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# OPERABILITY OF AN AUTOTHERMAL REACTOR LINKED TO A FLEXIBLE HEAT-EXCHANGER NETWORK

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**Abstract** - Operability of an autothermal fixed-bed catalytic reactor within a Heat-Exchanger Network (HEN) is investigated. A retrofit HEN is designed by considering the critical temperature deviations that cause run-away behavior for the reactor. The flexible retrofit design is of minimum cost (area) and keeps both the hot-spot temperature (maximum temperature rise) in the reactor within a strict safety margin and the overall conversion within a strict feasibility margin against a set of possible disturbance directions. The flexible retrofit HEN enables creation of favorable disturbance-propagation paths via optimal manipulation of bypass-stream flow rates, and thus, increases the operability and controllability of the autothermal reactor within the HEN.

## INTRODUCTION

Operability, flexibility, resiliency, and controllability issues must be carefully examined during preliminary- or retrofit-design stages of processes that involve heat integration. Heat-Exchanger Networks (HENs) are of major concern in heat integration; they determine, to a large extent, energy efficiency as well as operability and flexibility of a complete process. Steady-state synthesis methods (e.g., the pinch method) generate HENs for nominal values of stream supply temperatures and flow rates. However, a HEN, synthesized for nominal conditions, must be flexible/resilient to desired/undesired changes in supply temperatures and flow rates.

Various authors studied the flexibility, operability, and controllability problems of HENs. Saboo et al. (1985) and Swaney and Grossmann (1985) introduced flexibility/resiliency indexes to indicate largest deviations of uncertain variables from nominal values for which a HEN structure remains feasible. Colberg and Morari (1988) gave a comprehensive summary of the research on synthesis and analysis of flexible HENs. Huang and Fan (1992) applied a fuzzy-logic approach to incorporate controllability into synthesis of HEN structure by expressing effects of disturbance propagation on structural controllability in a controllability-assessment table that revealed fuzzy relations between disturbance sources and controlled variables. Mathisen (1994) suggested several optimization problems and proposed to take controllability/operability into account by adding control-related constraints to problem formulation. Papalexandri and Pistikopoulos (1994a, 1994b) presented a systematic framework for the synthesis and retrofit of flexible and structurally controllable HENs, and developed total disturbance-rejection criterion which was included within a MINLP model, based on a multiperiod hyperstructure network representation. Konukman et al. (1995a) demonstrated the possibility of creating alternate disturbance-propagation paths via bypass-fraction manipulations by imposing different range constraints on hot and cold targets. Recently, Konukman et al. (1995b) presented a method for flexible/controllable and minimum-cost retrofit design of HENs. Once locations of bypasses are decided upon, the method yields optimally updated exchanger areas and optimal bypass fractions. The resulting retrofit design satisfies target-temperature constraints (hard or soft) for a specified retrofit-design-resiliency-index (RDRI) which is a measure of the maximum tolerable magnitude of a set of disturbances pre-defined in all possible directions.

Decisions made during static structural design of a HEN, without any consideration of its flexibility and safety/feasibility margins of processes linked to its structure, may put severe limitations on achievable operability/controllability of downstream units such as reactors or separators. Static HEN synthesis methods do not necessarily accommodate a utility exchanger for each target stream outgoing to downstream process units. Therefore, necessary control actions in order to satisfy target-temperature constraints should be taken using the manipulated variables (split ratio, bypass fraction) that must be present in a HEN. The bypass or split manipulations can fully

or partially direct, or even reject, incoming disturbances by creating favorable disturbance-propagation paths within a HEN structure (Konukman et al., 1995a). Unfortunately, the static HEN synthesis methods never consider bypass of exchangers and generally yield HEN structures without any or sufficient number of stream splits.

In this work, it is demonstrated that processes operating within narrow safety and feasibility margins, such as fixed-bed autothermal reactors carrying out highly exothermic catalytic reactions, may be connected to HENs provided that operability/flexibility constraints are imbedded in formulating retrofit design of HENs.

## DESCRIPTION OF THE PROCESS

Figure 1 shows the connection of the fixed-bed reactor (FBR) to the HEN. The heat exchanger (E-3) is used to heat the cold feed stream (pre-heated in E-2 by the hot effluent of E-1) of FBR by the FBR's hot product stream. The temperature of the cold-effluent stream from E-1 and temperatures of the hot-effluent streams from E-2 and E-3 are to be controlled for the safety/operability of downstream process units. The FBR has to operate both within a strict safety margin with regard to run-away problem due to hot-spot formation and within a narrow feasibility margin with regard to desired conversion. The nominal values of the stream temperatures and flow rates were determined based on a steady-state operating point of the FBR, and a fictitious nominal HEN (that does not contain any bypass streams) was designed for these nominal operating conditions, which are indicated in Fig.1 in bold typeface.

