Available online at www.sciencedirect.com
SCIENCE DIRECT®
European Polymer Journal 41 (2005) 2893–2908
EUROPEAN POLYMER JOURNAL
www.elsevier.com/locate/europolj

Optimal control determination of MMA polymerization in non-isothermal batch reactor using bifunctional initiator

Simant R. Upreti *, Baranitharan S. Sundaram, Ali Lohi

Department of Chemical Engineering, Ryerson University, 350 Victoria Street, Toronto, Ont., Canada M5B 2K3

Received 7 April 2005; received in revised form 14 June 2005; accepted 16 June 2005
Available online 28 July 2005

Abstract

In this work, we determine the optimal control for free-radical methyl methacrylate polymerization using a bifunctional initiator in a non-isothermal batch reactor. A detailed unsteady-state model of the process is employed. Four different optimal control objectives are realized, each of which optimizes a given variable simultaneously with the specification of another. The first two objectives involve the maximization of monomer conversion in a specified operation time, and the minimization of operation time for a specified, final monomer conversion. The last two objectives involve the maximization of monomer conversion for specified, final number and weight average polymer molecular weights. The temperature of heat-exchange fluid inside reactor jacket is considered as a control function of an independent variable. To meet the specification of an optimization variable other than time, the differential model of batch process is derived in the range of specified variable. Equations are provided for Jacobian evaluations to help in the accurate solution of process model. A genetic algorithms-based optimal control method is applied to realize the four optimal control objectives. The results show that optimal control can significantly enhance the performance of the batch polymerization process.

Keywords: Optimal control; Batch reactor; Methyl methacrylate; Polymerization; Bifunctional initiation

1. Introduction

Poly(methylmethacrylate) or PMMA is a transparent thermoplastic, which is extensively used in manufacturing industry because of its high resistance to ultraviolet degradation and corrosion. PMMA is generally produced by the free radical polymerization of methyl methacrylate (MMA) in batch reactors, which are easily adaptable to production demands, and are simple to operate. The performance of batch reactors can be enhanced by optimizing various process parameters that are available for manipulation. Some of these parameters, e.g. the temperature of heat-exchange fluid, can be varied with time in an optimal fashion to achieve what is known as the optimal control of a process. In general, the optimal control of process denotes off-line determination of optimization function(s), the online application of which would achieve a desired objective. It must be noted that optimal control, also referred as dynamic optimization, is neither the usual (closed loop) process control nor optimization, which involves variables but not functions as optimization parameters.

* Corresponding author. Tel.: +1 416 979 5000x6344; fax: +1 416 979 5083.
E-mail address: supreti@ryerson.ca (S.R. Upreti).

0014-3057/$ - see front matter © 2005 Elsevier Ltd. All rights reserved.
doi:10.1016/j.eurpolymj.2005.06.019

Nomenclature

A	heat transfer area, m^2
C_p	specific heat of reactant mixture, J/g K
f	efficiency of initiator
i	concentration of initiator, mol/L
i^0	initial i, mol/L
$\underset{\sim}{i}$	normalized i
$\widetilde{I}$	initiator
J	performance index
K_{d1}	rate coefficient of chemical initiation, min^{-1}
K_{d2}	rate coefficient of chemical initiation with undecomposed radical, min^{-1}
K_p	rate coefficient of propagation, L/mol min
K_t	rate coefficient of termination, L/mol min
$K_{t,c}$	rate coefficient of termination by combination, L/mol min
$K_{t,d}$	rate coefficient of termination by disproportionation, L/mol min
$K_{tf,m}$	rate coefficient of chain transfer to monomer, L/mol min
$K_{tf,s}$	rate coefficient of chain transfer to solvent, L/mol min
$K_{tf,z}$	rate coefficient of chain transfer to inhibitor, L/mol min
m	monomer concentration, mol/L
m^0	initial m, mol/L
$\underset{\sim}{m}$	normalized m
$\underset{\sim}{m}_f$	final $\underset{\sim}{m}$
M	monomer
$\overline{M}_n$	number average molecular weight, g/mol
$\overline{M}_{n,f}$	final, specified $\overline{M}_n$, g/mol
$\overline{M}_w$	weight average molecular weight, g/mol
$\overline{M}_{w,f}$	final, specified $\overline{M}_w$, g/mol
M_m	monomer molecular weight, g/mol
P_l	dead polymer of chain length l
$\widetilde{P}_l$	dead polymer of chain length l, with one undecomposed peroxide
$\widetilde{\widetilde{P}}_l$	dead polymer of chain length l, with two undecomposed peroxide
$R^{\cdot}_{in}$	initiator radical
$\widetilde{R}^{\cdot}_{in}$	initiator radical with one undecomposed peroxide
$R^{\cdot}_l$	radical of chain length l
$\widetilde{R}^{\cdot}_l$	radical of chain length l, with one undecomposed peroxide
$R^{\cdot}_k$	radical of chain length k
$\widetilde{R}^{\cdot}_k$	radical of chain length k, with one undecomposed peroxide
s	solvent concentration, mol/L
s^0	initial s, mol/L
$\underset{\sim}{s}$	normalized s
$\widetilde{S}$	solvent
t	time, min
t_f	final, specified operation time, min
T	temperature of reactants (or reactor), °C
T^0	initial T, °C
T_{max}	upper limit to T, °C
$\underset{\sim}{T}$	normalized T
$\widetilde{T}_j$	temperature of heat exchange fluid in reactor jacket, °C
$T_{j,max}$	upper limit to T_j, °C
$T_{j,min}$	lower limit to T_j, °C
U	heat transfer coefficient for reactor wall and jacket, J/m^2 min K
V	volume of reactants inside reactor, L
V^0	initial V, L
$\underset{\sim}{V}$	normalized V
$\widetilde{X}$	monomer conversion, %
X_f	specified, final X
y_j	jth state variable
z	concentration of inhibitor, mol/L
z^0	initial z, mol/L
$\underset{\sim}{z}$	normalized z
$\widetilde{Z}$	inhibitor
$Z^{\cdot}$	inactive inhibitor radical

Greek symbols

$-\Delta H$	heat of polymerization, J/mol
λ_j	jth moment of live polymer radical
$\underset{\sim}{\lambda}_j$	normalized λ_j
$\tilde{\lambda}_j$	jth moment of live polymer radical with one undecomposed peroxide
$\underset{\sim}{\tilde{\lambda}}_j$	normalized $\tilde{\lambda}_j$
μ_j	jth moment of dead polymer
$\underset{\sim}{\mu}_j$	normalized μ_j
$\widetilde{\mu}_j$	jth moment of dead polymer with one undecomposed peroxide
$\underset{\sim}{\tilde{\mu}}_j$	normalized $\tilde{\mu}_j$