Numerical Methods in Chemistry
Solutions to Exercises 2

Problem 1

(a) We decompose the original rational function into partial fractions:

$$\frac{2\,(2s+7)}{(s+4)\,(s+2)} = \frac{A}{s+4} + \frac{B}{s+2},$$

$$2\,(2s+7) = (s+2)\,A + (s+4)\,B,$$

$$s = -4 \Longrightarrow 2(-8+7) = -2A \Longrightarrow A = 1,$$

$$s = -2 \Longrightarrow 2(-4+7) = 2B \Longrightarrow B = 3.$$

Therefore

$$\frac{2\,(2s+7)}{(s+4)\,(s+2)} = \frac{1}{s+4} + \frac{3}{s+2}.$$

The inverse Laplace transform is

$$\mathcal{L}^{-1}\left\{\frac{1}{s+4} + \frac{3}{s+2}\right\} \overset{\text{linearity}}{=} \mathcal{L}^{-1}\left\{\frac{1}{s+4}\right\} + 3\,\mathcal{L}^{-1}\left\{\frac{1}{s+2}\right\} \overset{1^{\text{st}}\text{shift theorem}}{=} e^{-4t} + 3e^{-2t}.$$

(b) Partial fraction decomposition:

$$\frac{s+9}{s^2-9} = \frac{s+9}{(s-3)\,(s+3)} = \frac{A}{s-3} + \frac{B}{s+3},$$

$$s+9 = (s+3)\,A + (s-3)\,B,$$

$$s = 3 \Longrightarrow 12 = 6A \Longrightarrow A = 2,$$

$$s = -3 \Longrightarrow 6 = -6B \Longrightarrow B = -1.$$

We get

$$\frac{s+9}{s^2-9} = \frac{s+9}{(s-3)\,(s+3)} = \frac{2}{s-3} - \frac{1}{s+3}.$$

The inverse Laplace transform is given by

$$\mathcal{L}^{-1}\left\{\frac{2}{s-3} - \frac{1}{s+3}\right\} \overset{\text{linearity}}{=} 2\,\mathcal{L}^{-1}\left\{\frac{1}{s-3}\right\} - \mathcal{L}^{-1}\left\{\frac{1}{s+3}\right\} \overset{1^{\text{st}}\text{shift theorem}}{=} 2e^{3t} - e^{-3t}.$$

Problem 2

The initial value theorem states that

$$\lim_{t \to 0} f(t) = \lim_{s \to \infty} sF(s).$$

(a) The left-hand side is given by

$$\lim_{t \to 0} f(t) = \lim_{t \to 0} (2 + \cos t) = 3.$$

The Laplace transform of $f(t)$ is

$$F(s) = \mathcal{L}\{f(t)\} = \mathcal{L}\{2 + \cos t\} = \mathcal{L}\{2\} + \mathcal{L}\{\cos t\} = \frac{2}{s} + \frac{s}{s^2 + 1},$$

and

$$sF(s) = 2 + \frac{s^2}{s^2 + 1}.$$

So the right-hand side is

$$\lim_{s \to \infty} sF(s) = \lim_{s \to \infty} \left(2 + \frac{s^2}{s^2 + 1}\right) = 3,$$

which verifies the initial value theorem.

(b) The limit on the left-hand side is

$$\lim_{t \to 0} f(t) = \lim_{t \to 0} (4 + t)^2 = 16.$$

The Laplace transform of $f(t)$ is

$$F(s) = \mathcal{L}\{f(t)\} = \mathcal{L}\left\{(4 + t)^2\right\} = \mathcal{L}\left\{16 + 8t + t^2\right\} = 16\,\mathcal{L}\{1\} + 8\,\mathcal{L}\{t\} + \mathcal{L}\left\{t^2\right\} = \frac{16}{s} + \frac{8}{s^2} + \frac{2}{s^3},$$

and

$$sF(s) = 16 + \frac{8}{s} + \frac{2}{s^2}.$$

Hence the limit on the right-hand side is

$$\lim_{s \to \infty} sF(s) = \lim_{s \to \infty} \left(16 + \frac{8}{s} + \frac{2}{s^2}\right) = 16,$$

and this verifies the initial value theorem for this example.

Problem 3

The final value theorem states that

$$\lim_{t\to\infty} f(t) = \lim_{s\to 0} sF(s)$$

(a) The limit on the left-hand side of the final value theorem is

$$\lim_{t\to\infty} f(t) = \lim_{t\to\infty} \left(3 + e^{-t}\right) = 3.$$

The Laplace transform of $f(t)$ is

$$F(s) = \mathcal{L}\left\{3 + e^{-t}\right\} = 3\,\mathcal{L}\left\{1\right\} + \mathcal{L}\left\{e^{-t}\right\} = \frac{3}{s} + \frac{1}{s+1},$$

so

$$sF(s) = 3 + \frac{s}{s+1},$$

and the limit on the right-hand side of the final value theorem is

$$\lim_{s\to 0} sF(s) = \lim_{s\to 0} \left(3 + \frac{s}{s+1}\right) = 3,$$

which verifies the theorem statement.
(b) The left-hand side is

$$\lim_{t\to\infty} f(t) = \lim_{t\to\infty} \left(t^3 e^{-t}\right) = 0.$$

The Laplace transform of $f(t)$ is

$$F(s) = \mathcal{L}\left\{t^3 e^{-t}\right\} \overset{1^{\text{st}}\text{shift theorem}}{=} \frac{3!}{(s+1)^4} = \frac{6}{(s+1)^4},$$

and

$$sF(s) = \frac{6s}{(s+1)^4}.$$

So the limit on the right-hand side is

$$\lim_{s\to 0} sF(s) = \lim_{s\to 0} \frac{6s}{(s+1)^4} = 0,$$

and this verifies the final value theorem for this example.

Problem 4

We calculate the Laplace transform of the Heaviside step function $h\left(t-a\right)$:

$$\mathcal{L}\left\{h\left(t-a\right)\right\} = \int_0^\infty h\left(t-a\right) e^{-st}\,\mathrm{d}t \overset{a\geq 0}{=} \int_a^\infty e^{-st}\,\mathrm{d}t = \left[-\frac{e^{-st}}{s}\right]_a^\infty = \frac{e^{-sa}}{s}.$$