HWRS 561b Homework Answer Keys #2

- Assigned: Sunday, 8 February 2026
- Due: Thursday, 19 February 2026 (upload answers in PDF or Jupyter Notebook to D2L)
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- Semester: Spring 2026

1. (20 points) Consider one-dimensional conservative solute transport in a saturated homogeneous porous medium (with a length of L) governed by the advection–dispersion equation with constant porewater velocity (V) and dispersion coefficient (D).

   - (a) (7 points) Starting from the advection–dispersion equation, use a scaling analysis to derive the characteristic time scale for:

     – advection, t_a
     – dispersion, t_d

     Clearly state the characteristic length scale you assume.

   - (b) (6 points) Define the Peclet number using these characteristic time scales and explain its physical meaning in one or two sentences.

   - (c) (7 points) A tracer is injected into a homogeneous sand column of length $L = 1$ m with porewater velocity $V = 0.5$ m/day.

     – Case A: $D = 5 \times 10^{-3}$ m^2/day
     – Case B: $D = 5 \times 10^{-2}$ m^2/day

     For each case:

     – Compute t_a, t_d, and Pe.
     – State whether transport is advection-dominated, dispersion-dominated, or transitional (i.e., advection and dispersion are comparable).
     – Predict qualitatively and sketch how the breakthrough curve shape would differ between the two cases.

Answers:

1(a) Start from

$$\frac{\partial C}{\partial t} + V \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2}.$$

Use characteristic scales $x \sim L$, $t \sim t_c$, and $C \sim C_*$:

$$\frac{C_*}{t_c} + V \frac{C_*}{L} \sim D \frac{C_*}{L^2}.$$

Balancing each transport term with the storage term gives

$$t_a = \frac{L}{V}, \qquad t_d = \frac{L^2}{D}.$$

Note that the column length L is used as the characteristic length scale.

1(b) Define

$$Pe = \frac{t_d}{t_a} = \frac{VL}{D}.$$

Pe is the ratio of advective transport strength to dispersive spreading strength. Large Pe means advection-dominated transport; small Pe means dispersion-dominated transport.

1(c) For $L = 1$ m and $V = 0.5$ m/day,

$$t_a = \frac{1}{0.5} = 2 \text{ days.}$$

- Case A ($D = 5 \times 10^{-3}$ m^2/day):

$$t_d = \frac{1^2}{5 \times 10^{-3}} = 200 \text{ days,} \qquad Pe = \frac{200}{2} = 100.$$

  Classification: strongly advection-dominated.

- Case B ($D = 5 \times 10^{-2}$ m^2/day):

$$t_d = \frac{1^2}{5 \times 10^{-2}} = 20 \text{ days,} \qquad Pe = \frac{20}{2} = 10.$$

  Classification: still advection-dominated, but dispersion is much more important than that in Case A.

- BTC shape comparison: Case A has a steeper rise and less tailing (closer to piston-like). Case B has earlier low-concentration arrival, a smoother breakthrough front, and stronger tailing.

2. (20 points) A conservative tracer is injected continuously at concentration C_0 into a saturated soil column of length ($L = 0.5$ m). The initial concentration is zero everywhere. The porewater velocity is constant, and transport can be approximated as one-dimensional.

   - (a) (5 points) Write the analytical solution for concentration $C(x, t)$ in a semi-infinite domain for continuous injection with a 3rd-type (flux) inlet boundary condition, $-D\, \partial C/\partial x + VC|_{x=0} = VC_0$.

   - (b) (5 points) What boundary condition would you assign to the outlet for the solute transport in the saturated soil column? Explain why the semi-infinite domain solution may be directly used to approximate the column experiment at early times before the solute arrives at the outlet.

   - (c) (5 points) After the solute arrives at the outlet, the semi-infinite concentration solution is no longer consistent with your outlet boundary condition. Using the class approach, define the outlet flux-based concentration by $-D\, \partial C/\partial x + VC|_{x=L} = VC_f$, then write the revised expression for $C_f(L, t)/C_0$ and compute/plot breakthrough curves for the following Peclet numbers:

     - $Pe = 5$
     - $Pe = 50$
     - $Pe = 500$

     $L = 0.5$ m and you can choose V and D accordingly.

   - (d) (5 points) On the same figure, compare the three breakthrough curves and answer:

     - How does increasing Peclet number affect the steepness of the breakthrough curve?
     - Which case best approximates piston flow?
     - Which case shows the strongest early breakthrough and tailing?

