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Modified two-phase model with hybrid control for gas phase propylene copolymerization in fluidized bed reactors

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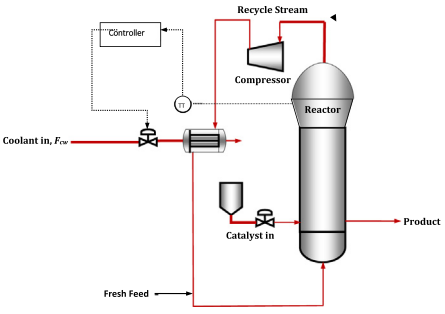
HIGHLIGHTS

- The two-phase model was modified by incorporating it with solid entrainment.
- The proposed modified two-phase model was validated with actual plant data.
- The hybrid controller performed better compared to the FLC and PID controllers.

GRAPHICAL ABSTRACT



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ABSTRACT

In order to explore the dynamic behavior and process control of reactor temperature, a modified two-phase dynamic model for gas phase propylene copolymerization in a fluidized bed reactor is developed in which the entrainment of solid particles is considered. The modified model was compared with well-mixed and two-phase models in order to investigate the dynamic modeling response. The modified two-phase model shows close dynamic response to the well-mixed and two-phase models at the start of the polymerization, but begins to diverge with time. The proposed modified two-phase and two-phase models were validated with actual plant data. It was shown that the predicted steady state temperature by the modified two-phase model was closer to actual plant data compared to those obtained by the two-phase model. Advanced control system using a hybrid controller (a simple designed Takagi–Sugeno fuzzy logic controller (FLC)) integrated with the adaptive neuro-fuzzy inference system (ANFIS) controller was implemented to control the reactor temperature and compared with the FLC and conventional PID controller. The results show that the hybrid controller (ANFIS and FLC controller) performed better in terms of set point tracking and disturbance rejection compared to the FLC and conventional PID controllers.

1. Introduction

Polymerization is an important process in the petrochemical and polymer industries. It is a complicated process with complex chemical kinetics and physical mechanisms [1,2], thus making its modeling and control a very challenging task. There are a number of papers about successful modeling and controlled of polymerization processes [3–19]. However, few attempts have been reported on modeling and the control of polypropylene (PP) copolymerization in fluidized bed reactors (FBR). Copolymerization is a process in the production of polymers from two (or more) different types of monomers which are linked in the same polymer chain.

