

# Dynamic Characteristics of Continuous Stirred Tank Reactor (CSTR) Part I: Adiabatic Reactor

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## Abstract

CSTR is a very common reactor type which is widely used in the chemical process industries. It is well-known that its dynamics are nonlinear with a multi-mode behavior. This aspect was and still is an active subject of research with the investigative approach being either mathematical or experimental involving specific reaction systems. In this work a different approach is adopted in which the variation of the damping coefficient value of the linearized reactor's transfer function is investigated over chosen values/ranges of relevant parameters. Our results indicate that an adiabatic type of such a reactor in which a liquid-phase, 1st-order, irreversible, exothermic chemical reaction takes place can be unstable or stable. If stable, it is either critically damped or overdamped with the latter mode being overwhelming; however, it is never underdamped. Furthermore, even when stable its dynamic behavior can be peculiar depending on certain values of some parameters.

**Keywords:** CSTR dynamics, Adiabatic reactor, Damping coefficient, Residence time, Stability.

## 1. Introduction

CSTRs are known for their operational complexity and challenging control schemes. They are classified dynamically as nonlinear systems. These features gave rise to numerous research works concerning their dynamics since the middle of the last century (e.g. Van Heerden [1]) up to the present (e.g. Suo et al. [2]). The majority of relevant papers were based on mathematical analysis (e.g. Uppal et al. [3, 4, 5]). Alternatively, few papers reflected the multi-mode dynamic behavior of CSTRs in which specific chemical reactions took place. Noteworthy among them is the work of Nagay et al. [6] concerning permanganate-hydroxylamine reaction.

Linearization is an essential mathematical tool to obtain transfer functions of nonlinear systems. Furthermore, the designs of control schemes are usually based on the analysis of linear systems. The characteristic equation of a linear 2nd-order system's transfer function is of the form,

$$\tau^2 s^2 + 2\zeta\tau s + 1 = 0 \quad (1)$$

Where  $\tau$  and  $\zeta$  represent the system's characteristic time and damping coefficient, respectively. It is well-known that such a system is dynamically stable if  $\zeta > 0$ ; with  $\zeta = 0$ , the system becomes self-sustained oscillatory when subjected to a step-change forcing function. Negative  $\zeta$  values render the system unstable.

As instructors of an undergraduate program, we felt that a different approach is needed to elucidate the multi-mode dynamic behavior of CSTRs to our students. This was the motive for the present work which is divided into two parts: this part I and the next part II concerning a non-adiabatic reactor.

Due to the complexity of the matter, a liquid-phase 1<sup>st</sup>-order, exothermic, irreversible chemical reaction  $A \rightarrow B$  is assumed to take place in the reactor which is in line with previous studies. For the adiabatic reactor, the transfer function considered (Seborg et al. [7])  $G(s) = \frac{T(s)}{C_{iA}(s)}$  where  $T(s)$  and  $C_{iA}(s)$  are deviations in outflow temperature and inflow reactant concentrations, respectively. This

transfer function was obtained as a result of linearization of the reactor's material and energy balance equations, which made the CSTR a linear 2<sup>nd</sup>-order system. Ranges of relevant parameters were used to determine  $\zeta$  values covering unstable and stable conditions. Additionally, the impact of these parameters on  $\zeta$  were determined and elucidated in tabular and graphical forms.

## 2. Material and energy balance equations

The following simplifying assumptions were made,

- The CSTR is perfectly mixed.
- The mass densities and specific heat capacities of inflow and outflow are equal and constant.
- The liquid content volume of the reactor is constant due to an overflow arrangement with a constant inflow equals outflow.
- The enthalpy of the exothermic chemical reaction is constant.
- The steady-state reactant concentration and reaction temperature are both linearly dependent on the reactor's residence time.
- The inflow temperature and its reactant concentration are constant.

