Homework 5 — Multiple Choice

ChE 132A

Exercise 1 (Fourier sine series of a triangle wave).

The triangle wave on $0 \le x \le 1$ is

$$f(x) = \begin{cases} x & x < 1/2 \\ 1 - x & x \ge 1/2 \end{cases}$$

We expand it in the sine basis as $f(x) = \sum_{n=1}^{\infty} \alpha_n \sin(n\pi x)$.

(a) Using the orthogonality relation $\int_0^1 \sin(n\pi x)\sin(m\pi x)\ \mathrm{d}x = \frac{1}{2}\delta_{nm}$, the coefficient α_n is given by

- (A) $\dfrac{1}{2}\int_0^1 f(x)\sin(n\pi x)\ \mathrm{d}x$
- (B) $2\int_0^1 f(x)\sin(n\pi x)\ \mathrm{d}x$
- (C) $\int_0^1 f(x)\cos(n\pi x)\ \mathrm{d}x$
- (D) $\dfrac{2}{n\pi}\int_0^1 f(x)\sin(n\pi x)\ \mathrm{d}x$

(b) The triangle wave is even about $x = 1/2$, while $\sin(n\pi x)$ is symmetric or antisymmetric about $x = 1/2$ depending on whether n is odd or even. As a consequence,

- (A) $\alpha_n = 0$ for odd n
- (B) $\alpha_n = 0$ for even n
- (C) All α_n are nonzero
- (D) α_n is nonzero only for $n = 1$

(c) For odd n, the symmetry of f about $x = 1/2$ reduces the coefficient to

$$\alpha_n = 4\int_0^{1/2} x\ \sin(n\pi x)\ \mathrm{d}x$$

Integration by parts (the boundary term vanishes since $\cos(n\pi/2) = 0$ for odd n) gives

- (A) $\alpha_n = \dfrac{4}{n\pi}$
- (B) $\alpha_n = \dfrac{4\,(-1)^{(n-1)/2}}{(n\pi)^2}$
- (C) $\alpha_n = \dfrac{4(-1)^n}{n\pi}$
- (D) $\alpha_n = \dfrac{2}{(n\pi)^2}$

(d) The nonzero coefficients α_n decay as

- (A) $1/n$

(B) $1/n^2$
(C) $1/n^3$
(D) exponentially in n

This decay rate is one power faster than for the square wave's Fourier series, reflecting that f is continuous (only the slope is discontinuous, at $x = 1/2$).

Exercise 3 (Fourier series of a narrow triangle wave).

Taken from (Graham and Rawlings, 2022, Exercise 2.10).

A narrow triangle wave is supported on $[0.4, 0.6]$ with peak value 1 at $x = 1/2$. Its Fourier sine series is $f(x) = \sum_{n=1}^{\infty} a_n \sin(n\pi x)$.

(a) On the interval $[0.4, 0.5]$ the rising leg is a straight line passing through $(0.4, 0)$ and $(0.5, 1)$. Its equation is

(A) $f(x) = 10x$
(B) $f(x) = 5x - 2$
(C) $f(x) = 10x - 4$
(D) $f(x) = 2x - 0.8$

(b) The triangle is even about $x = 1/2$, while $\sin(n\pi x)$ is symmetric or antisymmetric about $x = 1/2$ depending on n. Therefore

(A) $a_n = 0$ for even n
(B) $a_n = 0$ for odd n
(C) All a_n are nonzero
(D) $a_n = 0$ except for $n = 1$

(c) For odd n, this symmetry also gives

$$\int_0^1 f(x)\sin(n\pi x)\,\mathrm{d}x = 2\int_{0.4}^{0.5} f(x)\sin(n\pi x)\,\mathrm{d}x$$

Using $f(x) = 10x - 4$ on $[0.4, 0.5]$ and the integration-by-parts identity

$$\int (mx+b)\sin(n\pi x)\,\mathrm{d}x = -\frac{mx+b}{n\pi}\cos(n\pi x) + \frac{m}{(n\pi)^2}\sin(n\pi x)$$

the coefficient evaluates to

(A) $a_n = \dfrac{4(-1)^{(n-1)/2}}{(n\pi)^2}$
(B) $a_n = \dfrac{40\,(-1)^{(n-1)/2}\big[1 - \cos(n\pi/10)\big]}{(n\pi)^2}$
(C) $a_n = \dfrac{10\sin(n\pi/10)}{(n\pi)^2}$

(D) $a_n = \dfrac{40\left[1 - \cos(n\pi/10)\right]}{n\pi}$

(d) Roughly how many terms in the partial sum f_N are required to obtain visually-good convergence?

