ONLINE DYNAMIC OPTIMIZATION STUDIES OF CATALYZED ESTERFICATION OF PROPIONIC ANHYDRIDE WITH 2-BUTANOL IN THE PRESENCE OF DISTURBANCE AND UNCERTAINTY

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by

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LIST OF ABBREVIATIONS

ADP	Approximate dynamic programming
CKF	Cubature Kalman filter
CPU	Computation time
CVI	Control vector iteration
CVP	Control vector parameterization
DAE	Differential algebraic equation
DDKF	Divided difference Kalman filter
DE	Differential evolution
DM	Dual mode
DOF	Degree of freedom analysis
EKF	Extended Kalman filter
Em,	Specified percent of the desired reactor temperature
EnKF	Ensemble kalman filter
ELO	Extended Luenberg observer
fmincon	Find minimum of constrained nonlinear multivariable function
GHKF	Gauss–Hermite Kalman filter
Hi	High
HJB	Hamilton Jacobi Bellman
HS	Hybrid strategy

IAE	Integrated absolute error
IDP	Iterative dynamic programming
IVP	Initial value problem
L	Low
MHE	Moving horizon kalman estimator
Me	Medium
MS	Multiple-shooting
NCO	Necessary conditions optimality
NLP	Nonlinear programming problem
NMPC	Nonlinear model predictive control
OC	Orthogonal collocation
ODE	Ordinary differential equation
pdf	Probability density function
PID	Proportional-integral-derivative
PL	Period value
PMP	Pontryagin's Minimum Principle
RLS	Recursive Least Square
RMSE	Root mean square error
SQP	Sequential quadratic programming
sUKF	Scaled unscented Kalman filter
SUNDIALS	Suite of Nonlinear and Differential/Algebraic equation Solvers

TC	Full cooling
TD1	Time delay
TD2	Time delay
TH	Full heating
TolFun	Tolerance of objective function
TolX	Tolerance of searching step
TPBVP	Two-point boundary value problem
UKF	Unscented Kalman Filter
UT	Unscented transformation

LIST OF SYMBOLS

Symbol	Description	Unit
A	Heat exchange area	dm^2
C_A	Concentration of 2-butanol	M
C_B	Concentration of propionic anhydride	M
C_C	Concentration of propionic acid	M
C_{cat1}	Concentration of sulphuric acid	M
C_{cat2}	Concentration of mono-butyl sulphuric acid	M
C_j	Heat capacity of solution in jacket	J/kg K
C_p	Heat capacity of solution in reactor	J/kg K
CR	Cross over	-
e_i	Unit vector to the direction of coordinate axis	-
E_{ai}	Energy activation constant	J mol^{-1}
f	Process dynamic model	-
F	Set discretized equations of objective function	-
Fa	Scalar multiplication	-
F_j	Jacket flowrate	L/s
Fo	Feed flowrate,	L/s
G	Set discretized equations of equality constraints	-
G_k	One generation of NP	-
g	Inequality design constraint vector	-
H	Set discretized equations of inequality constraints	-
ΔHr	Heat of reaction	J mol^{-1}
h	Equality design constraint vector	-

h_M	Measurement model function	-
K	Kalman gain	-
k_{0i}	Frequency factor	L mol^{-1} s^{-1}
M	Number of control collocation	-
m_0	Mean the states	-
n	Number of sigma points	-
n_C	Number of cubature points	-
N	Number of states collocation	-
NP	Number of members in a population	-
n_A	Molar ratio of propionic anhydride	-
n_B	Molar ratio of 2-butanol	-
n_C	Molar ratio of propionic acid	-
$xcat1$	Molar fraction of sulphuric acid	-
P_i	Prices of i	RM/min
P_0	Initial covariance of the states	-
P_x	Covariance of states P_x	-
P_y	Covariance of measurements P_y	-
P_{xy}	Covariance of cross covariance of P_{xy} .	-
Q	Process noise covariance	-
p_i	Parameter	-
p^L, p^U	Time independent parameter bounds.	-
R	Measurement noise covariance	-
$r(j)$	jth evaluation of a uniform random generator number	-

S	Square root of positive definite covariance matrix	-
SC	Convergence criteria	-
t_f	Final time	min
t_{feed}	Feed time	min
Δt_k	Time interval	-
t_n	Number interval time	-
T_{feed}	Feed temperature	K
T_j	Jacket temperature	K
T_{jin}	Inlet jacket temperature	K
U	Heat exchange coefficient	W/dm^2 K
$u(t)$	Vector of control (decision) variables	-
$u(t)^L$, $u(t)^U$	Control (decision) profile bounds	-
$u_i^{G\,k}$	Trial vector	-
Vj	Volume of jacket	-
v	Interval length of interpolation	-
v_i^{Gk}	Mutated vector	-
$x(t)$	Vector of state (measurable) variables	-
$\overline{x}$	Mean of states	-
X_i	Sigma-point	-
yk	Measurement function	-
y	Actual value	-
$\hat{y}$	Simulated value of y	-
$\overline{y}$	Mean of the y values	-