### 2.1. Reactant A mass balance

Steady-state (ss)

$$q(\bar{C}_{iA})_{ss} + V(r_A)_{ss} - q(\bar{C}_A)_{ss} = 0 \quad (2)$$

With  $(r_A)_{ss} = -k_{ss}(\bar{C}_A)_{ss}$  and since  $\frac{V}{q} = \tau$

the reactor's residence time, eq. (2) becomes,

$$(\bar{C}_{iA})_{ss} - \tau k_{ss}(\bar{C}_A)_{ss} - (\bar{C}_A)_{ss} = 0 \quad (3)$$

from which,

$$k_{ss} = \frac{(\bar{C}_{iA})_{ss} - 1}{(\bar{C}_A)_{ss} - 1} \tau \quad (4)$$

Transient state

$$\bar{C}_{iA}(t) - \tau k_{ss} \bar{C}_A(t) - \bar{C}_A(t) = \tau \frac{d\bar{C}_A(t)}{dt} \quad (5)$$

where the specific reaction rate  $k = k_0 \exp\left(\frac{-E}{RT}\right)$  according to Arrhenius equation. Linearization of the 2<sup>nd</sup>-term on the LHS of Eq. (5) and noting that  $k_{ss} = k_0 \exp\left(\frac{-E}{RT_{ss}}\right)$  leads to,

$$\bar{C}_{iA}(t) - \tau k_{ss} \bar{C}_A(t) - \tau k_{ss} (\bar{C}_A)_{ss} \left( \frac{E}{RT_{ss}^2} \right) (\bar{T} - \bar{T}_{ss}) - \bar{C}_A(t) = \tau \frac{d\bar{C}_A(t)}{dt} \quad (6)$$

Subtracting Eq. (3) from Eq. (6), introducing the deviation variables  $C_{iA}(t) = [\bar{C}_{iA}(t) - (\bar{C}_{iA})_{ss}]$ ,  $C_A(t) = [\bar{C}_A(t) - (\bar{C}_A)_{ss}]$ ,  $T(t) = [\bar{T}(t) - \bar{T}_{ss}]$ , and rearranging result in,

$$\tau \frac{dC_A(t)}{dt} + (\tau k_{ss} + 1)C_A(t) + \tau k_{ss} (\bar{C}_A)_{ss} \left( \frac{E}{RT_{ss}^2} \right) T(t) = C_{iA}(t) \quad (7)$$

Laplace transforming Eq. (7) leads to,

$$(\tau s + \tau k_{ss} + 1)C_A(s) + \tau k_{ss} (\bar{C}_A)_{ss} \left( \frac{E}{RT_{ss}^2} \right) T(s) = C_{iA}(s) \quad (8)$$

### 2.2 Reactor thermal balance

$$\rho q C_p \bar{T}_i(t) + \Delta H_r V r_A - \rho q C_p \bar{T}(t) = \rho V C_p \frac{d\bar{T}(t)}{dt} \quad (9)$$

Or

$$\bar{T}_i(t) - \frac{\Delta H_r}{\rho C_p} \tau k_{ss} \bar{C}_A(t) - \bar{T}(t) = \tau \frac{d\bar{T}(t)}{dt} \quad (10)$$

Linearization of the 2<sup>nd</sup>-term on the LHS of eq. (10), introducing deviation variables, and rearranging result in,

$$\tau \frac{dT(t)}{dt} + \left[ \frac{\Delta H_r}{\rho C_p} \tau k_{ss} (\bar{C}_A)_{ss} \left( \frac{E}{RT_{ss}^2} \right) + 1 \right] T(t) + \frac{\Delta H_r}{\rho C_p} \tau k_{ss} C_A(t) = T_i(t) = 0 \quad (11)$$

Noting that  $T_i(t) = 0$  because  $\bar{T}_i$  is constant as pointed out in the simplifying assumptions. Following Laplace transformation and rearrangement of eq. (11), eq. (12) is obtained,

$$C_A(s) = \left\{ \left( \frac{\rho C_p}{\Delta H_r k_{ss}} \right) s + (\bar{C}_A)_{ss} \left( \frac{E}{RT_{ss}^2} \right) + \left( \frac{\rho C_p}{\Delta H_r \tau k_{ss}} \right) \right\} T(s) \quad (12)$$

Eq. (12) is substituted into Eq. (8) to obtain the desired transfer function  $G(s) = \frac{T(s)}{C_{iA}(s)}$  following simplification. This

transfer function is then put in the standard form,

$$G(s) = \frac{T(s)}{C_{iA}(s)} = \frac{\frac{C_1}{C_4}}{\left(\frac{C_2}{C_4}\right)s^2 + \frac{C_3}{C_4}s + 1} \quad (13)$$

where  $C_1$ - $C_4$  are constants for specific values of the parameters in eqs. (8) and (12). The CSTR's steady-state gain  $K = \frac{C_1}{C_4}$ , its characteristic time  $\tau = \sqrt{\frac{C_2}{C_4}}$ , and its damping coefficient  $\zeta = \frac{C_3}{2\sqrt{\frac{C_2}{C_4}}}$ . The values of  $K$  and  $\tau$  were not registered; being of no consequence to this work.

