Chemical Reactor Analysis and Design Fundamentals

Errata for First Edition, First Printing

September 19, 2020

1. cover, change sign on $\dot{W}_r$ term and add $\dot{W}_0$ term to energy balance at bottom of cover.

2. cover, remove minus sign in front of $D_l$.

3. p. 43, three lines above first equation, change "Equation 2.27" to "Reaction 2.26." Thanks to Manos Mavrikakis of UW for pointing out this erratum.

4. p. 78, last equation, replace $\Delta C_f$ with $\Delta C_f'$. Thanks to Carlos Henao of UW for pointing out this erratum.

5. p. 91. Change $\varepsilon_i, \varepsilon_j$ to $\varepsilon_i', \varepsilon_j'$, respectively, in second to last displayed equation and sentence preceding it.

6. p. 91, last paragraph, change "the production of 2,2,4 is preferable" to "the production of 2,2,3 is preferable." Thanks to Manos Mavrikakis of UW for pointing out this erratum.

7. p. 103, Exercise 3.10, change equation in (a) to

$$\frac{k_j}{k_0} = \frac{K \phi_j}{R T \phi_0}$$

in which $x$ is the compressibility factor of the mixture.

8. p. 103, Exercise 3.10 (b), change "ideal mixture" to "ideal-gas mixture."

9. p. 104, line after Equation 3.86. Change $\pi (n - 1)$ to $\pi (n + 1)$.

10. p. 104, last equation, change $\sum_j \mu_j n_j$ to $\sum_j \mu_j \phi_j$.

11. p. 106, in Exercise 3.14, matrix $H$ is positive definite, but matrix $H$ is only positive semidefinite. Therefore change parts (c) and (e) to the following. Also include the definition of a positive semidefinite matrix in the problem statement.

A matrix $H$ is positive semidefinite if

$$x^T H x \geq 0, \text{ for every } x \neq 0$$

(c) To show $H$ is positive semidefinite, we must show that the following quadratic form is nonnegative

$$x^T H x = \sum_j x_j H_{jj} x_j \geq 0, \text{ for every } x \neq 0$$

Substitute Equation 3.92 into the above equation and show

$$x^T H x = \frac{R T}{n_f} \left[ \sum_j \frac{x_j^2}{Y_j} + \left( \sum_j x_j \right)^2 \right]$$

12. p. 109, sentence after Equation 4.40, should read "One can divide Equation 4.39 through by $Q_f$ . . ." Thanks to Nathan Knapp of Oregon State University for pointing out this erratum.

13. p. 115, sentence before Equation 4.51, should read the probability for the two reactions are

14. p. 170, Equation 4.102, add units of 1/day to the rate constants. Thanks to Elise Huang of UW for pointing out this erratum.

15. p. 178, Exercise 4.6, Equation 4.115 is missing a term; it should read

$$x(t) = x_0 e^{\lambda t} - \frac{A}{1} \left[ 1 - e^{-\lambda t} \right]$$

and the partial fraction formula after Equation 4.115 is missing a minus sign; it should read

$$\frac{1}{s(x - A)} = \frac{1}{A} \left[ \frac{1}{x} - \frac{1}{x - A} \right]$$

16. p. 178, Exercise 4.6, change units of $E_A$ to kcal/mol. Thanks to Ryan West of UW for pointing out this erratum.

17. p. 180, Exercise 4.8, part (a), change "production rate of propylene glycol" to "the total reactor production rate of propylene glycol."

18. p. 181, Exercise 4.10, Add the phrase "starting with pure A" to the question in (a).

19. p. 182, Exercise 4.12 (b), change "gas flowrate" to "volumetric flowrate." Thanks to Charlie Hill of UW for pointing out this erratum.

20. p. 183, Exercise 4.13, second line, should read "from 5% to 5 ppm."

21. p. 183, Exercise 4.14, third sentence should read "What happens if one attempts to achieve a higher conversion than this limiting value by recycling more material?"
26. p. 183, Figure 4.36. Replace the figure with the following to make the separation more clear.

27. p. 184, Exercise 4.17, change units of $k_1$ from mol/L-min to L/mol-min. Thanks to Yong Ku Cho of UW for pointing out this erratum.