(A) $N \approx 5$
(B) $N \approx 10$
(C) $N \approx 50$
(D) $N \approx 1000$

The convergence is much slower than for the wide triangle of Exercise 1 because the narrow triangle's slopes are steeper and confined to a small region.

Exercise 8 (Effectiveness factor of a cylindrical catalyst pellet).

A long cylindrical catalyst pellet of radius R supports a first-order isothermal reaction with rate constant k (s^{-1}). The reactant has surface concentration c_s and diffusivity D. The dimensionless steady species balance is

$$\frac{1}{r'}\frac{d}{dr'}\left(r'\frac{d\hat{c}}{dr'}\right) = \phi^2\,\hat{c}, \qquad \hat{c}(1) = 1, \qquad \hat{c} \text{ bounded at } r' = 0$$

where $r' = r/R$, $\hat{c} = c/c_s$, and ϕ is the Thiele modulus.

(a) The Thiele modulus is given by

(A) $\phi = R\,k\,D$
(B) $\phi = R\sqrt{k/D}$
(C) $\phi = \sqrt{kR/D}$
(D) $\phi = (k/D)\,R^2$

Physically, ϕ^2 compares the diffusion time R^2/D to the reaction time $1/k$.

(b) The substitution $z = \phi r'$ converts the ODE to the modified Bessel equation of order zero, $z^2\hat{c}'' + z\,\hat{c}' - z^2\,\hat{c} = 0$. Its two linearly independent solutions are

(A) $J_0(z)$ and $Y_0(z)$
(B) $I_0(z)$ and $K_0(z)$
(C) $\sin(z)$ and $\cos(z)$
(D) e^z and e^{-z}

(c) Of the two terms in $\hat{c}(r') = A\,I_0(\phi r') + B\,K_0(\phi r')$, one coefficient is forced to zero by the boundedness requirement at the centerline $r' = 0$. Specifically,

(A) $A = 0$ because $I_0(0) = 0$
(B) $B = 0$ because K_0 diverges logarithmically at the origin
(C) $A = 0$ because the solution must decay at large r'
(D) Both A and B must be nonzero to satisfy the surface BC

Applying the surface BC $\hat{c}(1) = 1$ then gives $\hat{c}(r') = I_0(\phi r')/I_0(\phi)$.

(d) The effectiveness factor is the ratio of the actual reaction rate to the rate that would obtain at uniform surface concentration:

$$\eta = 2 \int_0^1 \hat{c}(r')\, r' \, \mathrm{d}r'$$

Using the integral identity $\int_0^x z\, I_0(z)\, \mathrm{d}z = x\, I_1(x)$ this evaluates to

- (A) $\eta(\phi) = I_0(\phi)/\phi$
- (B) $\eta(\phi) = I_1(\phi)/I_0(\phi)$
- (C) $\eta(\phi) = \dfrac{2\, I_1(\phi)}{\phi\, I_0(\phi)}$
- (D) $\eta(\phi) = 1 - \dfrac{I_1(\phi)}{\phi\, I_0(\phi)}$

(e) In the slow-reaction limit $\phi \to 0$, using $I_0(\phi) \approx 1$ and $I_1(\phi) \approx \phi/2$,

- (A) $\eta \to 0$
- (B) $\eta \to 1$
- (C) $\eta \to 2$
- (D) $\eta \to \infty$

The pellet sits at essentially uniform $\hat{c} \approx 1$, so it performs as well as a well-mixed reactor at c_s.

(f) In the fast-reaction limit $\phi \to \infty$, the asymptotic $I_\nu(\phi) \sim e^\phi/\sqrt{2\pi\phi}$ is independent of ν to leading order, so $I_1/I_0 \to 1$ and

- (A) $\eta \to 0$ exponentially
- (B) $\eta \to 2/\phi$
- (C) $\eta \to \phi$
- (D) $\eta \to 1$

Reactant is consumed in a thin shell near the surface and the bulk of the pellet is starved. Effectiveness drops as $1/\phi$ — the classical scaling of diffusion-limited heterogeneous catalysis.

References

M. D. Graham and J. B. Rawlings. *Modeling and Analysis Principles for Chemical and Biological Engineers*. Nob Hill Publishing, Santa Barbara, CA, 2nd, paperback edition, 2022. 560 pages, ISBN 978-0-9759377-6-1.