### 3. Ranges / values of Parameters

The following ranges / values of relevant parameters were employed,

- Reactor's residence time  $5 \leq \tau \leq 50$  min, with one minute variation leading to 46 values (assumed).
- Inflow reactant concentration  $\bar{C}_{iA} = 12 \frac{\text{kmol}}{\text{m}^3}$  (assumed, constant).
- Steady-state outflow reactant concentration  $6 \leq (\bar{C}_A)_{ss} \leq 0.6 \frac{\text{kmol}}{\text{m}^3}$ , corresponding to  $5 \leq \tau \leq 50$  min, based on the assumed linear relationship  $(\bar{C}_A)_{ss} = 6.6 - 0.12\tau$  (calculated).
- Steady-state specific reaction rate  $0.2 \geq k_{ss} \geq 0.0923 \text{ min}^{-1}$  corresponding to  $5 \leq \tau \leq 22$  min, and  $0.0924 \leq k_{ss} \leq 0.38 \text{ min}^{-1}$  corresponding to  $23 \leq \tau \leq 50$  min [calculated using eq. (4)].
- Inflow temperature  $\bar{T}_i = 300 \text{ K}$  (assumed, constant).
- Steady-state reaction temperature  $303 \leq \bar{T}_{ss} \leq 312 \text{ K}$ , corresponding to  $5 \leq \tau \leq 50$  min, based on the assumed linear relationship  $\bar{T}_{ss} = 302 + 0.2\tau$  (calculated).
- E/R values were calculated using two values of the preexponential factor  $k_0 = 7.0 \times 10^{10}$ ,  $k_0 = 2.4 \times 10^{15} \text{ min}^{-1}$

(Seborg et al. [7]) with the corresponding  $\bar{T}_{ss}$  and  $k_{ss}$  values using Arrhenius equation. Table 1 shows the results,

**Table 1. Used E/R values based on two  $k_0$  values for the full range of CSTR residence time.**

$k_0 = 7.0 \times 10^{10} [\text{min}^{-1}]$	$k_0 = 2.4 \times 10^{15} [\text{min}^{-1}]$
$8054 \leq \frac{E}{R} \leq 8401 \text{ K}$	$11218 \leq \frac{E}{R} \leq 11618 \text{ K}$
$5 \leq \tau \leq 29 \text{ min}$	$5 \leq \tau \leq 32 \text{ min}$
$8400.5 \leq \frac{E}{R} \leq 8093 \text{ K}$	$11617 \leq \frac{E}{R} \leq 11351 \text{ K}$
$30 \leq \tau \leq 50 \text{ min}$	$33 \leq \tau \leq 50 \text{ min}$

The above E/R values are well within the common range  $5000 \leq \frac{E}{R} \leq 25000 \text{ K}$  according to Denbigh [8]. For simplicity lower and higher E/R values shall be designated "low" and "high", respectively.

- Two values of the specific heat capacity per unit volume  $\rho C_p$  were considered, a low value of  $(800)(1.25) = 1000$  and a high value of  $(1250)(4.2) = 5250 \text{ kJ}/(\text{m}^3 \text{ K})$  (assumed, constant).
- Five values of the exothermic reaction enthalpy were employed, namely  $-1 \times 10^3$ ,  $-2 \times 10^3$ ,  $-3 \times 10^3$ ,  $-4 \times 10^3$ , and  $-5 \times 10^3 \text{ kJ}/\text{kmol}$  (assumed, constant).

Combinations of the aforementioned parameters values led to 20 values of  $\zeta$  for each value of  $\tau$ , with a total of 920 results using MATLAB ver. R2017b.  $\zeta$  values for  $\tau = 50$  min are given as appendix to clarify the combinations leading to the 20 values.

### 4. Results and Analysis

Figure 1 and 2 show  $\zeta$  variation vs.  $\tau$  for  $\rho C_p = 1000 \text{ kJ}/(\text{m}^3 \text{ K})$ , with Fig. 1 based on the low E/R range and Figure 2 on the high E/R range. As can be seen, each fig. contains five curves, one for each  $\Delta H_r$  value. Figs. 3 and 4 are similar to Figs. 1 and 2 but for  $\rho C_p = 5250 \text{ kJ}/(\text{m}^3 \text{ K})$ .