Answers:

2(a) For continuous injection with a 3rd-type (flux) inlet boundary condition,

$$-D\frac{\partial C}{\partial x} + VC\Big|_{x=0} = VC_0,$$

the semi-infinite-domain solution $(x \geq 0)$ is

$$C(x,t) = \frac{C_0}{2}\left[\text{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \left(\frac{V^2t}{\pi D}\right)^{1/2}\exp\left(-\frac{(x - Vt)^2}{4Dt}\right) - \frac{1}{2}\left(1 + \frac{Vx}{D} + \frac{V^2t}{D}\right)\exp\left(\frac{Vx}{D}\right)\text{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right].$$

2(b) At the outlet of a finite column $(x = L)$, use an outflow (zero-gradient) boundary:

$$-D\left.\frac{\partial C}{\partial x}\right|_{x=L} = 0 \quad \Longleftrightarrow \quad \left.\frac{\partial C}{\partial x}\right|_{x=L} = 0.$$

Before the plume reaches $x = L$, the downstream boundary has negligible influence, so the semi-infinite solution is a good approximation.

2(c) To make the semi-infinite solution consistent with outlet interpretation in a finite column, use the flux-based concentration

$$\left(-D\frac{\partial C}{\partial x} + VC\right)\Big|_{x=L} = VC_f, \qquad C_f = \left(C - \frac{D}{V}\frac{\partial C}{\partial x}\right)\Big|_{x=L}.$$
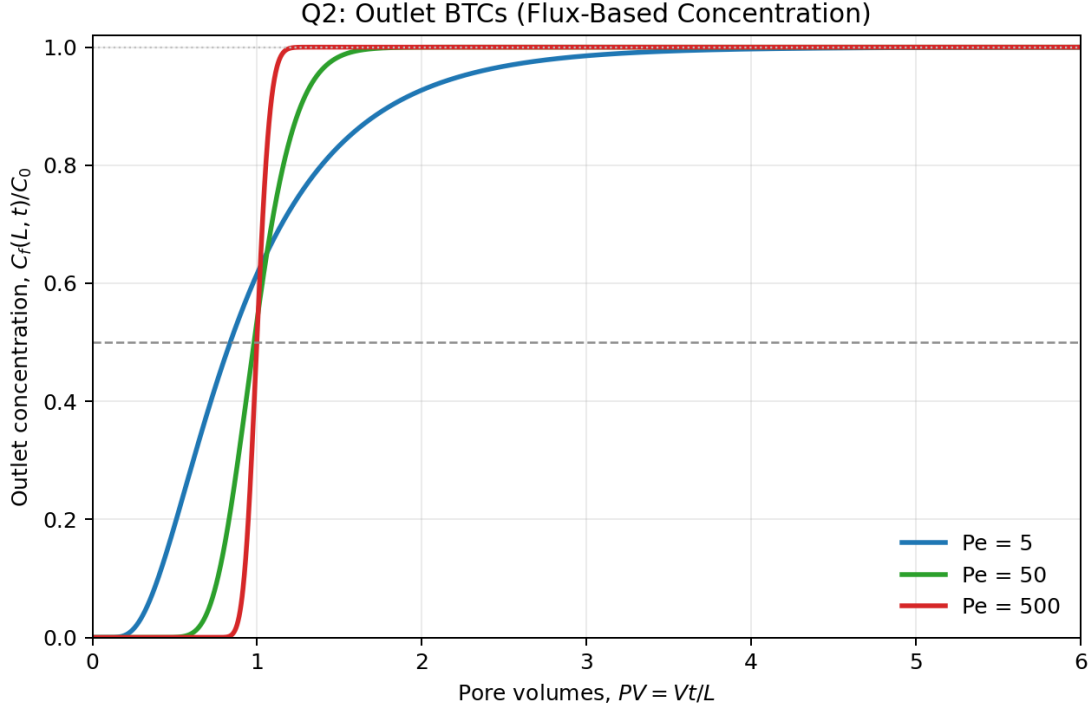
Substituting the solution from 2(a) gives

$$\frac{C_f(x,t)}{C_0} = \frac{1}{2}\left[\text{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{Vx}{D}\right)\text{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right].$$

For outlet BTCs, evaluate at $x = L = 0.5$ m, chose $V = 1$ m/day, and set

$$D = \frac{VL}{Pe}.$$

So $D = 0.1$, 0.01, and 0.001 m^2/day for $Pe = 5$, 50, and 500, respectively.

Computed outlet BTCs using $C_f(L, t)/C_0$:

Q2: Outlet BTCs (Flux-Based Concentration)

Representative results:

- $Pe = 5$: $C_f/C_0 = 0.5$ at about 0.837 pore volumes (strong spreading).

- $Pe = 50$: $C_f/C_0 = 0.5$ at about 0.980 pore volumes.

- $Pe = 500$: $C_f/C_0 = 0.5$ at about 0.998 pore volumes (near piston-like).

2(d) Increasing Pe makes the breakthrough curve steeper and shifts behavior toward advective piston flow.

