DYNAMIC OPTIMIZATION OF LOW DENSITY POLYETHYLENE PRODUCTION IN TUBULAR REACTOR UNDER THERMAL SAFETY AND FOULING RESISTANCE CONSTRAINTS

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LIST OF ABBREVIATIONS

CH_2	Methylene
CP	Compression Power
CPU	Computer processor unit
CTA	Chain transfer agent
CVI	Control vector iteration
CVP	Control vector parameterization
DAE	Differential algebraic equation
FD	Finite Difference
GDP	Gross domestic product
HJB	Hamilton–Jacobi–Bellman
HP	High pressure
IDP	Iterative dynamic programming
IVP	Initial value problem
JG	Jumping gene
LDPE	Low density polyethylene
LP	Low pressure
MFI	Melt flow index
Me	Methyl
MW	Molecular weight
NCO	Necessary conditions optimality

NLP	Non-linear programming
NSGA-II	Non-dominated sorting genetic algorithm
OC	Orthogonal collocation
ODE	Ordinary differential equation
OI	Oxygen initiation
PCLDPE	PETRONAS Chemicals Sdn. Bhd.
PMP	Pontryagin’s Minimum Principle
PI	Peroxide initiation
PRO	Chain propagation
QN	Quasi-Newton
R	Regression
Re	Reynolds number
SCB	Short chain branches
SP	Side products
SQP	Sequential quadratic programming
SSE	Sum square of error
TC	Termination by combination
TD	Termination by disproportionation
TDT	Thermal degradation
THI	Thermal initiation

TM	Chain transfer to monomer
TP	Chain transfer to polymer
TS	Chain transfer to solvent
TPBVP	Two-point boundary value problem
V_i	Vinyl group
V_{id}	Vinylidene group
XM	Monomer conversion
ZHA	Zurich Hazard Analysis

LIST OF SYMBOLS

A_i	Inside pipe area	cm^2
A_o	Outside pipe area	cm^2
$A_{x,i}$	Frequency factor of x process with i-th number	l/s; cm^3/mol.s
bb	Backbiting	-
$C_{x,i}$	Concentration *x* component with *i*-th number	mol/cm^3
D	Diameter	cm
D_{in}	Inside diameter of reactor,	cm
D_e	Equivalent diameter	cm
D_{Ji}	Inner diameter of jacket wall	cm
$E_{x,i}$	Activation energy of *x* process with *i*-th number	cal/mol
e	Ethylene	-
F_x	Mass flow rate of *x* component	kg/h
f_x	Initiation efficiency of *x*-th peroxide	-
f_r	Fanning friction factor	-
G_c	Jacket volumetric flux rate	$cm^3.cm^{-2}.s^{-1}$
h_i	Reactor side heat transfer coefficient	cal/cm^2.s.K
h_o	Outside film heat transfer coefficient	cal/cm^2.s.K
h_w	Heat transfer coefficient of reactor wall	cal/cm^2.s.K
$K_{d,i}$	Rate constant of peroxide initiation with *i*-th number	l/ s

K_{th}	Rate constant of monomer thermal initiation,	l/ s
K_p	Rate constant of propagation,	l/mol.s
K_{td}	Rate constant of termination by thermal degradation	l/mol.s
K_{thd}	Rate constant of termination by disproportionation	l/mol.s
K_{trm}	Rate constant of chain transfer to monomer	l/mol.s
K_{trp}	Rate constant of chain transfer to polymer	l/mol.s
K_{trs}	Rate constant of chain transfer to solvent	l/s
K_{β}	Rate constant of β-scission to secondary radical	l/s
$K_{\beta 1}$	Rate constant of β -scission to tertiary radical	l/s
K_m	Thermal conductivity of reaction mixture	cal/cm.s.K
K_w	Thermal conductivity of reactor wall	cal/cm.s.K
K_J	Thermal conductivity of jacket water	cal/cm.s.K
L	Length of reactor [IE2:S,1]	cm
I	Initiator	-
M	Monomer	-
m	Reaction mixture	-
$\dot{m}_x$	Mass flow rate of x-th component	g/s
Nu	Nusselt number	-
P	Reaction pressure	Bar
pe	Polyethylene	-

P_{in}	Reactor inlet pressure	Bar
Pr	Prandtl number	-
p_x	Input variable of *x* component	
$P(x)$	Dead polymer with chain length *x*	-
Q	Heat transfer	Joules
r_o	Outside radius of tubular reactor area	cm
r_i	Inside radius tubular reactor area	cm
R	Ideal gas constant	cal/mol.K
$R(x)$	Live radical with chain length *x*	-
Re	Reynolds number	-
R_f	Fouling resistance	cm^2. s.K /cal
R_{f_m}	Maximum fouling resistance	cm^2. s.K /cal
S	Solvent	-
T	Temperature	◦C
T_{in}	Reactor inlet temperature	◦C
T_J	Reactor jacket temperature	◦C
T_{max}	Maximum reaction temperature	◦C
T_{c_m}	Maximum reaction critical temperature	◦C
T_{c_p}	Peak critical temperature	◦C
U	Overall heat transfer coefficient,	cal/cm2.s.K
u_x	Control variable of x component	

v	Linear velocity of the reaction mixture in reactor	cm/s
V_i	Vinyl group	
V_{id}	Vinylidene group	
V_m	Specific volume of monomer	cm^3/g
V_p	Specific volume of polymer	cm^3/g
$\Delta V_{x,i}$	Activation volume of x component with i-th number	l/mol
X_M	Monomer conversion	%
z	Axial distance from reactor inlet	cm

Greek Symbols

ΔH_p	Heat of polymerization	cal/mol
ΔT_{ad}	Adiabatic temperature rise	℃
ΔT_{lm}	Log mean temperature	-
λ_x	x-th moment of the live polymer radical	-
μ_x	x-th moment of dead polymer radical	-
β	Beta scission of secondary radical	-
$\beta 1$	Beta scission of tertiary radical	-
Ø	Diameter	
ρ	Reaction mixture density	g/cm^3
η_s	Viscosity of reactant mixture	Poise
η_r	Relative viscosity of monomer	Poise

η_o	Viscosity of monomer	Poise
η_s	Viscosity of reaction	Poise
w_m	Weight fraction of monomer	-
w_p	Weight fraction of polymer	-