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เครื่องปฏิกรณ์อะเซทิลีนไฮโดรจีเนชัน



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PROCESS MODELING, DYNAMIC DATA RECONCILIATION AND CONTROL
OF ACETYLENE HYDROGENATION REACTORS

Miss Tarawipa Saurod

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for the Degree of Master of Engineering in Chemical Engineering

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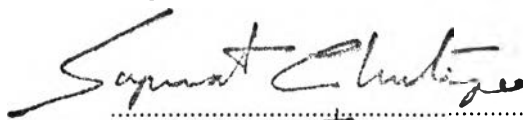
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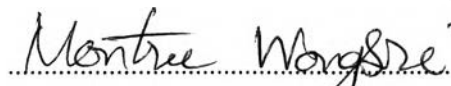
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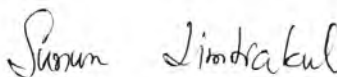

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งานวิจัยนี้เสนอแบบจำลองทางคณิตศาสตร์ของกระบวนการอะเซทีลีนไฮโดจีเนชัน โดยเขียนบนโปรแกรมสปีดอัป (SPEEDUP) ซึ่งเป็นโปรแกรมสภาวะจำลองแบบไดนามิก เครื่องปฏิกรณ์อะเซทีลีนไฮโดจีเนชันถูกจำลองด้วยชุดลำดับเครื่องปฏิกรณ์แบบถังกวนต่อเนื่อง ข้อมูลที่นำมาใช้ในการสร้างแบบจำลองได้จากข้อมูลโรงงานที่ผ่านการปรับให้สอดคล้องของข้อมูลด้วยตัวแปรเกินจากสมการสมดุลมวลสารและพลังงาน จำนวนชุดลำดับเครื่องปฏิกรณ์แบบถังกวนต่อเนื่องที่เหมาะสมเท่ากับยี่สิบถัง ซึ่งให้ผลการเปรียบเทียบการเปลี่ยนแปลงของอุณหภูมิภายในเครื่องปฏิกรณ์ และผลการทำนายค่าความเข้มข้นของอะเซทีลีนกับข้อมูลโรงงานเหมือนที่สุด สามารถเขียนชุดสมการการเกิดปฏิกิริยาของกระบวนการได้หกแบบ และทำการเลือกชุดสมการที่เหมาะสมจากการพิจารณาเปรียบเทียบผลการทำนายจากแบบจำลองกับข้อมูลโรงงาน พบว่าชุดสมการที่เขียนจากกระบวนการเกิดปฏิกิริยาแบบที่ขึ้นกับความเข้มข้นไฮโดเจนกำลังหนึ่ง, ไฮโดเจนมีการแตกตัวก่อนเกิดปฏิกิริยา, ผลิตภัณฑ์ที่เกิดไม่ถูกดูดซับบนตัวเร่งปฏิกิริยา, และความสามารถของตัวเร่งปฏิกิริยาขึ้นกับผลรวมของปริมาณอะเซทีลีนที่เข้าระบบ ให้ผลเปรียบเทียบผลการทำนายจากแบบจำลองกับข้อมูลโรงงานดีที่สุด

การปรับให้สอดคล้องของข้อมูลแบบไดนามิกที่สร้างใช้สมการสมดุลมวลสารและพลังงานเป็นเงื่อนไขของการปรับ พบว่าค่าเวลาย้อนหลังที่ใช้ในการปรับข้อมูลที่ดีที่สุดเท่ากับสิบเท่าของช่วงเวลาในการเก็บข้อมูล สามารถลดค่าเบี่ยงเบนมาตรฐานของข้อมูลโรงงานได้ 40-70%, สามารถลดค่าเบี่ยงเบนมาตรฐานของข้อมูลที่ได้จากการจำลองได้ 90% และทดสอบโปรแกรมด้วยการใช้ข้อมูลที่มีสัญญาณรบกวน และข้อมูลที่ปรับให้สอดคล้องแล้วในการประมาณค่าตัวแปรของแบบจำลองใหม่ ผลการทำนายอุณหภูมิของแบบจำลองที่ใช้ข้อมูลที่ปรับให้สอดคล้องแล้วคาดเคลื่อนไป 0.16% และผลการทำนายอุณหภูมิของแบบจำลองที่ใช้ข้อมูลมีสัญญาณรบกวนคาดเคลื่อนไป 2.13%