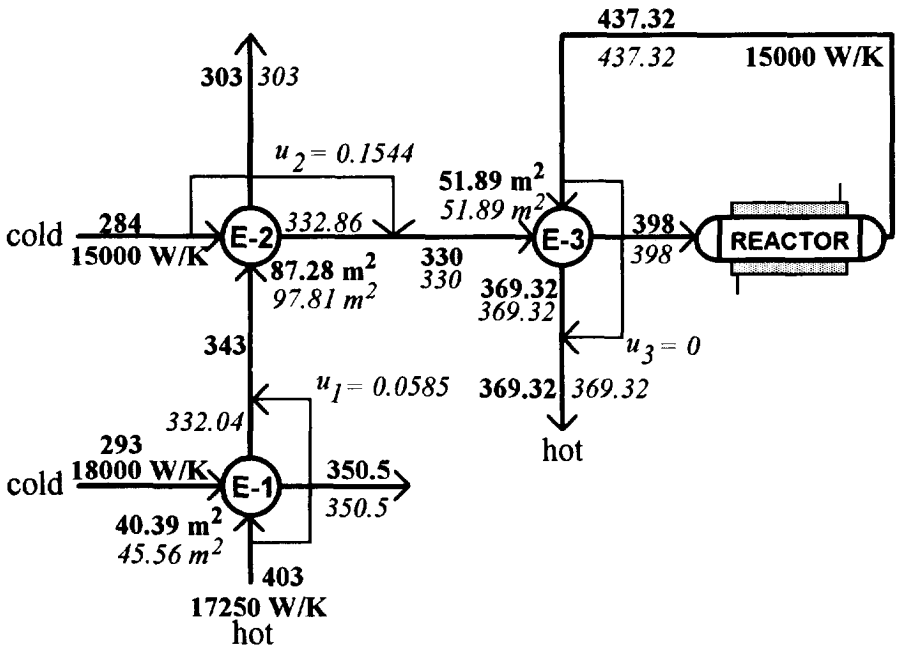



Fig. 1. Process consisting of heat-exchanger network and autothermal fixed-bed reactor.

## MODEL AND BEHAVIOR OF THE FIXED-BED REACTOR

A one-dimensional, homogeneous, steady-state model of the FBR (Froment and Bischoff, 1979), in which a reversible catalytic reaction $A \leftrightarrow B$ is taking place, can be put into the following dimensionless form:

$$\frac{dx_i}{d\xi} = \mp\alpha r \quad i = A,B \qquad \frac{dy}{d\xi} = -\gamma(y - y_w) + \beta r \qquad y_w = 1 - \Delta T_w / T_r^i \qquad \Delta T_w = T_r^i - T_w \tag{1}$$

$$x_i = C_i / C_A^i \qquad y = T_r / T_r^i \qquad y_w = T_w / T_r^i \qquad \xi = z/L \qquad \alpha = \frac{\rho_p L \pi d_c^2}{4 W \bar{C}_A^i} \qquad \beta = \frac{\rho_p (-\Delta H) L \pi d_c^2}{4 W \rho c_p \bar{T}_r^i} \qquad \gamma = \frac{U L \pi d_c}{W \rho c_p} \tag{2}$$

$$r = \frac{10^{-1} k (C_A - C_B / K_e)}{(1 + K_A C_A + K_B C_B)^2} \qquad \begin{aligned} &\ln k = 7.5 - 5000/T_r \qquad \ln K_e = 1500/T_r + 3.5 \\ &\ln K_A = 500/T_r - 0.5 \qquad \ln K_B = 800/T_r - 1.5 \end{aligned} \tag{3}$$

It was assumed that the temperature of the reactor wall can be kept $\Delta T_w$ (constant) degrees lower than the feed temperature of the reactor. The values of the parameters at the nominal operating condition of the FBR are given in Table 1.

Figure 2 shows the behavior of FBR (effluent conversion, and change in effluent and hot-spot temperatures with respect to feed temperature) against deviations in feed temperature and flow rate. Parameters $\alpha$, $\beta$, $\gamma$ have to be updated for flow variations (see Eq.2). Operational requirements of FBR are that the overall conversion should not be lower than $\eta^{min}$ = % 92.5 and the maximum temperature rise at the hot spot location should not exceed $T_r^{max}(\xi)$ = 480.5 K within FBR for the safety of the catalyst. The narrow feasibility and safety margins dictated by these constraints can be identified in Fig.2.