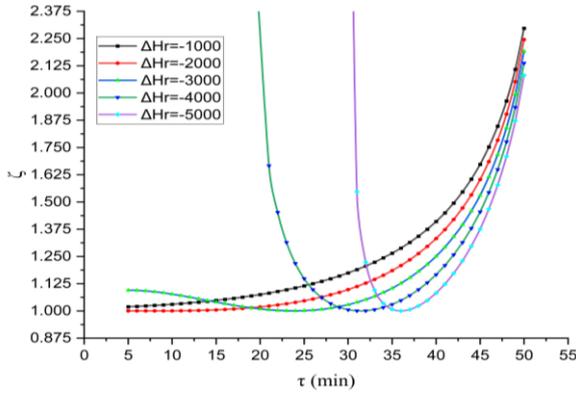


Fig 1.  $\zeta$  variation vs.  $\tau$  for  $\rho C_p = 1000 \text{ kJ}/(\text{m}^3 \text{ K})$  &  $k_0 = 7 \times 10^{10} \text{ min}^{-1}$

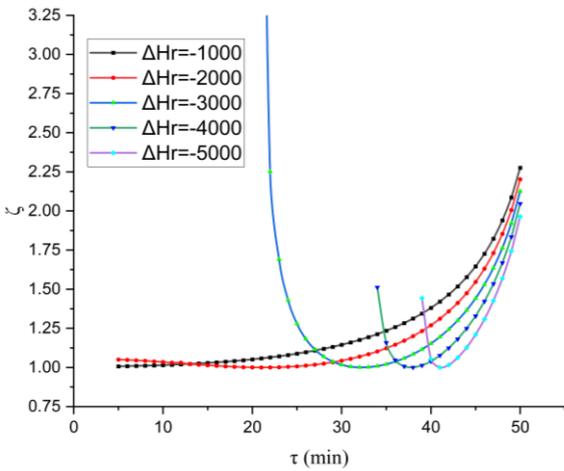


Fig 2.  $\zeta$  variation vs.  $\tau$  for  $\rho C_p = 1000 \text{ kJ}/(\text{m}^3 \text{ K})$  &  $k_0 = 2.4 \times 10^{15} \text{ min}^{-1}$

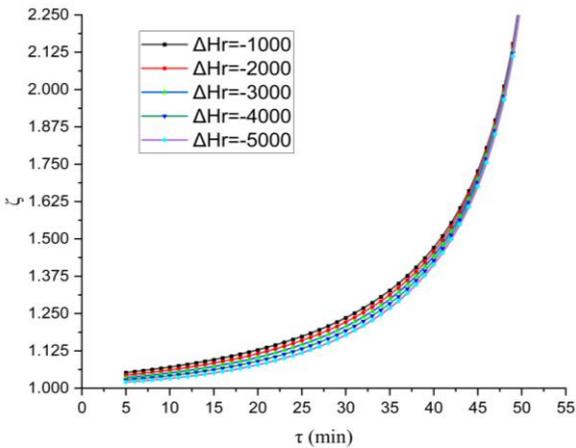


Fig 3.  $\zeta$  variation vs.  $\tau$  for  $\rho C_p = 5250 \text{ kJ}/(\text{m}^3 \text{ K})$  &  $k_0 = 7 \times 10^{10} \text{ min}^{-1}$

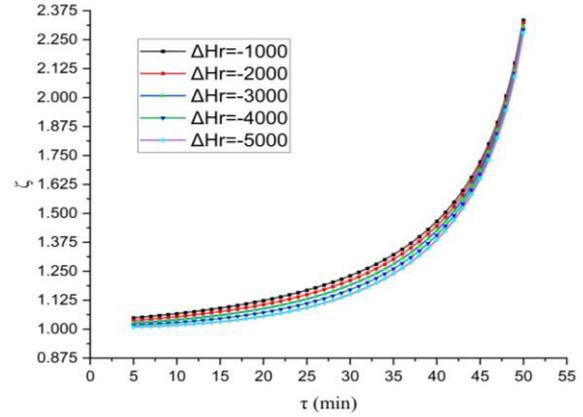


Fig 4.  $\zeta$  variation vs.  $\tau$  for  $\rho C_p = 5250 \text{ kJ}/(\text{m}^3 \text{ K})$  &  $k_0 = 2.4 \times 10^{15} \text{ min}^{-1}$

### 4.1 Instability Ranges

Table 2 specifies the reactor's instability ranges as shown in Figs. 1 and 2; noting the distinct feature of no instability in Figs. 3 and 4 due to the higher  $\rho C_p$  value of  $5250 \text{ kJ}/(\text{m}^3 \text{ K})$ .