แบบจำลองทางคณิตศาสตร์ของกระบวนการอะเซทีลีนไฮโดจีเนชันที่สร้างถูกนำมาใช้ในการออกแบบระบบควบคุมแบบไดนามิกเมทริก และการทดสอบผลการควบคุม ตัวควบคุมที่ดีที่สุดคือ ตัวควบคุมที่มีค่าขั้นการทำนายผลล่วงหน้าเท่ากับสามเท่าของช่วงเวลาในการเก็บข้อมูล และมีค่าขั้นการควบคุมสำหรับผลในอนาคตเท่ากับสองเท่าของช่วงเวลาในการเก็บข้อมูล ตัวควบคุมที่ได้มีประสิทธิภาพในการควบคุมกระบวนการ ผลการควบคุมให้ค่าผลรวมความคาดเคลื่อนจากค่ากำหนด (set point) เท่ากับ 3.33% ของค่าจากตัวควบคุมแบบพีไอดี ช่วยลดปริมาณการสูญเสียเอทรีลีนได้ 80-98% เมื่อเทียบกับตัวควบคุมแบบพีไอดี

ภาควิชา วิศวกรรมเคมี
สาขาวิชา วิศวกรรมเคมี
ปีการศึกษา 2541.....

ลายมือชื่อนิสิต ธรวิภา เสือรอด
ลายมือชื่ออาจารย์ที่ปรึกษา [ลายมือ]
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KEY WORD: ACETYLENE HYDROGENATION / DATA RECONCILIATION / PROCESS MODELING

TARAVIPA SAUROD : PROCESS MODELING, DYNAMIC DATA RECONCILIATION AND CONTROL OF ACETYLENE HYDROGENATION REACTORS. THESIS ADVISOR : MONTREE WONGSRI, D.Sc., THESIS CO-ADVISOR : PAISAN KITTISUPAKORN, Ph. D., 245 pp. ISBN 974-639-506-8

The mathematical model of the industrial acetylene hydrogenation process is developed and formulated on SPEEDUP program which is a dynamic simulation program. The fixed bed acetylene hydrogenation reactor is modeled as the CSTRs connected in series. The data using in modeling, the actual data from the ethylene plant are reconciled first using material and energy balance redundancy. The best number of CSTRs is found to be twenty which is given the best agreement in temperature profile and the output acetylene concentration of each bed. The six kinetic models with the different reaction mechanism are derived and selected for the best one by comparing their predicted outputs with the actual data. The kinetic model which its reaction mechanism are the reaction rate depends on the first order of H_2 , H_2 break to free atoms before react, the product are not adsorbed on the catalytic surface, and the catalytic activity depend on the accumulation of the inlet acetylene, gives the best agreement of the predicted result with the actual data.

The dynamic data reconciliation using the material and energy balance constrains of process is performed. The best time history horizon is found to be ten steps. It can reduce the standard deviation of the actual data and the simulated data to about 40-70% and 90% in series. The noised data and the reconciled data are then used to obtain the new parameters of the model, i.e. the reconstruction of the model. The noised model gives 2.13% of temperature error and the reconciled model gives 0.16% of temperature error.

The obtained model of acetylene hydrogenation reactor is used to demonstrate the design, implementation, and performance of Dynamic Matrix controller by simulation. The Dynamic Matrix controller is tuned for best performance with the control horizon, $U=2$, the prediction horizon, $V=3$. The integral error of Dynamic Matrix controller is only 3.33 % of the PID controller's error. The ethylene loss is reduced by 80-98% by using Dynamic Matrix controller over PID controller. The degree of the benefit of using the Dynamic Matrix Control is illustrated.

