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Dynamic simulation and control of auto-refrigerated CSTR and tubular reactor for bulk styrene polymerization

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ABSTRACT

Dynamic simulation and control of a two-stage continuous bulk styrene polymerization process is developed to predict the performance of auto-refrigerated CSTR and tubular reactors. The tubular reactor is subdivided into three temperature-control jacket zones. In this paper temperature control of auto-refrigerated continuous stirred tank reactor and tubular reactor are carried out, simultaneously. Two strategies are proposed for the control of tubular reactor. At the first strategy the controlled variable is jacket temperature and in the second strategy the controlled variable is the reactor temperature at the exit of each section. The set points for polymer grade transition are obtained using optimization of reactors temperatures via genetic algorithm (GA). Simulation results show that both of the control strategies are successful but second strategy has better performance in the control of polymer properties in the presence of disturbance and model mismatch.

Keywords: Polystyrene; Auto-refrigerated reactor; Tubular reactor; Optimization; Dynamic simulation; Control process

1. Introduction

Different types of reactors are used for continuous bulk styrene polymerization such as autorefrigerated stirred reactors, stirred tubular with internal cooling coils and plug flow reactors (Chen, 1994).

Industrial reactors for continuous bulk styrene polymerization can be categorized into two groups: the back mixed reactors and the linear-flow reactors (LFR). Continuous stirred-tank reactors (CSTR) are a perfect back-mixed reactor while a tubular reactor with recycle flow is a partially back-mixed reactor. Since the LFR has a desirable radial mixing and poor back-mixing in the axial direction, these reactors can be assumed as a plug-flow reactor (PFR). One of the major problems associated with bulk styrene polymerization is the large amount of heat generation (Chen, 2000). Although using tubular reactors for polymerization seems to be more suitable due to simple design and low cost, but these reactors have some major problems, with highly exothermic reaction, high viscosity and laminar flow (Vasco de Toledo et al., 2006). Although the continuous stirred tank reactor can resolve the above mentioned drawbacks of tubular reactors but, a continuous or batch stirred tank reactor is not a good choice when we are dealing with production of variety of polymer grades. Type and number of reactors in the process depend on quality of products and number of production. Most producers are interested to use several reactors in series to provide production flexibility (Chen, 2000). The properties of a polymer are mainly determined by number and weight average molecular weights and polydispersity index, which depends on the reaction conditions. Hence, it is essential to be able to control polymerization reactors conditions for desirable polymer properties (Vasco de Toledo et al., 2005).

Many works have been done in the modeling, simulation and control of styrene polymerization reactors, but a limited number of works are performed to simulate a combination of reactors.

There are several papers about simulation of styrene polymerization in tubular reactors, for instance Costa et al. (2003), Nogueira et al. (2004), and Yoon and Choi (1996). Modeling, simulation and control of autorefrigerated CSTRs with highly exothermic reactions, including polymerization by Henderson and Cornejo (1989), Luyben (1999), Vasco de Toledo et al. (2000, 2005, 2006), and Waschler et al. (2003). Control of styrene polymerization reactors can be found in other researches such as Asteasuain et al. (2007,2006), Cetinkaya et al. (2006), Hur