Table 2. CSTR instability ranges,  $\rho C_p = 1000 \text{ kJ}/(\text{m}^3 \text{ K})$ .

Fig	$\tau$ [min]	$\Delta H_r$ [ $\frac{\text{kJ}}{\text{kmol}}$ ]	$\frac{E}{R}$ [K]
1	5--18	$-4 \times 10^3$	low
1	5--29	$-5 \times 10^3$	low
2	5--20	$-3 \times 10^3$	high
2	5--33	$-4 \times 10^3$	high
2	5--38	$-5 \times 10^3$	high

Two effects can be deduced from Table 2. The first is that  $\tau$  instability range increases as the value of  $\Delta H_r$  increases. The second effect is the increase in  $\Delta H_r$  range in which instability occurs as the value of  $E/R$  becomes higher.

### 4.2 Stability ranges and peculiarity of CSTR dynamics

Figs. 1 and 2 indicate the well-known stability effect of increasing the reactor's residence time. Furthermore, this effect is corroborated in Figs. 3 and 4 where the value of  $\zeta$  increases as  $\tau$  is increased. Notwithstanding this general trend, Figs. 1 and 2 depict a peculiar dynamic behavior which is entirely absent in Figs. 3 and 4. The details of this behavior are as follows,

- The  $\zeta$  vs.  $\tau$  curves for the lowest  $\Delta H_r$  value of  $-1 \times 10^3$  kJ/kmol is similar to the trend in Figs. 3 and 4.
- The curves for  $\Delta H_r$  of  $-2 \times 10^3$ ,  $-3 \times 10^3$  (Fig. 1) and  $-2 \times 10^3$  kJ/kmol (Fig. 2) start with decreasing  $\zeta$  values down to a minimum of  $\zeta = 1.0$  (critically damped) followed by increasing  $\zeta$  values up to a maximum at  $\tau = 50$  min.
- For the higher  $\Delta H_r$  values of  $-4 \times 10^3$ ,  $-5 \times 10^3$  Figure. 1;  $-3 \times 10^3$  to  $-5 \times 10^3$  kJ/kmol (Fig.2), following instability (Table 1),  $\zeta$  shoots up to a high value then drops sharply to unity and shoots up again reaching a maximum at  $\tau = 50$  min. Table 3 gives  $\tau$  values at which  $\zeta = 1.0$  in Figs. 1 and 2,

**Table 3. Conditions at which  $\zeta = 1.0$ ,  $\rho C_p = 1000$  kJ/(m<sup>3</sup> K)**

Fig.	$\Delta H_r$ [ $\frac{kJ}{kmol}$ ]	$\frac{E}{R}$ [K]	$\tau$ [min]
1	$-2 \times 10^3$	low	10
1	$-3 \times 10^3$	low	25
1	$-4 \times 10^3$	low	31--33
1	$-5 \times 10^3$	low	35--37
2	$-2 \times 10^3$	high	20
2	$-3 \times 10^3$	high	32--33
2	$-4 \times 10^3$	high	38
2	$-5 \times 10^3$	high	41

Two aspects are noticeable in Table 3. The first is related to  $\Delta H_r$  value at a specific E/R range, whether low or high, which is the shift to a higher  $\tau$  value as  $\Delta H_r$  increases. The second aspect is related to the E/R range at a specific  $\Delta H_r$ , which is again the shift to a higher  $\tau$  value as E/R range increases. These two aspects can be seen in Figs. 1 and 2.

An interesting feature can be seen in Figs. 3 and 4, which is the diminishing variation among the five  $\zeta$  vs.  $\tau$  curves as the reactor's residence time increases, such that they virtually become a single curve in the form of a straight line for  $\tau > 45$  min. Additionally, these two lines of Figs. 3 and 4 are practically congruent. The implication of this feature is that the impact of both  $\Delta H_r$  and E/R on the  $\zeta$  vs.  $\tau$  relation ceases to exist if the residence time is high enough. This trend can also be seen in Figs. 1 and 2, but only partially, requiring more than 50 min residence time for full manifestation due to the lower  $\rho C_p$  value.