- Best piston-flow approximation: $Pe = 500$.

- Strongest early breakthrough and tailing: $Pe = 5$.

3. (20 points) Consider solute transport in a semi-infinite domain ($x \geq 0$) with constant velocity V and dispersion coefficient D. The initial concentration is zero everywhere. At the inlet ($x = 0$), impose a flux boundary condition corresponding to two identical pulses of concentration: $VC - D\partial C/\partial x = VC_0$.

    - Pulse 1: $t = 0$ to $t = t_0$
    - Pulse 2: $t = T$ to $t = T + t_0$, where $T > t_0$

    Far-field boundary condition: $\lim_{x \to \infty} \partial C/\partial x$ is finite.

    - (a) (5 points) Write the analytical expression for concentration $C(x,t)$ due to a single pulse using the step-change continuous injection solution and the principle of superposition.

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- (b) (5 points) Using your result from (a), write the full analytical solution for the two-pulse injection at any location x and time t.
- (c) (5 points) Sketch (no computation required) the expected breakthrough curve at a fixed observation point $x = x_{obs}$, clearly indicating:
  - arrival of each pulse
  - overlap or separation depending on the relative magnitude of T, t_0, and dispersion
- (d) (5 points) Briefly explain why superposition is valid for this problem and under what conditions it would no longer be valid.

Answers:

Define the continuous step-response solution for the inlet flux boundary as

$$S(x,t) = \frac{C_0}{2} \left[\operatorname{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}} \right) + \exp\left(\frac{Vx}{D} \right) \operatorname{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}} \right) \right], \quad t > 0,$$

and $S(x,t) = 0$ for $t \leq 0$.

3(a) A single pulse from $t = 0$ to $t = t_0$ is

$$C_{\text{pulse}}(x,t) = S(x,t) - S(x, t - t_0)H(t - t_0),$$

where $H(\cdot)$ is the Heaviside function.

3(b) Two identical pulses (second starts at $t = T$) are

$$C(x,t) = C_{\text{pulse}}(x,t) + C_{\text{pulse}}(x, t - T)H(t - T),$$

which can be expanded as

$$\begin{aligned} C(x,t) = {} & S(x,t) - S(x, t - t_0)H(t - t_0) \\ & + S(x, t - T)H(t - T) - S(x, t - T - t_0)H(t - T - t_0). \end{aligned}$$

3(c) Expected BTC at $x = x_{obs}$:

- first rise/peak from pulse 1 arrival,

- second rise/peak from pulse 2 arrival,

- if T is large relative to pulse width and dispersive spreading, two peaks are clearly separated,

- if T is small (or dispersion is large), peaks overlap and may merge into one broad BTC.

3(d) Superposition is valid because the ADE here is linear, with constant coefficients and linear boundary forcing. It breaks down for nonlinear systems (for example, concentration-dependent D or V, nonlinear reactions, nonlinear sorption/kinetics).

4. (20 points) Consider one-dimensional transport of a solute in a saturated porous medium with equilibrium sorption described by a linear isotherm

$$C_s = K_d C$$

where C_s is the sorbed concentration (mass per mass of solid) and C is the aqueous concentration.

- (a) (7 points) Starting from the mass balance equation that includes both aqueous and sorbed phases,

$$\phi\frac{\partial C}{\partial t} + \rho_b\frac{\partial C_s}{\partial t} + \phi V\frac{\partial C}{\partial x} - \phi D\frac{\partial^2 C}{\partial x^2} = 0,$$

  derive the advection–dispersion equation with a retardation factor R. Explain what parameters control R.

- (b) (7 points) A tracer test is conducted in a sand column with:

  - porosity $\phi = 0.35$
  - bulk density $\rho_b = 1.65$ g/cm^3
  - pore water velocity $V = 0.4$ m/day
  - dispersion coefficient $D = 0.02$ m^2/day

  Two solutes are injected separately continously at a concentration of 1 mg/L

  - Solute A: $K_d = 0$
  - Solute B: $K_d = 0.8$ L/kg

  For each solute:

  - compute the retardation factor
  - compute the effective advective velocity (after accounting for the retardation factor R, i.e., $V_{\text{eff}} = V/R$)
  - predict qualitatively how the breakthrough curves would differ (Try your best to be as quantitative as possible). Explain why, under equilibrium sorption, the shape of the breakthrough curve is unchanged but the arrival time is delayed.

- (c) (6 points) Now suppose that the solute B does not follow linear adsorption, instead, it follows the Freundlich adsorption. $K_f = 0.8$ and $N = 0.7$. Sketch the breakthrough curve and contrast it with that from linear adsorption.