28. p. 212, change the two equations at the bottom of the page to

$$\frac{dz_1}{dt} = r_1 \quad \frac{dz_2}{dt} = \frac{K_2}{1 + K_2} r_1$$

29. p. 246, Equation 5.140, change $K_{CO}$ to $K_1$. Thanks to Irene Chen of UW for pointing out this erratum.

30. p. 261, Exercise 5.6, 3 lines from end. Change the list $(CH_3, CH_3CO$ and $CHO)$ to $(CH_3$ and $CH_3CO)$. Thanks to Tania Deb and Chris Barrett of UW for pointing out this erratum.

31. p. 269, Exercise 5.19, first line. Change "hydrogen" to "ethane." Thanks to Kevin Hennock of Princeton University for pointing out this erratum.

32. p. 270, add "S" to the right-hand side of the last reaction in Exercise 5.19. Thanks to Andrew Stella of Princeton University for pointing out this erratum.

33. p. 281, second line of Example 6.1. Change "elementary and irreversible" to "exothermic, elementary, and irreversible." 

34. p. 289, last line. Change $-5.33$ to $-5.4$. Thanks to Sam Toan of U. Minnesota-Duluth for pointing out this erratum.

35. p. 297, change $Q_a$ under Equation 6.38 to $-Q_a$.

36. p. 300, change $U^m$ to $U^m A/V_k$ in Equation 6.40

37. p. 301, change $U^m$ to $U^m A/V_k$ in Equation 6.44

38. p. 305, Add $T_a = 298$ K to Table 6.3

39. p. 305, Add $T_a = 298$ K to Table 6.3. Thanks to Mike Donnelly of UW for pointing out this erratum.

40. p. 316, First paragraph of Section 6.4. Should read "...Equations 6.82-6.83 in the semi-batch reactor Table 6.9 are identical to the corresponding Equations 6.73-6.74 in the CSTR Table 6.8."

41. p. 324, $E/R$ in Table 6.5 should be $E_a/R$ or simply $E$.

42. pp. 324-325, Table 6.5, change $k_{10}$ value from 1922.6 to 2082; change $\Delta H_a$ value from $-1.361 \times 10^9$ to $-1.284 \times 10^9$. With these changes the corrected Figures 6.35 and 6.36 are shown here. Thanks to Matt Kipper of Colorado State for pointing out this erratum.
43. p. 327, Partial pressures in Equation 6.55 are divided by 1.0 atm.
44. p. 329, Table 6.4, units of $\alpha_{\text{ch}}$ are atm/s.
45. p. 329, Add $x_{\text{AF}} = 0.015, x_{\text{NF}} = 0.985 \cdot (1/4), x_{\text{HF}} = 0.985 \cdot (3/4)$ to Table 6.6. The feed consists of 1.5% ammonia and 98.5% stoichiometric mixture of nitrogen and hydrogen. Thanks to graduate student Jim Plaendner of Northwestern for pointing out this omission and the next typo.
46. p. 329, Change the sign of $\Delta G^*$ in Table 6.6.
47. p. 328, Table 6.6, Change $Q_f$ to 0.05713 m$^3$/s.
48. p. 329. Figure 6.38 is not quite correct. The corrected figure is shown here in Figure 6.38.
49. p. 330. The middle steady-state profiles in Figures 6.39 and 6.40 are not quite correct. The corrected figures are shown here in Figures 6.39 and 6.40.
50. p. 332, Equation 6.65, change $V$ to $V_p$
51. p. 333, Equation 6.75, change $\alpha$ to $\alpha_f$
52. p. 333, missing terms in Equation 6.75 and Equation 6.76 of Table 6.8 are underlined below. Note $P_0 = (P_0/P_{\text{total}})_{\text{atm}}$ has been added to the list of symbols.
b. Constant-volume reactor
\[
V_R \frac{dT}{dt} = - \sum_j (\Delta H_{\text{R}j} - \alpha T V_R \sum_i v_i P_{e_i}) r_i V_R + \sum_j c_{ij} Q_j (H_{\text{R}j} - H_j) \\
+ \alpha T V_R \sum_i P_{e_i} (c_{ij} Q_j - c_j Q_i) + \dot{Q} \quad (6.75)
\]

b.1 Constant-volume reactor, ideal gas
\[
V_R \frac{dT}{dt} = - \sum_j (\Delta H_{\text{R}j} - R T V_R) r_i V_R + \sum_j c_{ij} Q_j (H_{\text{R}j} - H_j) \\
+ R T \sum_j (c_{ij} Q_j - c_j Q_i) + \dot{Q} \quad (6.76)
\]

