혼합모델을 이용한 스타이렌 모노머 반응기의 최적화

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Dynamic Optimization of for a Styrene Monomer Reactor Using Hybrid Model

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Introduction

The rigorous styrene monomer(SM) reactor model is highly valuable because it can be used in optimizing the current operation, which has high operating cost due to the use of a large amount of expensive high-pressure steam. In this study, a PC based simulator for a styrene monomer reactor has been introduced. The mathematical kinetic model for an adiabatic radial-flow styrene monomer reactor has been used as a first principle model. A neural network model has been developed for the catalyst deactivation model. Consequently these two models are combined for simulation and optimization of the SM reactor. Some examples are tested with this simulator and the potential usages of this program are investigated.

System Description

Fig. 1. shows the adiabatic radial flow reactor which is the target process in this study. In this SM reactor, three major competing reactions((1)~(3)) and three side reactions((4)~(6)) are known.

$$C_6H_5CH_2CH_3 \leftrightarrow C_6H_5CHCH_2 + H_2 \quad (1)$$

$$C_6H_5CH_2CH_3 \rightarrow C_6H_6 + C_2H_4 \quad (2)$$

$$C_6H_5CH_2CH_3 + H_2 \rightarrow C_6H_5CH_3 + CH_4 \quad (3)$$

$$H_2O + \frac{1}{2}C_2H_4 \rightarrow CO + 2H_2 \quad (4)$$

$$H_2O + CH_4 \rightarrow CO + 3H_2 \quad (5)$$

$$H_2O + CO \rightarrow CO_2 + H_2 \quad (6)$$

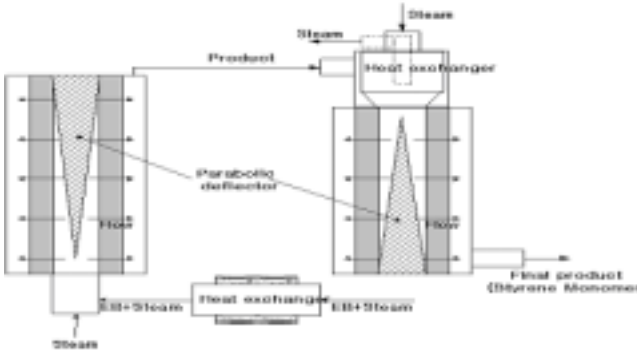


Fig. 1 Current adiabatic radial flow reactor

Hybrid Modeling of SM Reactor

1. First Principle Model

The kinetic model for the reactions is shown below.

Reaction amounts in reaction j is f_j.

$$f_1 = \Phi k_1 (P_{EB} - P_{SM}P_{H2}/K_P),\ f_2 = \Phi k_2 P_{EB},\ f_3 = \Phi k_3 P_{EB}P_{H2},\ f_4 = k_4 P_{H_2O}P_{ET},\ f_5 = k_5 P_{H_2O}P_{ME},$$

$$f_6 = k_6 \frac{P}{T^3} P_{H_2O}P_{CO} \quad (7)$$

Reaction amounts of components i is f_i.

$$f_i = \sum_{j=1}^{6} \nu_{ij} f_j \quad (8)$$

Reaaction rate constant

$$k_i = k_{i0} exp\left(\frac{-E_i}{RT}\right) \quad (9)$$

The governing equations are formulated like below.[5]

Mass balance

$$\frac{dg_i}{dr} = \frac{1}{F}\left(2\pi rL\sum_{j=1}^{m} f_{ij} MW_i\right), \sum_{i=1}^{NC} g_i = 1 \quad (10)$$

Energy balance

$$\frac{dT}{dr} = 2\pi rL\sum_{j=1}^{m}(-\Delta H_j) f_j/(FC_P) \quad (11)$$

Pressure drop

$$\frac{dP}{dr} = \frac{P_{out} - P_{in}}{R_{out} - R_{in}} \quad (12)$$

2. Neural Network Model

The neural network model consists of a set of processing units called neurons, connected to one another. The neural network in thisstudy is a feed-forward network with one hidden layer, five input variables and one output variable. By adjusting parameters in the coupling between neurons, the network is capable of learning from a set of numerical data corresponding to the input and desired output.[6] Because of the time-varying characteristics of catalyst activity, the recurrent neural network is used in this hybrid model.