Table 1. Nominal operating conditions of FBR.

| Parameter | Nominal Value | max. temperature rise |
|---|---|---|
| $\alpha$ | 13500 kg-s/kmol | $T_{r,max}$ = 480.076 K |
| $\beta$ | 10000 kg-s/m | hot-spot location |
| $\gamma$ | 5 | $\xi$ = 0.758 |
| $C_A^i$ | 4 kmol/m$^3$ | outlet temperature |
| $C_B^i$ | 0 | $T_{r\|\xi=1}$ = 437.315 K |
| $T_r^i$ | 398 K | overall conversion |
| $\Delta T_w$ | 5 K | $\eta_{\xi=1}$ = 1−$x_A$ = % 94.52 |

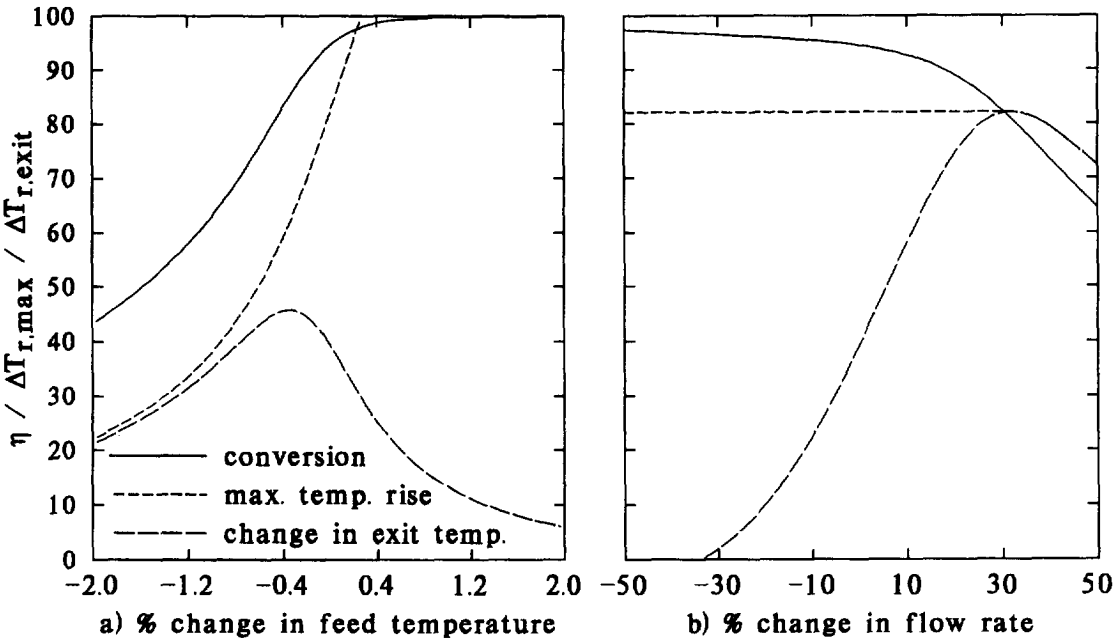



Fig. 2. Behavior of FBR against deviations in a) feed temperature, b) flow rate.

## FLEXIBILITY OF THE ORIGINAL PROCESS

For the nominal designs of the HEN (no bypass streams) and FBR, Table 2 shows the maximum flexibilities, $S^{max}$ (maximum allowable common ± % deviations in temperatures and heat-capacity-flow-rates of the source-streams from their nominal values), for some selected combinations of the disturbance directions in temperatures and heat-capacity-flow-rates of the source-streams (hot stream to E-1, cold stream to E-1, and cold stream to E-2) when the deviations in temperatures of the target streams (cold stream from E-1, hot stream from E-2, and hot stream from E-3) were constrained within ± 1 K. Out of 80 disturbance directions studied, directions No:1-8 and No:9-16 consider disturbances only in source-stream temperatures and flow rates, respectively. Directions No:55 and No:78 were selected for presentation out of 64 simultaneous disturbances in source-stream temperatures and flow rates as the directions yielding the maximum and minimum flexibilities among such disturbances.