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Nomenclature

A	cross sectional area of the reactor (m^2)
$ALEt_3$	triethyl aluminum cocatalyst
Ar	Archimedes number
B_i	moles of reacted monomer of type i bound in the polymer in the reactor
C_{pi}	specific heat capacity of component i (J/kg K)
C_{pg}	specific heat capacity of gaseous stream (J/kg K)
$C_{p,pol}$	specific heat capacity of product (J/kg K)
C_{pMi}	specific heat of component i (J/kmol K)
d_b	bubble diameter (m)
d_{b0}	initiate bubble diameter (m)
d_p	particle diameter (m)
d_p^*	dimensionless particle size
D_g	gas diffusion coefficient (m^2/s)
D_t	reactor diameter (m)
F_{cat}	catalyst feed rate (kg/s)
f_i	fraction of total monomer in the reactant gas which is monomer M_I
g	gravitational acceleration (m/s^2)
H	height of the reactor (m)
H_{be}	bubble to emulsion heat transfer coefficient (W/m^3 K)
H_{bc}	bubble to cloud heat transfer coefficient (W/m^3 K)
H_{ce}	cloud to emulsion heat transfer coefficient (W/m^3 K)
H_2	hydrogen
I_m	impurity such as carbon monoxide
i	monomer type
J	active site type
kf (j)	formation rate constant for a site of type j
kfh_i (j)	transfer rate constant for a site of type j with terminal monomer M_I Reacting with hydrogen
kfm_i (j)	transfer rate constant for a site of type j with terminal monomer M_i Reacting with monomer M_K
kfr_i (j)	transfer rate constant for a site of type j with terminal monomer M_i Reacting with $Aiet_3$
kfs_i (j)	spontaneous transfer rate constant for a site of type j with terminal monomer M_I
k_g	gas thermal conductivity (W/m K)
kh_i (j)	rate constant for reinitiation of a site of type j by monomer M_I
kh_r (j)	rate constant for reinitiation of a site of type j by cocatalyst
ki_i	rate constant for initiation of a site of type j by monomer M_I
kp_{ik} (j)	propagation rate constant for a site of type j with terminal monomer Mire acting with monomer M_K
kp_{Ti}	propagation rate constant (m^3/kmol s)
K_b	elutriation constant in bubble phase (kg m^2 s^{-1})
K_{be}	bubble to emulsion mass transfer coefficient (s^{-1})
K_{bc}	bubble to cloud mass transfer coefficient (s^{-1})
K_{ce}	cloud to emulsion mass transfer coefficient (s^{-1})
K_e	elutriation constant in emulsion phase (kg m^2 s^{-1})
mw_i	molecular weight of monomer i (g/mol)
M_i	concentration of component i in reactor (kmol/m^3)
$[M_i]_{in}$	concentration of component i in the inlet gaseous stream
N (j)	potential active site of type j
N ($0, j$)	uninitiated site of type j produced by formation at sites of type j reaction
$N_d(j)$	spontaneously deactivated site of type j
$N_{d,IH}(0, j)$	impurity killed sites of type j
N_H	uninitiated site of type j produced by transfer to hydrogen reaction
$N_j(r, j)$	living polymer molecule of length r, growing at an active site of type j , with terminal monomer m_i
Q (r ,j)	dead polymer molecule of length r produced at a site of type j
P	pressure (Pa)
PP	polypropylene
R	number of units in polymer chain
R_i	instantaneous consumption rate of monomer i (kmol/s)
R_p	production rate (kg/s)
R_v	volumetric outflow rate of polymer (m^3/s)
Re_{mf}	Reynolds number of particles at minimum fluidization condition
T	time (s)
T	temperature (K)
T_{in}	temperature of the inlet gaseous stream (K)
T_{ref}	reference temperature
U_b	bubble velocity (m/s)
U_{br}	bubble rise velocity (m/s)
U_e	emulsion gas velocity (m/s)
U_0	superficial gas velocity (m/s)
U_{mf}	minimum fluidization velocity (m/s)
U_t	terminal velocity of falling particles (m/s)
U_t^*	dimensionless terminal falling velocity coefficient
V	reactor volume (m^3)
V_p	volume of polymer phase in the reactor (m^3)
W_b	weight of solids in the bubble phase (kg)
W_e	weight of solids in the emulsion phase (kg)
Y (n, j)	Nth moment of chain length distribution for living polymer produced at a site of type j
X (n, j)	Nth moment of chain length distribution for dead polymer produced at a site of type j

Greek letters

ΔH_R	heat of reaction (J/kg)
ε_b	void fraction of bubble for Geldart B particles
δ	volume fraction of bubbles in the bed
ε_e	void fraction of emulsion for Geldart B particles
ε_{mf}	void fraction of the bed at minimum fluidization
μ	gas viscosity (Pa s)
ρ_g	gas density (kg/m^3)
ρ_{pol}	polymer density (kg/m^3)
$\varnothing_s$	sphericity for sphere particles

Subscripts and superscripts

1	propylene
2	ethylene
I	component type number
In	inlet
J	active site type number
mf	minimum fluidization
pol	polymer
ref	reference condition

In the industrial PP copolymerization, the most commonly used reactor configuration is the FBR [20–22]. With this reactor configuration, shown schematically in Fig. 1, catalyst (Ziegler–Natta and triethyl aluminum) and reactants (propylene, ethylene and hydrogen) are fed continuously into the reactor with nitrogen as the carrier gas. Conversion of monomers is low for a single pass through the FBR and it is necessary to recycle the unreacted monomers. Unreacted monomer gases are removed from the top of the reactor. A cyclone is used to separate the solid particles (i.e., catalyst and low molecular weight polymer particles) from the gas in order to