53. p. 342, replace \( A_h \) with \( A \) in the table for Exercise 6.6.
55. p. 345, Exercise 6.14 (c), replace "If the equilibrium conversion of component A determined in 6.14(d) is achieved in the adiabatic reactor, calculate the outlet temperature using the inlet conditions specified in 6.14(d)." with "Calculate the minimal inlet temperature of an adiabatic reactor required to achieve the equilibrium conversion of component A determined in 6.14(d)."
56. p. 346, Exercise 6.16, replace "In a PFR" with "in an adiabatic PFR."
57. p. 330, Figure 6.41 is not quite correct. The corrected figure is shown here in Figure 6.41.
58. p. 330, 11 lines from bottom. Change \( x = \Phi r \) to \( x = \Phi r \). Thanks to Matthew Lenz of UCSB for pointing out this erratum.
59. p. 373, add \( x 10^{-5} \) after \( = 2.125 \) in second equation after Equation 7.37.
60. p. 382, change the upper limit of integration from \( c \) to \( \tau \) in the equation preceding Equation 7.56.
61. p. 388, Table 7.4, in top block under Thiele modulus heading, replace \( B \) with \( \sqrt{B} \). Thanks to UCSB students for pointing out this erratum.
62. p. 390, Equation 7.67. Change \( \frac{D}{n} \) to \( D_0 \). Thanks to Fox Bernhard of UCSB for pointing out this erratum.
63. p. 391, replace the last sentence of the first paragraph with the following.

We even obtain an incorrect reaction order: the first-order reaction is correct, but a second-order reaction appears 3/2 order, and so on.

Figure 6.41: Coolant temperature at reactor outlet versus temperature at reactor inlet, \( T_0(f) \) versus \( T_0(o) \), at the critical value of heat-transfer coefficient; upper and middle steady-state solutions have coalesced.

64. p. 393, Add the definitions of dimensionless variables,

\[
\tau = \frac{C_A}{C_{A0}} \quad \Phi = \frac{T - T_f}{T_0}
\]

to the definitions of dimensionless parameters \( \psi, \beta, \) and \( \Phi \).
65. p. 393, in Equation 7.74, \( d\tau/d\Phi = 0 \) at \( \tau = 0 \), and \( \tau = 1 \) at \( \tau = 3 \).
66. p. 399, Table 7.5, change the units of \( k_0 \) and \( k_B \) to \( \text{cm}^3/\text{mol} \cdot \text{s} \). Thanks to Ralph White of South Carolina for pointing out this erratum.
67. p. 400, third equation. Insert a minus sign on the right-hand side. Fourth and fifth equations: change minus sign to plus sign. Thanks to Ralph White of South Carolina for pointing out this erratum.
68. p. 405, replace \( (1 - C_A) \) in second equation with \( 1/(1 - C_A) \).
69. p. 405, replace \( \left( \frac{D_i}{D} \right) \) in third equation with \( \frac{D_i}{D} \).
70. p. 408, replace \( \frac{D_i}{D} \) in second equation after Equation 7.104. Factor of \( \sqrt{\Phi} \) missing from numerator. Thanks to Amy Claas of UW for pointing out this erratum.
71. pp. 409±411, Example 7.6. Change the reactor feed sentence to "The feed to the reactor consists of 16.7 mol% CO, 83.3 mol% O\(_2\), and zero CO\(_2\), with volumetric flowrate \( Q_j = 712 \) L/s." Thanks to Khalifa Yousif of UW for reporting this erratum. The rate constant should
be $k = 1.3828 \times 10^{10} \exp(-13,500/T)$. With the adjusted rate constant and flowrate given above, the reactor volume should be $V_R = 233 \text{ cm}^3$ instead of $L$. Also change the units on the x-axis from $L$ to $\text{cm}^3$ in Figures 7.27 and 7.28. Thanks to Jason Haugh and the students at NC State for reporting this erratum.