The input variables are Temperature (T (k-1)), Feed rate (F (k-1)), Partial pressure of steam in feed (PSTM (k-1)), Feed flowrate of ethylbenzene(EB) in feed (FEB (k-1)), Deactivation factor at time point k-1 ((k-1))

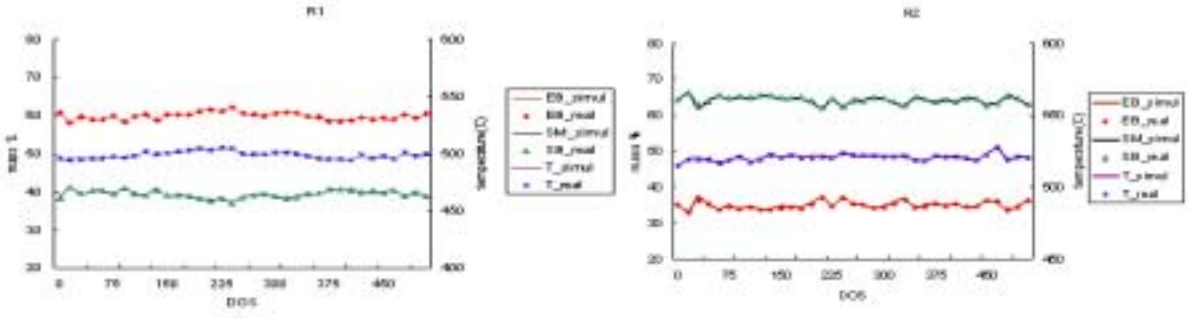
The output variable is Deactivation factor at time point k ((k))

3. Hybrid Model

After training, the proposed neural network model supplies the catalyst deactivation factor (Φ) at any operating conditions. Mass balance, energy balance and pressure drop equations can be solved using given plant data. From these equations, we can obtain reactor output data such as temperatures and composition of the product from each reactor. The structure of the hybrid model couples the first principle model and the neural network model.

Simulation Results

The proposed hybrid model is well fitted with the real plant data. Fig. 2 compares a real plant data with simulation results using predicted catalyst deactivation factor (Φ). These figures show the performance of styrene monomer and ethylbenzene that are the main materials of this process. The simulation results show good performance within error. The simulation results show good performance of 0.4% relative error, compared with 1.7% relative error of the first principle model [7].



a) Reactor 1 **b) Reactor 2**

Fig. 2 Comparison of simulation data and real data of reactors

Optimization of Operating Conditions

1. Problem formation

The objective function for optimization is the profit of the styrene monomer process.

(Profit)=(Product sales)-(Variable cost)-(Fixed cost) (12)

Objective function

$$Profit = Pr_1 Fg_1 + Pr_3 Fg_3 - Pr_{raw} F - \frac{Pr_{NTH}}{C_1}[F(T_{inR2} - T_{outR1})\sum_i^{NC}(Cp_i g_i) + Cp_{10} Fg_{10}(T_{inR1} - C_2)] - C_3 \quad (13)$$

Equality Constraints

$$f_1 = \Phi k_1 (P_{EB} - P_{SM} P_{H2}/K_P),\ f_2 = \Phi k_2 P_{EB},\ f_3 = \Phi k_3 P_{EB} P_{H2},\ f_4 = k_4 P_{H_2O} P_{ET},\ f_5 = k_5 P_{H_2O} P_{ME},$$

$$f_6 = k_6 \frac{P}{T^3} P_{H_2O} P_{CO}, \qquad k_i = k_{i0} exp\left(\frac{-E_i}{RT}\right), \qquad \frac{dg_i}{dr} = \frac{1}{F}\left(2\pi r L \sum_{j=1}^{m} f_{ij} MW_i\right) \quad , \quad \sum_{i=1}^{NC} g_i = 1,$$

$$\frac{dT}{dr} = 2\pi r L \sum_{j=1}^{m}(-\Delta H_j) f_j/(FC_P), \frac{dP}{dr} = \frac{P_{out} - P_{in}}{R_{out} - R_{in}}, \Phi = \Phi(t, F, X_{10}, X_1, P) \quad (14)$$

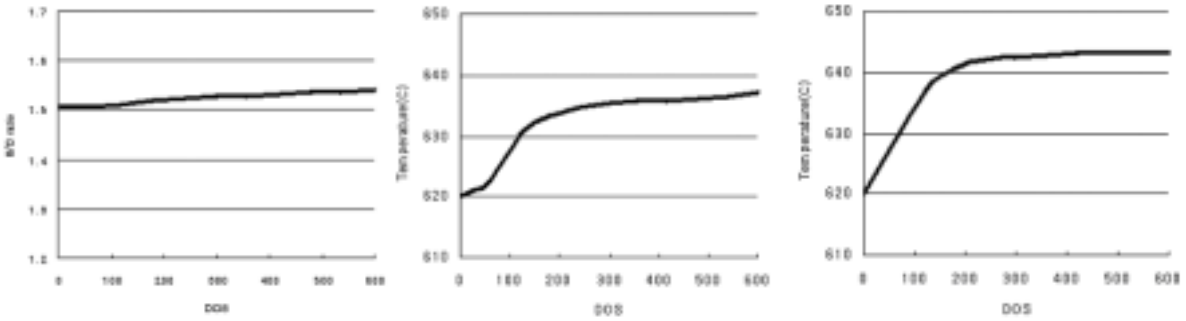
Inequality Constraints

$$600 \leqq T_{inR2} \leqq 650, 600 \leqq T_{inR1} \leqq 650, 0.5 \leqq g_{10} \leqq 0.63, 0 \leqq g_i \leqq 1 \quad (15)$$