It should be pointed out that an adiabatic CSTR in which an exothermic chemical reaction takes place is impractical since heat must be removed to

sustain the desired conversion. Nevertheless, such a reactor is of educational usefulness due to its simpler mathematical analysis in comparison with the practical non-adiabatic reactor which is the subject of part II of this work. It will be shown later that there are similarities and significant differences between these two reactor types.

### 5. Conclusions

- Eight parameters affect the CSTR stability / instability as well as its dynamic behaviour. Seven of them are present in the reactor's material / energy balance equations in addition to Arrhenius equation preexponential factor.
- Adiabatic CSTR instability is influenced by low residence time, high reaction exothermicity, low specific heat per unit volume, and high reaction activation energy.
- Since three of the four parameters of the previous point are reaction-specific, their adverse values would leave only the reactor's residence time as means of achieving stability. In this case, a relatively large tank volume should be used since the inflow rate is usually process-related.
- Over the ranges/values of parameters used in this work, an adiabatic CSTR if stable is never underdamped. It is either critically damped or overdamped with the latter dynamic mode being overwhelming.
- Following instability, as the reactor's residence time is increased and stability sets in,  $\zeta$  could shoot up to a relatively high value, then shoots down to a value of unity, and then shoots up again if the reactor's residence time keeps increasing.

### Notation

- A reactant
- $C_1 - C_4$  constants
- $\bar{C}_{iA}$  inflow reactant concentration
- $C_{iA}$  deviation in inflow reactant concentration
- $\bar{C}_A$  outflow reactant concentration
- $C_A$  deviation in outflow reactant concentration



$C_p$  specific heat capacity  
 $E/R$  ratio of activation energy to universal gas constant  
 $G(s)$  transfer function  
 $\Delta H_r$  heat of reaction  
 $k$  specific reaction rate  
 $k_o$  preexponential factor  
 $q$  volumetric inflow or outflow rate  
 $r_A$  reaction rate  
 $\bar{T}$  reaction temperature  
 $T$  deviation in reaction temperature  
 $V$  reactor's content volume

### Greek symbols

$\rho$  density  
 $\zeta$  damping coefficient  
 $\tau$  residence time

### Subscript

ss steady-state

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### Appendix

Example illustrating the combination of parameters values leading to 20 values of the damping coefficient  $\zeta$  for each value of the reactor's residence time  $\tau$ .

$\tau = 50$  min,  $(\bar{C}_A)_{ss} = 0.6$  kmol/m<sup>3</sup>,  $\bar{T}_{ss} = 312$  K,  $k_{ss} = 0.38$  min<sup>-1</sup>

**I**  $\rho C_p = 1000$  kJ/(m<sup>3</sup> K),  $k_o = 7.0 \times 10^{10}$  min<sup>-1</sup>,  $E/R = 8093$  K

$\Delta H_r$ :  $-1 \times 10^3$   $-2 \times 10^3$   $-3 \times 10^3$   $-4 \times 10^3$   $-5 \times 10^3$  kJ/kmol

$\zeta$  : 2.297 2.245 2.1917 2.1372 2.0813

**II**  $\rho C_p = 5250$  kJ/(m<sup>3</sup> K),  $k_o = 7.0 \times 10^{10}$  min<sup>-1</sup>,  $E/R = 8093$  K

$\Delta H_r$ :  $-1 \times 10^3$   $-2 \times 10^3$   $-3 \times 10^3$   $-4 \times 10^3$   $-5 \times 10^3$  kJ/kmol

$\zeta$  : 2.3383 2.3286 2.3189 2.3092 2.2994

**III**  $\rho C_p = 1000$  kJ/(m<sup>3</sup> K),  $k_o = 2.4 \times 10^{15}$  min<sup>-1</sup>,  $E/R = 11351$  K

$\Delta H_r$  :  $-1 \times 10^3$   $-2 \times 10^3$   $-3 \times 10^3$   $-4 \times 10^3$   $-5 \times 10^3$  kJ/kmol

$\zeta$  : 2.2762 2.2022 2.1257 2.0464 1.9639

**IV**  $\rho C_p = 5250$  kJ/(m<sup>3</sup> K),  $k_o = 2.4 \times 10^{15}$  min<sup>-1</sup>,  $E/R = 11351$  K

$\Delta H_r$  :  $-1 \times 10^3$   $-2 \times 10^3$   $-3 \times 10^3$   $-4 \times 10^3$   $-5 \times 10^3$  kJ/kmol

$\zeta$  : 2.3344 2.3208 2.3072 2.2935 2.2797