72. p. 409, seventh line from bottom. Replace "The catalyst pellet radius is $0.1 \text{ cm}"$ with "The spherical catalyst pellet radius is $0.1 \text{ cm}$, and the densities are $\rho_p = 0.84, \rho_b = 0.60 \text{ g/cm}^3"$.

73. p. 412, Table 7.6, delete $K$ in the units of the two heats of reaction, $\Delta H_{R1}, \Delta H_{R2}$.

74. p. 418. Change $k_{jm}$ to $k_{jn}$. Thanks to Robert Erickson of UW for pointing out this erratum.

75. p. 422, Exercise 7.4, change the units on the rate constant to cm$^3$/mol s.

76. p. 428, Exercise 7.18 (b), change "...two derivatives with respect to $\xi$..." to "...two derivatives with respect to $x$...".

77. p. 430, Exercise 7.19. In order to make the simulation more realistic, change the second paragraph to the following. In order to get reasonable pressure drops at these higher engine loads, let's assume the catalyst bed porosity is $\varepsilon_b = 0.4$, and the inlet pressure and temperature are $P_i = 1.5 \text{ atm}, T_f = 570 \text{ K}$. Assume the cross-section of the catalytic converter bed has a diameter four times as large as the exhaust pipe. Therefore the velocity in the entrance to the converter $v = 1/4$ the velocity in the exhaust pipe.

(a) Calculate the fluid and pellet profiles in the bed for $u_f = 5 \text{ m/sexhaust pipe velocity at the entrance to the catalytic converter.}$ How much catalyst is required to reach $97.0\%$ conversion of CO and $\text{C}_3\text{H}_8$ under the new engine operation? What is the pressure drop for this case?

(b) Using the bed size from the previous part, resolve the problem with the idling speed, $u_f = 0.75 \text{ m/s exhaust pipe velocity at the entrance to the catalytic converter.}$ What is the conversion of CO and $\text{C}_3\text{H}_8$ at the end of the bed? What is the pressure drop across the bed?

78. p. 451, add the phrase "for the reaction $A \rightarrow B$, $r = k_1$" with second-order, irreversible kinetics" to the last sentence on page 451.

79. p. 452, Figure 8.12, time should have units of minutes. Thanks to Ralph White of U, South Carolina, for pointing out this erratum.

80. p. 453, change $p(t) \rightarrow P(t)$ (two places).

81. p. 453, change $I$ to $\theta$ in both $P(t)$ equations (two places in each equation).

82. p. 461, change $\alpha$ to $\lambda$ in first two equations after the start of the numerical solution section (two places).

83. p. 461, change $\theta$ to $\lambda$ two lines before Example 8.3.
Chemical Reactor Analysis and Design Fundamentals

Other Changes from the First to Second Printing

September 19, 2020

1. The parameter $V_R/Q_j$ is now denoted by $\tau$ instead of $\theta$ in Chapters 4 and 6. The variable $\theta$ is now mainly used in Chapter 8 as the residence time variable.

2. We adopted the overbar notation to denote partial molar quantities such as partial molar volume, enthalpy, entropy, Gibbs energy and heat capacity.

3. One example was added to Chapter 6, Example 6.3, which shows how to write the mass and energy balances for systems with multiple phases.

4. One section was added to Chapter 7, Section 7.7.2, which shows how to use a logarithmic transformation to calculate the catalyst pellet concentrations when there are steep concentration profiles.

5. One new exercise was added to Chapter 6. Exercise 6.22, "CSTR steady-state isola."

6. One new exercise was added to Chapter 7, Exercise 7.20, "Logarithmic transformation."

7. Noise was added to the data in Exercise 9.6, the title of the exercise was changed to "Estimating rate constant from catalyzed CSTR reaction data," and the exercise now asks for a plot of the model’s fit to the data.

8. Four new exercises were added to Chapter 9. The corresponding exercise numbers are listed below:

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