Products of this process are styrene monomer and toluene. But the productivity of toluene is not important factor because productivity of toluene is much smaller than the productivity of styrene, while the prices are almost the same. Variable cost contains the cost for steam production and raw material cost. To keep the feed at a fixed temperature, steam cost for reactor 1 and naphtha cost for preheater of reactor 2 are needed. Variable cost increases as the operating temperature increases. Fixed cost, raw material prices and empirical equations for profit calculation are quoted from the real plant.

2. Single variable optimization

To determine the optimum trajectory of each operating variable, the other variables except one operating variable are remained constant during the whole operating horizon. Fig. 3 shows results for single variable optimization.



(a) S/O Ratio (b) T_{in} of R1 (c) T_{in} of R2

Fig. 3 Optimization Results for single variable

To simplifythe optimization problem of the multi operating variables, a mathematical equation form, (10) was selected

$$y = a_1 Log(t + C_1) a_2 t^2 + a_3 t + a_4 + \frac{a_5}{t + C_2} \quad (10)$$

In this equation, y is an operating variable and t is DOS(days on stream). And a1~a5 are variables and C1 and C2 are constants. The fitted variables a1~a5 in each equation are shown in table 3

y	S/O ratio	TinR1	TinR2
a1	-0.4618	44.9057	45.5467
a2	-6.126E-8	6.58E-5	3.10E-5
a3	1.307E-4	-0.09028	-0.07295
a4	3.2464	548.339	547.145
a5	1.0072E-2	1.6088	1.5644
error	0.077%	0.016%	0.017%

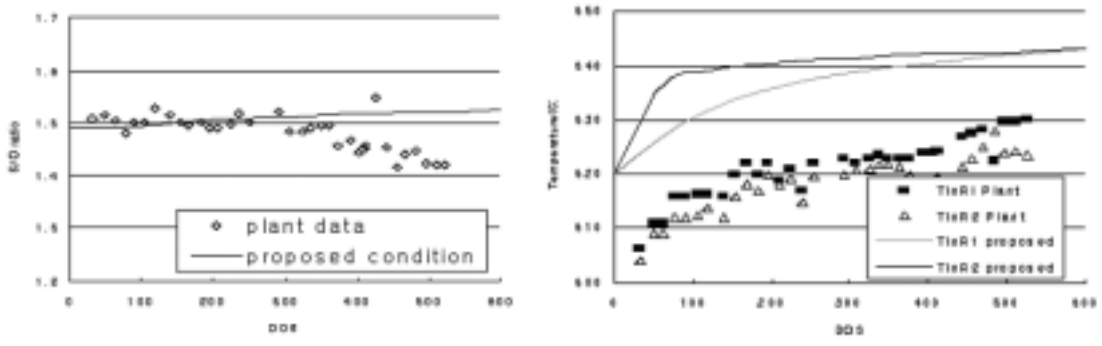
Table. 1 Fitting results

3. Multi-Variable Optimization

Results of previous section are single variable optimization because variables become numerous when using neural network method as time goes by. In this section, threevariables are optimized using previously fitted

equations. To reduce the complexity of multi variable optimization problem, the proposed equations are used. Since the number of time dependent variables is constant, this problem can be solved easier and more stable than the optimization which changes all variables.

Fig. 4 shows optimization results. As shown in Fig. 4, S/O ratio should be increased slowly and inlet temperature of each reactor should be increased. The optimum profit is 65.2×10^8won/yr while the current profit is 52.0×10^8won/yr.



(a) S/O Ratio (b) T_{in} of R1 and T_{in} of R2

Fig. 4 Profile optimization results and current operating data

Concusion

The hybrid model combining the first principle model with neural networks has been developedfor an adiabatic radial-flow dehydrogenation reactor in the styrene monomer production process. The neural network model has predicted the catalyst deactivation factors and the first principle model calculates the reactor outlet data.

From simulation data, the maximum profit of this process has been calculated using real prices. Optimum trajectories of all operating variables have been proposed.

Acknowledgment

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