ภาควิชา..... ภาควิชาวิศวกรรมเคมี

สาขาวิชา..... วิศวกรรมเคมี

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ลายมือชื่ออาจารย์ที่ปรึกษา..... อ.นพ

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NOMENCLATURE

C_{total}	=	the total concentration of sites, sites/weight
C_v	=	the concentration of free sites
$C_{A,S}$	=	the A specie adsorbed sites
$C_{B,S}$	=	the B specie adsorbed sites
C_{Ac}	=	acetylene concentration, mol/M ³
C_{Eth}	=	ethylene concentration, mol/M ³
C_{H_2}	=	hydrogen concentration, mol/M ³
C_{MA}	=	methyl acetylene concentration, mol/M ³
C_{PD}	=	propadiene concentration, mol/M ³
C_{CO}	=	carbonmonoxide concentration, mol/M ³
C_E	=	ethane concentration, mol/M ³
C_{Pr}	=	propylene concentration, mol/M ³
C_{Me}	=	methane concentration, mol/M ³
C_{BD}	=	butadiene concentration, mol/M ³
C_p	=	heat capacity of feed stream
C_m	=	heat capacity of the reacting system including catalyst
D	=	fluid density
f	=	differential equation constraints
F_i	=	outlet volumetric flow rate of the feed at i th stage, M ³ /hr
g	=	inequality constraints including simple upper and lower bounds
h	=	algebraic equality constraints
H	=	the history horizon time
Hr_{Ac}	=	heat of acetylene hydrogenation
Hr_{Eth}	=	heat of ethylene hydrogenation
Hr_{MA}	=	heat of methyl acetylene hydrogenation

$H_{r_{PD}}$	=	heat of propadiene hydrogenation
i	=	i th stage
K_{Ac}	=	adsorption equilibrium constant of acetylene
K_{Eth}	=	adsorption equilibrium constant of ethylene
K_{H_2}	=	adsorption equilibrium constant of hydrogen
K_{CO}	=	adsorption equilibrium constant of carbonmonoxide
k	=	reaction rate constant
M_i	=	mass of reacting system at i th stage including catalyst
N_p	=	the degrees of freedom
N_v	=	the total number of variables (unspecified inputs plus outputs)
N_E	=	the number of independent equations
NV	=	the number of variables in the type section
NI	=	the number of input stream variables
NE	=	the number of equations
NS	=	the number of set variables that should expect to set for a simulation.
$NDYN$	=	the number of the dynamic run
NSS	=	the number of the steady state run
NT	=	the number of the time step of the actual input-output data
NM	=	the number of the the output variables
P_i	=	the elements of the projection vector
Q_i	=	heat loss at i^{th} stage
R_{Ac}	=	rate of acetylene hydrogenation
R_{Eth}	=	rate of ethylene hydrogenation
R_{MA}	=	rate of methyl acetylene hydrogenation
R_{PD}	=	rate of propadiene hydrogenation
R_{CO}	=	adsorption rate of carbonmonoxide
t_c	=	the current time

Δt	=	time step size
$t_{1/2}$	=	the half-life time
T	=	temperature
U	=	the control horizon
V	=	the prediction horizon
\mathbf{V}	=	the variance-covariance matrix
V_r	=	volume of one CSTR stage, M^3
w	=	the weight fraction
Y	=	discrete measurement
y	=	estimate function
y^L	=	lower limit of y
y^U	=	upper limit of y
y_j	=	the estimated value of estimation equation at time t_j
Y_j	=	the measured value at time t_j
z	=	the actual output data
\hat{z}	=	the predic output
θ	=	the catalyst activity
ϕ	=	objective function equation
σ	=	measurement noise standard deviation