Mathematical methods in chemistry. Exam for Part II.

Total = 90 points

May 28, 2024

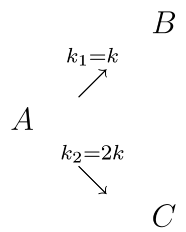
You do not need to derive any formulas in the provided **formula sheet** or **hints** on page 2.

Problem 1 (30 points)

Let $f(x) = \cos(2x)$. Find the
(a) Laplace transform $\mathcal{L}[f(t)]$,
(b) cosine Fourier series of $f(x)$ on the interval $(0, \pi)$, and
(c) sine Fourier series of $f(x)$ on the interval $(0, \pi)$.

Problem 2 (30 points)

Consider the **parallel reactions**



with the indicated rate constants ($k_1 = k$ and $k_2 = 2k$) and initial concentrations $[A]_0 = a_0$ and $[B]_0 = [C]_0 = 0$. The concentrations $a(t) := [A]_t$, $b(t) := [B]_t$, and $c(t) := [C]_t$ at time t satisfy the following system of ordinary differential equations (ODEs):

$$\begin{aligned}\dot{a}(t) &= -(k_1 + k_2)a(t),\\ \dot{b}(t) &= k_1 a(t),\\ \dot{c}(t) &= k_2 a(t).\end{aligned}$$

(a) Use the **Laplace transform** to solve this system and find the concentrations $a(t)$, $b(t)$, and $c(t)$ at time t.
(b) What is the branching ratio of this reaction [i.e., $c(t)/b(t)$]?
(c) What are the concentrations of A, B, and C reached at infinitely long times $t \to \infty$?
Note: The answers to (a), (b), and (c) should be expressed in terms of a_0, k, and t alone.
(d) Draw a figure of the concentrations $a(t)$, $b(t)$, and $c(t)$ as functions of time t for $a_0 = k = 1$.

EXAM CONTINUES ON PAGE 2 !

Problem 3 (30 points)

Use the **method of separation of variables** and **Fourier series** to solve the Laplace equation

$$u_{xx}(x,y) + u_{yy}(x,y) = 0, \quad x \geq 0,\, 0 \leq y \leq \pi,$$

describing the steady temperatures in a semi-infinite plate, whose edges are kept at fixed temperatures

$$\begin{aligned} &u(x,0) = 0 \quad \text{and} \quad u(x,\pi) = 0 \quad \text{for} \quad x \geq 0, \text{ and} \\ &u(0,y) = \sin(y) - \sin(2y) \quad \text{for } 0 \leq y \leq \pi. \end{aligned}$$

Moreover, the temperature in the plate is bounded, i.e., $|u(x,y)| \leq M$, where $M \in \mathbb{R}$.
(a) Find $u(x,y)$, that is, the dependence of temperature on coordinates.
(b) What is the temperature at the point $(x,y) = (\ln 2, \pi/2)$ inside the plate?

Hints for Problems 1 to 3

You can use these formulas without deriving them:
Inverse Laplace transforms:

$$\mathcal{L}^{-1}\left[\frac{1}{s}e^{-a\sqrt{s}}\right] = \operatorname{erfc}\left(\frac{a}{2\sqrt{t}}\right),$$

$$\mathcal{L}^{-1}\left[e^{-a\sqrt{s}}\right] = \frac{a}{2\sqrt{\pi t^3}}e^{-a^2/(4t)}.$$

General solutions of homogeneous ODEs ($k \in \mathbb{R}$; $n \in \mathbb{N}$; a and b are arbitrary constants):

$$\frac{d}{dx}y(x) + k\,x^n\,y(x) = 0 \quad \text{has a general solution} \quad y(x) = ae^{-kx^{n+1}/(n+1)},$$

$$\frac{d^2}{dx^2}y(x) + k^2 y(x) = 0 \quad \text{has a general solution} \quad y(x) = a\cos(kx) + b\sin(kx),$$

$$\frac{d^2}{dx^2}y(x) - k^2 y(x) = 0 \quad \text{has a general solution} \quad y(x) = ae^{kx} + be^{-kx}.$$

Particular solutions of inhomogeneous ODEs ($k, A, B, C \in \mathbb{R}$; a and b are suitable constants):

$$\frac{d^2}{dx^2}y(x) \pm k^2 y(x) = A\cos(Cx) + B\sin(Cx) \quad \text{has a particular solution} \quad y(x) = a\cos(Cx) + b\sin(Cx),$$

$$\frac{d^2}{dx^2}y(x) \pm k^2 y(x) = Ae^{Cx} \quad \text{has a particular solution } y(x) = ae^{Cx}.$$