Formulation of the optimization problem for each disturbance direction is summarized by Eq.(4-8). Equality constraint, Eq.5, was included since the convergence loop for E-3 and FBR was handled via infeasible-path optimization strategy. Inequality constraint, Eq.6, was imposed only on the three target streams. The optimization problem was solved using the package ADS (Vanderplaats, 1984), and the differential equations of the FBR (Eq.1) were integrated with the package LSODES. Heat exchanger calculations were based on an analytic solution that avoided the use of log-mean temperature differences which allowed removal of some thermodynamic constraints (Boyaci, 1995; Boyaci et al., 1996).

Table 2 shows that the minimum-conversion constraint is not binding, instead, either the maximum hot-spot temperature or the target-temperature range constraints are active for some disturbance directions. As the table reveals, the original process possesses quite low flexibility, mainly due to the constraint on the maximum allowable hot-spot temperature.

Table 2. Disturbance directions and corresponding flexibilities of the original process

| No: | Disturbance Directions in Source Stream: Temperatures $T^s_{H,1}$ | $T^s_{C,1}$ | $T^s_{C,2}$ | Flow Rates $F_{H,1}$ | $F_{C,1}$ | $F_{C,2}$ | $S^{max}$ (%) | Deviations in Target Temperatures $\Delta T^t_n = \bar{T}^t_n - T^t_n$: $\Delta T^t_{C,1}$ | $\Delta T^t_{H,2}$ | $\Delta T^t_{H,3}$ | $\eta$ (%) | $T_{r,max}$ (K) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | – | – | – | 0 | 0 | 0 | 0.285 | 1.00 | 0.86 | 0.43 | 94.23 | 479.03 |
| 2 | – | – | + | 0 | 0 | 0 | 0.285 | 1.00 | -0.23 | 0.26 | 94.35 | 479.43 |
| 3 | – | + | – | 0 | 0 | 0 | 0.499 | 0.35 | 1.00 | 0.18 | 94.40 | 479.63 |
| 4 | – | + | + | 0 | 0 | 0 | 0.540 | 0.38 | -1.00 | -0.11 | 94.59 | 480.34 |
| 5 | + | – | – | 0 | 0 | 0 | 0.540 | -0.38 | 1.00 | 0.11 | 94.45 | 479.81 |
| 6 | + | – | + | 0 | 0 | 0 | 0.479 | -0.33 | -0.95 | -0.17 | 94.64 | 480.50 |
| 7 | + | + | – | 0 | 0 | 0 | 0.189 | -0.66 | 0.15 | -0.17 | 94.64 | 480.50 |
| 8 | + | + | + | 0 | 0 | 0 | 0.117 | -0.41 | -0.35 | -0.17 | 94.64 | 480.50 |
| 9 | 0 | 0 | 0 | – | – | – | 1.876 | -0.50 | 0.36 | 1.00 | 93.14 | 474.54 |
| 10 | 0 | 0 | 0 | – | – | + | 0.204 | -0.05 | 0.11 | -0.04 | 94.61 | 480.50 |
| 11 | 0 | 0 | 0 | – | + | – | 1.548 | 0.90 | 0.45 | 1.00 | 93.27 | 475.10 |
| 12 | 0 | 0 | 0 | – | + | + | 0.234 | 0.13 | 0.15 | -0.02 | 94.61 | 480.50 |
| 13 | 0 | 0 | 0 | + | – | – | 1.529 | -0.90 | -1.00 | 0.13 | 93.93 | 477.27 |
| 14 | 0 | 0 | 0 | + | – | + | 0.136 | -0.08 | -0.04 | -0.08 | 94.62 | 480.50 |
| 15 | 0 | 0 | 0 | + | + | – | 1.812 | 0.48 | -1.00 | 0.36 | 93.66 | 476.24 |
| 16 | 0 | 0 | 0 | + | + | + | 0.149 | 0.04 | -0.02 | -0.07 | 94.62 | 480.50 |
| 55 | + | + | + | + | – | + | 0.782 | -0.33 | 1.00 | 0.30 | 94.07 | 478.07 |
| 78 | + | – | – | + | + | – | 0.063 | -0.25 | -0.21 | -0.13 | 94.63 | 480.50 |