Greek letters

θ	Parameter vector of identification	-
∇	Specified Jacobian function	-
ρ	the density of solution in reactor	kg/L
ρ_j	the density of jacket solution	kg/L
σ	Radius of the reactor, dm	-
$\Im(.)$	Optimization criterion	-
$\wp(.)$	Component of objective function evaluated at final conditions	-
ε	Small nonnegative constant	-
$\kappa^i(.)$	Inequality path constraint	-
$\kappa^e(.)$	Equality path constraint	-
μ^k	Control polynomial	-
μ_0^k	Initial control collocation	-
μ^L, μ^U	Control bounds for each collocation points	-
ω	Decision variables	-
ω_i^{Gk}	Parent vector	-
χ^k	Lagrange Interpolating Polynomial	-
$\delta_{i,q}$	Kronecker delta.	-
η^L, η^U	Bounds for each collocation points	-
η^k	Collocation coefficients for the state profiles	-
ζ_0^k	Multiple shooting nodes on the same interval time	-

$[\zeta_0^L, \zeta_0^U]$	Bound of MS nodes	-
α^n	Relaxation factor	-
α	Scaling parameters	-
β	Scaling parameters	-
κ	Scaling parameters	-
λ	Scaling parameter	-

KAJIAN PENGOTIMUMAN DINAMIK DALAM TALIAN TERHADAP PENGESTERAN BERMANGKIN PROPIONIK ANHIDRIDA DENGAN 2-BUTANOL DALAM KEWUJUDAN GANGGUAN DAN KETIDAK PASTIAN

ABSTRAK

Dalam kehadiran gangguan dan ketidakpastian yang ketara, loji boleh menghadapi masalah dengan produk luar spesifikasi yang menyebabkan kerugian yang ketara dalam keuntungan. Bagi mengatasi masalah tersebut, pengoptimuman dinamik dalam talian merupakan strategi yang terbaik untuk dilaksanakan. Oleh kerana itu, dalam kajian ini, strategi pengoptimuman dinamik dalam talian yang mudah iaitu pengoptimuman berasaskan lata bersyarat telah dicadangkan.

Dalam kerangka pengoptimuman berasaskan lata bersyarat yang dicadangkan, pengoptimuman semula dan masalah kawalan diselesaikan secara berasingan dalam dua lapisan. Masalah kawalan diselesaikan dengan menggunakan pengawal PID penyesuaian. Manakala, penyelesaian masalah melalui pengoptimuman semula merangkumi kemaskini bersyarat dan mekanisma pengoptimuman semula dinamik. Satu pencetus mudah untuk mengaktifkan pengoptimuman semula dinamik diperkenalkan apabila sisihan ± 5% dari pernukaran berlaku dalam loji yang bertindak sebagai kemaskini bersyarat. Mekanisma pengoptimuman semula dinamik yang dicadangkan turut terdiri daripada penganggar dan pengoptimum semula dinamik. Penganggar terbenam adalah untuk memberi maklumat penuh tentang keadaan

pembolehubah utama yang terkini dan input pembolehubah kawalan yang diperlukan dalam pengoptimuman semula dinamik untuk mengira trajektori optimal yang baru.

Bagi menentukan teknik pengoptimuman dinamik yang paling efektif, satu kajian pengoptimuman dinamik secara luar talian telah dijalankan. Lima teknik pengoptimuman dinamik iaitu control vector parameterization (CVP), orthogonal collocation (OC), multiple shooting (MS), differential evolution (DE) and hybrid strategy (HS) telah dilaksanakan untuk mengoptimumkan tiga fungsi objektif yang berbeza, iaitu memaksimumkan penukaran, meminimumkan masa akhir dan memaksimumkan keuntungan operasi. Trajektori optimal yang paling efektif yang telah dicapai adalah yang diperolehi daripada teknik OC dalam memaksimumkan keuntungan. Nilai optimum penukaran, masa akhir dan keuntungan yang diperolehi daripada teknik OC adalah 99.9%, 60 min dan RM12.84/min.

Sementara itu, untuk menentukan teknik penganggar yang paling berkesan, penganggar terbitan bebas, iaitu Penyaring Kalman Tidak Berbau Berskala (sUKF), Penyaring Kalman Perbezaan Terbahagi (DDKF) dan Penyaring Kalman Kekubusan (CKF) telah dinilai dalam enam kes yang berlainan. Hasil kajian telah menunjukkan bahawa CKF ialah penganggar yang paling berkesan kerana ia boleh memberikan anggaran dengan darjah ketepatan yang tertinggi dengan RMSE terendah untuk kebanyakan kes yang diuji.

Akhirnya, strategi pengoptimuman dinamik dalam talian yang dicadangkan itu telah dilaksanakan dan dinilai dalam pengesteran bermangkin Propionik Anhidrida dengan 2-Butanol. Apabila gangguan yang ketara dan ketidaktentuan berlaku, strategi pengoptimuman dinamik dalam talian yang dicadangkan telah berjaya menjana trajektori optimum yang baru untuk mengekalkan penukaran dalam julat yang dikehendaki (dalam-specifikasi).