymerization reactors. In our papers, we investigated the dynamics of continuous polymerization reactors with mixed initiators in a single and in a train of CSTRs.

Also, some of the following publications present the dynamic optimization of semibatch copolymerization reactors and model-based control of polymerization reactors using extended Kalman filter.

1. Analysis of steady state of free radical solution polymerization in a continuous stirred tank reactor (K.Y. Choi), **Polym. Eng. Sci**., 26(14), 975-981 (1986).
2. Kinetics of bulk free radical polymerization of methyl methacrylate using potassium peroxydisulfate with 18-crown-6 as phase transfer catalyst (K.Y. Choi and C.Y. Lee), **Ind. Eng. Chem. Res**., 26, 2079-2086 (1987).
3. Multiobjective dynamic optimization of semibatch free radical copolymerization process with interactive CAD tools (D.N. Butala, M.K.H. Fan and K.Y. Choi), **Computers & Chem. Eng**., 12(11), 1115-1127 (1988).
4. Synthesis of open loop controls for semibatch copolymerization reactors (D.N. Butala and K.Y. Choi), **Automatica**, 25(6), 917-923 (1989).
5. Copolymer composition control policies for semibatch free radical copolymerization processes (K.Y. Choi), **J. Appl. Polym. Sci**., 37, 1429-1433 (1989).
6. Dynamics of a CSTR for styrene polymerization initiated by a binary initiator system (K.J. Kim, K.Y. Choi and J.C. Alexander), **Polym. Eng. Sci**., 30(5), 279-290 (1990).
7. Dynamics of a cascade of two continuous stirred tank styrene polymerization reactors with a binary initiator system (K.J.Kim, K.Y. Choi and J.C. Alexander), **Polym. Eng. Sci.**, 31(5), 333-352 (1990).
8. An experimental study of multiobjective dynamic optimization of a semibatch copolymerization process (K.Y. Choi and D.N. Butala), **Polym. Eng. Sci**., 31(5), 353-364 (1991).
9. On-line estimation and control of a continuous stirred tank polymerization reactor (K.Y. Kim and K.Y. Choi), **J. Process Control**, 1(3), 96-110 (1991).
10. Multiobjective dynamic optimization of batch free radical polymerization process by mixed initiator systems (D.N. Butala, W.R. Liang and K.Y. Choi), **J. Appl. Polym. Sci**., 44, 1759-1778 (1992).
11. Dynamics of a CSTR for styrene polymerization initiated by a binary initiator mixture. II. Effect of viscosity dependent heat transfer coefficient (K.J. Kim, K.Y. Choi and J.C. Alexander), **Polym. Eng. Sci**., 32(7), 494-505 (1992).
12. Effect of initiator characteristics on high pressure ethylene polymerization in autoclave reactors (B.G. Kwag and K.Y. Choi), **Ind. Eng. Chem. Res**., 33(2), 211-217 (1994).
13. Modeling of a multistage high pressure ethylene polymerization reactor (B.G. Kwag and K.Y. Choi), **Chem. Eng. Sci**., 24B, 4959-4969 (1995).
14. In-line dielectric monitoring of monomer conversion in a batch polymerization reactor (T.J. Crowley and K.Y. Choi), **J. Appl. Polym. Sci**., 55, 1361-1365 (1995).
15. Polymerization of styrene in a continuous filled tubular reactor (W.J. Yoon and K.Y. Choi), **Polym. Eng. Sci**., 36(1), 65-77 (1996).
16. On-line monitoring and control of polymerization reactors (T.J. Crowley and K.Y. Choi), **J. Process Control**, 6(2/3), 119-127 (1996).

17. Calculation of molecular weight distribution from molecular weight moments in free radical polymerization (T.J. Crowley and K.Y. Choi), **Ind. Eng. Chem. Res**., 36, 1419-1423 (1997).
18. Discrete optimal control of molecular weight distribution in a batch free radical polymerization process (T.J. Crowley and K.Y. Choi), **Ind. Eng. Chem. Res**., 36, 3676-3684 (1997).
19. Calculation of molecular weight distribution in a batch thermal polymerization of styrene (W.J. Yoon, J.H. Rhu, C.H. Cheong and K.Y. Choi), **Macromol. Theory and Simulations**, 7, 327-332 (1998).
20. Control of molecular weight distribution and tensile strength in a free radical styrene polymerization process (T.J. Crowley and K.Y. Choi), **J. Appl. Polym. Sci**., 70, 1017-1026 (1998).
21. Experimental studies on optimal molecular weight distribution control in a batch free radical polymerization process (T.J. Crowley and K.Y. Choi), **Chem. Eng. Sci**., 53(15), 2769-2790 (1998).
22. Copolymer hydrodynamic volume distribution in free radical copolymerization processes (T.J. Crowley and K.Y. Choi), **Polym. React. Eng**., 7(1), 43-70 (1999).
23. Control of copolymer hydrodynamic volume distribution in a semibatch free radical copolymerization process (T.J. Crowley and K.Y. Choi), **Computers and Chem. Eng**., 23, 1153-1165 (1999).
24. Modeling, design and control of polymerization reactions (K.Y. Choi), *Encyclopedia of Chemical Processing*, accepted for publication (to be published in 2004).
25. Recent advances in polymer reaction engineering: Modeling and control of polymer properties (W.J. Yoon, Y.S. Kim, I.S. Kim, and K.Y. Choi), **Korean J. Chem. Eng**., 21(1), 147-167 (2004).
26. New Developments in Polymer Reaction Engineering (K.Y.Choi), Proc. of APCRE'05 (4th Asia Pacific Chemical Reaction Engineering Conference, Gyeongju, Korea), 17-18 (2005).