## FLEXIBLE OPTIMAL RETROFIT DESIGN

An optimal retrofit HEN was designed on the basis of the original structure of the HEN in order to increase the flexibility of the overall process against external disturbances. First the number and location of the bypass streams were decided on, as shown in Fig.1, by following the heuristics outlined in Mathisen (1994). The objectives of the retrofit design were set as follows: i) it should be a minimum cost (area) design; ii) it should yield the nominal operating conditions of the HEN and FBR exactly under zero-disturbance case; iii) it should posses maximum flexibility in each disturbance direction; iv) it should satisfy target-temperature range constraints for all disturbance directions; and v) it should be able to satisfy the safety and feasibility constraints on conversion and maximum temperature rise for each disturbance direction. The decision variables to achieve these objectives were the bypass fractions (a different set for each disturbance direction) and the increments in heat exchanger areas (common for each disturbance direction).

objective function:

$$\underset{S,\,T_r^i}{\textit{maximize}}\ S \tag{4}$$

equality constraint:

$$T^o_{C,3} - T^i_r = 0 \tag{5}$$

inequality constraints:

$$\bar{T}^t_n - \Delta T^t_n \le T^t_n \le \bar{T}^t_n + \Delta T^t_n \tag{6}$$

$$\eta \ge \eta^{min} \tag{7}$$

$$T_{r,max} \le T_r^{max} \tag{8}$$

Formulation of the optimal retrofit design problem is summarized by Eq.(9-16). Disturbance directions are identified by the index $k$. For the purpose of presentation, the retrofit design was performed by considering only the source-temperature disturbances. Therefore, only 8 disturbance directions were considered. Zero-disturbance direction (nominal operating condition) is identified by $k = 0$. Equality constraints, Eq.10, was included since the convergence loop for E-3 and FBR was handled via infeasible-path optimization strategy. Equality constraint, Eq.11, guarantees that, under zero disturbance, the conversion and maximum-temperature-rise values will be equal to their nominal values which are already feasible and safe. Equality constraints, Eq.12, guarantee that the target temperatures of the HEN under zero disturbance will be exactly those at the nominal operating condition. Inequality constraints, Eq.13, guarantee that the target-temperature range constraints are satisfied for all disturbance directions. Inequality constraints, Eq.(14-15) guarantee that the safety and feasibility constraints on conversion and maximum temperature rise are satisfied for each disturbance direction. Side constraints, Eq.16, put an upper limit on bypass openings so that each exchanger will be functioning for each disturbance direction and for the zero-disturbance case. The optimization problem was solved as explained before.

The operating conditions and new exchanger areas of the retrofit HEN (that contains bypass streams) are indicated in Fig.1 in italic typeface. Table 3 shows the flexibilities, $S^k$ (common allowable ± % deviations from nominal values), and the optimal openings of the bypass streams of the retrofit process for all combinations of the disturbance directions in temperatures of the source-streams when the deviations in temperatures of the target

streams were constrained within ±1 K. Compared to the flexibilities of the original process shown in Table 2, Table 3 reveals that the retrofit design enables notable increase in the flexibility of the process for all disturbance directions. Flexibility increase due to retrofit design is bounded mainly by the minimum conversion and maximum (hot-spot) temperature constraints which were found binding except for the fourth disturbance direction where only the target-temperature range constraints were found active. Although not presented here, similar results were obtained when the retrofit design was performed by considering flow-rate disturbances as well. Overall conclusion is that the operational requirements of the FBR restricts further flexibility enhancement of the HEN and the complete process.

objective function:

$$\underset{S^k,\mathbf{u}^j,\mathbf{A},T_r^{i,j}}{maximize} \left\{ \sum_k S^k \Big/ \sum_n A_n \right\} \quad k=1,...,8 \quad j=0,...,8 \qquad (9)$$

equality constraints:

$$T_{C,3}^{o,k} - T_r^{i,k} = 0 \qquad k=1,...,8 \qquad (10)$$

$$T_{C,3}^{o,0} - \bar{T}_r^{i} = 0 \qquad (11)$$

$$T_n^{t,0} - \bar{T}_n^{t} = 0 \qquad (12)$$

inequality constraints:

$$\bar{T}_n^t - \Delta T_n^t \le T_n^{t,k} \le \bar{T}_n^t + \Delta T_n^t \qquad k=1,...,8 \qquad (13)$$

$$\eta^k \ge \eta^{min} \qquad k=1,...,8 \qquad (14)$$

$$T_{r,max}^k \le T_r^{max} \qquad k=1,...,8 \qquad (15)$$

$$0 \le u_n^j \le 0.95 \qquad j=0,...,8 \qquad (16)$$

Table 3. Disturbance directions and corresponding flexibilities of the retrofit process