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Nomenclature

A_1, A_2, A_3	gel effect coefficients
A_C	area of cross section of tubular reactor (m^2)
A_H	heat-transfer area (m^2)
C_p	specific heat of the reaction mixture ($J\,kg^{-1}\,K^{-1}$)
$Cp_{Dow,c}$	specific heat of the cold oil ($J\,kg^{-1}\,K^{-1}$)
$Cp_{Dow,h}$	specific heat of the hot oil ($J\,kg^{-1}\,K^{-1}$)
C_{Pm}	specific heat of styrene monomer ($J\,kg^{-1}\,K^{-1}$)
C_{Pw}	specific heat of the water ($J\,kg^{-1}\,K^{-1}$)
D_A	diameter of liquid return vessel (m)
D_l	diameter of liquid return pipe (m)
D_V	diameter of vapor transmitter pipe (m)
E_1	defined parameter
F_{CC}	cooling water flowrate ($kg\,s^{-1}$)
F_{CCSS}	steady-state cooling water flowrate ($kg\,s^{-1}$)
$F_{h,i}$	inlet hot oil flowrate to the ith jacket ($kg\,s^{-1}$)
$F_{c,i}$	inlet cold oil flowrate to the ith jacket ($kg\,s^{-1}$)
$F_{j,i}$	inlet total oil flowrate to the ith jacket ($kg\,s^{-1}$)
F_{in}	feed flowrate ($kg\,s^{-1}$)
F_{out}	reaction mixture flowrate from autorefrigerated reactor ($kg\,s^{-1}$)
k	thermal conductivity of the reaction mass ($W\,m^{-1}\,K^{-1}$)
k_C	proportional band (tuning constant of controller)
k_D	derivative time constant (tuning constant of controller)
k_s	thermal conductivity of styrene ($W\,m^{-1}\,K^{-1}$)
k_{ps}	thermal conductivity of polystyrene ($W\,m^{-1}\,K^{-1}$)
k_{fm0}	rate constant for chain transfer at zero conversion of styrene ($m^3\,mol^{-1}\,s^{-1}$)
k_{fm}	rate constant for chain transfer ($m^3\,mol^{-1}\,s^{-1}$)
k_i	rate constant for initiation ($m^6\,mol^{-2}\,s^{-1}$)
k_p	rate constant for propagation ($m^3\,mol^{-1}\,s^{-1}$)
k_{t0}	rate constant for termination at zero conversion of styrene ($m^3\,mol^{-1}\,s^{-1}$)
k_t	rate constant for termination ($m^3\,mol^{-1}\,s^{-1}$)
L_C	liquid flow rate from the condenser ($kg\,s^{-1}$)
L_p	liquid flow rate from the return vessel ($kg\,s^{-1}$)
L_{pss}	steady-state liquid flow rate from the return vessel ($kg\,s^{-1}$)
L_T	total length of the tubular reactor (m)
$L_{j,i}$	length of the tubular reactor at the ith section (m)
M	molar flow rate of styrene in the autorefrigerated reactor at the outlet, and at any z in the tubular reactor ($mol\,s^{-1}$)
M_n	number-average molecular weight of polystyrene ($kg\,kmol^{-1}$)
M_{nf}	number-average molecular weight of polystyrene at the output of tubular reactor ($kg\,kmol^{-1}$)
M_0	molar flow rate of monomer feed to the Autorefrigerated reactor ($mol\,s^{-1}$)
M_w	weight-average molecular weight of polystyrene ($kg\,kmol^{-1}$)
Nu	Nusselt number
P_0	vapor pressure of the monomer (Pa)
P_{cond}	pressure in condenser (Pa)
P_R	pressure in autorefrigerated reactor (Pa)
PDI	polydispersity index
PDI_f	polydispersity index at the output of tubular reactor
Pr	Prandtl number
Q	volumetric flow rate in the autorefrigerated reactor at the outlet, and at any z in the tubular reactor ($mol\,s^{-1}$)
Q_C	heat transfer rate ($J\,s^{-1}$)
r	inner radius of the tubular reactor (m)
r_0	inner radius of the jackets (m)
R	universal gas constant ($J\,mol^{-1}\,K^{-1}$)
Re	Reynolds number
t	reaction time in the batch reactor (s)
T	temperature of the reaction mixture (K)
$T_{av,i}$	average temperature of tubular reactor at length of ith section (K)
T_C	temperature of the reaction mixture in the autorefrigerated reactor (K)
T_{cond}	temperature of condenser (K)
T_{CC}	temperature of coolant in condenser (°C)
T_{CC0}	temperature of inlet coolant (°C)
T_d	set point of Autorefrigerated reactor temperature (°C)
$T_{d,i}$	set point of ith jacket temperature (°C)
$TT_{d,i}$	set point of tubular reactor temperature at length of ith section (°C)
TT_i	tubular reactor temperature at length of ith section (°C)
T_{in}	temperature of feed (°C)
$T_{Dow,c}$	temperature of the cold oil
$T_{Dow,h}$	temperature of the cold oil
$T_{j,i}$	temperature of oil in the ith jacket (°C)
T_m	temperature of vapor in condenser (°C)
T_w	wall temperature of the tubular reactor (K)
h	overall heat transfer coefficient of the tubular reactor ($W\,m^{-2}\,K^{-1}$)
U_c	overall heat transfer coefficient of condenser ($W\,m^{-2}\,K^{-1}$)
u_{Dow}	velocity of oil at the inlet of jacket ($kg\,m^{-3}$)
V_{tube}	volume of cooling water in condenser (m^3)
V_c	volume of autorefrigerated reactor holdup (m^3)
v_P	polymer volume fraction
V_V	effective volume of vapor space in condenser (m^3)
W_M	molecular weight of styrene (kg/mol)
W_v	vapor flowrate from the autorefrigerated reactor ($kg\,s^{-1}$)
w_i	weighting factors of optimization objective functions
X	conversion of styrene
X_f	conversion of styrene at the output of tubular reactor
Y_i	optimization objective functions
z	length along the axial direction in the tubular reactor (m)

Greek letters

ΔH	heat of polymerization ($J\,kg^{-1}$)
ΔH_V	latent heat of vaporization ($J\,kg^{-1}$)
β	defined parameter
λ_k	kth moment of radicals (k = 0, 1, 2)