| | Disturbance Directions in Source Stream Temperatures | | | | Deviations in Target Temperatures $\Delta T_n^t = \bar{T}_n^t - T_n^t$ | | | Optimal Bypass Fractions | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| k | $T_{H,1}^s$ | $T_{C,1}^s$ | $T_{C,2}^s$ | $S^k$ (%) | $\Delta T_{C,1}^t$ | $\Delta T_{H,2}^t$ | $\Delta T_{H,3}^t$ | $u_{H,1}$ | $u_{C,2}$ | $u_{H,3}$ | $\eta$ (%) | $T_{r,max}$ (K) |
| 0 | 0 | 0 | 0 | - | 0 | 0 | 0 | 0.1544 | 0.0585 | 0 | 94.52 | 480.08 |
| 1 | − | − | − | 0.574 | 1.00 | 1.00 | 1.00 | 0.1103 | 0.1080 | 0.0240 | 92.50 | 473.63 |
| 2 | − | − | + | 1.188 | 1.00 | 1.00 | 1.00 | 0 | 0.0029 | 0.0240 | 92.50 | 473.63 |
| 3 | − | + | − | 1.593 | 1.00 | 1.00 | 1.00 | 0.1485 | 0.1482 | 0.0240 | 92.50 | 473.63 |
| 4 | − | + | + | 1.473 | -1.00 | -1.00 | -0.47 | 0.0507 | 0 | 0.0119 | 94.38 | 479.49 |
| 5 | + | − | − | 3.664 | 1.00 | 1.00 | 1.00 | 0.2621 | 0.2057 | 0.0240 | 92.50 | 473.63 |
| 6 | + | − | + | 0.899 | -1.00 | -1.00 | -1.00 | 0.1399 | 0.0239 | 0.0139 | 94.64 | 480.50 |
| 7 | + | + | − | 0.670 | -1.00 | -1.00 | -1.00 | 0.2071 | 0.1036 | 0.0139 | 94.64 | 480.50 |
| 8 | + | + | + | 0.324 | -1.00 | -1.00 | -1.00 | 0.1600 | 0.0573 | 0.0139 | 94.64 | 480.50 |

## CONCLUSIONS

When the operability constraints of the reactor are included in the retrofit-design formulation, the optimal retrofit HEN design enables robust operation of the HEN as well as the reactor against disturbances entering from all possible directions. The flexible retrofit HEN design enables creation of favorable disturbance propagation paths which increase the operability and controllability of the autothermal reactor via bypass manipulations.

## NOTATION

$A$ = heat exchanger area, $m^2$
$c_p$ = fluid heat capacity in reactor, kJ/kg-K
$C$ = concentration, kmol/$m^3$
$d_c$ = diameter of reactor, m
$F$ = heat-capacity-flow-rate, J/s-K
$\Delta H$ = heat of reaction, kJ/kmol
$k$, $K_e$, $K_A$, $K_B$ = temperature-dependent parameters of rate equation
$L$ = length of reactor, m
$r$ = global rate of reaction, kmol/kg-s
$S$ = flexibility index (% deviations from nominal values)
$T$ = temperature of stream related to exchanger $n$, K
$\Delta T$ = deviation of temperature from nominal its value related to exchanger $n$, K
$T_r$ = temperature of reactor, K
$T_{r,max}$ = maximum temperature in reactor, K
$T_r^{max}$ = maximum allowable temperature in reactor, K

$T_w$ = wall temperatures of reactor, K
$\Delta T_w$ = difference between feed and wall temperatures of reactor, K
u = bypass fraction
U = overall fluid-wall heat-transfer coefficient, kJ/m$^2$-s-K
W = (reactor) volumetric flow rate, m$^3$/s
x = dimensionless concentration
y = dimensionless reactor temperature
$y_w$ = dimensionless reactor-wall temperature
z = axial position along reactor, m

*Greek Letters*

$\alpha, \beta, \gamma$ = parameters of dimensionless reactor model
$\eta$ = conversion
$\eta^{min}$ = minimum acceptable conversion
$\rho$ = fluid density in reactor, kg/m$^3$
$\rho_p$ = catalyst density, kg/m$^3$
$\xi$ = dimensionless length of reactor

*Superscripts*

i = inlet (feed) location identifier
j, k = disturbance direction identifier
n = heat exchanger number
o = outlet location identifier
t = identifier for target value
$\bar{}$ = identifier showing nominal (zero-disturbance) value
0 = identifier for zero-disturbance direction ( $k = 0$ )

*Subscripts*

i = component identifier
r = identifies that variable is related to reactor
w = identifies that variable is related to reactor wall

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