Answers:

4(a) With linear equilibrium sorption $C_s = K_d C$,

$$\frac{\partial C_s}{\partial t} = K_d\frac{\partial C}{\partial t}.$$

Substitute into

$$\phi\frac{\partial C}{\partial t} + \rho_b\frac{\partial C_s}{\partial t} + \phi V\frac{\partial C}{\partial x} - \phi D\frac{\partial^2 C}{\partial x^2} = 0:$$

$$(\phi + \rho_b K_d)\frac{\partial C}{\partial t} + \phi V\frac{\partial C}{\partial x} - \phi D\frac{\partial^2 C}{\partial x^2} = 0.$$

Divide by ϕ:

$$R\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = 0, \qquad R = 1 + \frac{\rho_b K_d}{\phi}.$$

So R is controlled by ϕ, ρ_b, and K_d.

4(b) Given $\phi = 0.35$, $\rho_b = 1.65$ g/cm$^3 = 1.65$ kg/L, $V = 0.4$ m/day, $D = 0.02$ m^2/day.

- Solute A ($K_d = 0$):

$$R_A = 1, \qquad V_{\text{eff},A} = \frac{V}{R_A} = 0.4 \text{ m/day}.$$

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- Solute B ($K_d = 0.8$ L/kg):

$$R_B = 1 + \frac{1.65 \times 0.8}{0.35} = 4.771, \qquad V_{\text{eff},B} = \frac{0.4}{4.771} = 0.0838 \text{ m/day}.$$

Solute B arrives about 4.77× later than Solute A. Under linear equilibrium sorption, advection and dispersion are both scaled by $1/R$ in time, so BTC shape in appropriately normalized time is unchanged; the main effect is delay.

4(c) For Freundlich sorption,

$$C_s = K_f C^N, \qquad K_f = 0.8, \ N = 0.7.$$

The local slope is

$$\frac{dC_s}{dC} = K_f N C^{N-1},$$

so apparent retardation becomes concentration-dependent:

$$R_{\text{app}}(C) = 1 + \frac{\rho_b}{\phi} \frac{dC_s}{dC}.$$

Because $N < 1$, low concentrations are relatively more retarded than high concentrations. Compared with linear sorption, this generally yields a more asymmetric BTC (sharper front with stronger late-time tailing).

5. (20 points) Consider one-dimensional solute transport in a saturated porous medium column with first-order kinetic sorption. The sorbed concentration evolves according to

$$\frac{\partial C_s}{\partial t} = k(K_d C - C_s),$$

where k is a first-order rate constant.

- (a) (5 points) Write the coupled system of equations governing aqueous concentration $C(x,t)$ and sorbed concentration $C_s(x,t)$.

- (b) (5 points) Explain why a single, constant retardation factor R can no longer be defined for this system.

- (c) (5 points) Consider a pulse injection at the inlet ($x = 0$) with duration t_0. Qualitatively describe how the breakthrough curve at a fixed observation point changes as:
  - $k \to \infty$
  - $k \to 0$

  On the same plot, also sketch the breakthrough curve with equilibrium sorption. In your answer, discuss peak arrival time, tailing, and mass recovery.

- (d) (5 points) Briefly explain why kinetic sorption often produces long late-time tails in breakthrough curves, even when dispersion is small.

Answers:
5(a) The coupled system is

$$\phi \frac{\partial C}{\partial t} + \rho_b \frac{\partial C_s}{\partial t} + \phi V \frac{\partial C}{\partial x} - \phi D \frac{\partial^2 C}{\partial x^2} = 0,$$

$$\frac{\partial C_s}{\partial t} = k(K_d C - C_s).$$

(plus initial and boundary conditions for pulse input at $x = 0$.)

5(b) A single constant retardation factor R requires an algebraic equilibrium relation $C_s = C_s(C)$ at every instant. Here sorption is rate-limited, so C_s depends on kinetic history (memory), not only on instantaneous C. Therefore, effective retardation is time-dependent and no single constant R fully describes the system.

5(c) Pulse BTC behavior at fixed x:

- $k \to \infty$: recovers equilibrium sorption; delayed peak (relative to conservative case), limited tailing.

- $k \to 0$: little exchange during experiment; BTC approaches conservative transport (earlier peak, much less retardation).

- finite/intermediate k: typically earlier peak than equilibrium, lower peak concentration, and stronger late-time tailing due to slow desorption.

For reversible sorption, total mass can eventually approach full recovery, but finite-time observations may not recover all the mass.

5(d) Kinetic sorption creates long tails because solute partitions into slower domains/phases and is released gradually. This slow back-transfer sustains low concentrations long after the main advective front has passed, even when hydrodynamic dispersion is small.

6. (20 points) Use the notebook `Resources->Numerical solution for solute transport [Jupyter Notebook]` on the GitHub website to investigate one-dimensional solute transport in a finite domain. For all parts below, include your modified parameter values, plots, and concise interpretation.
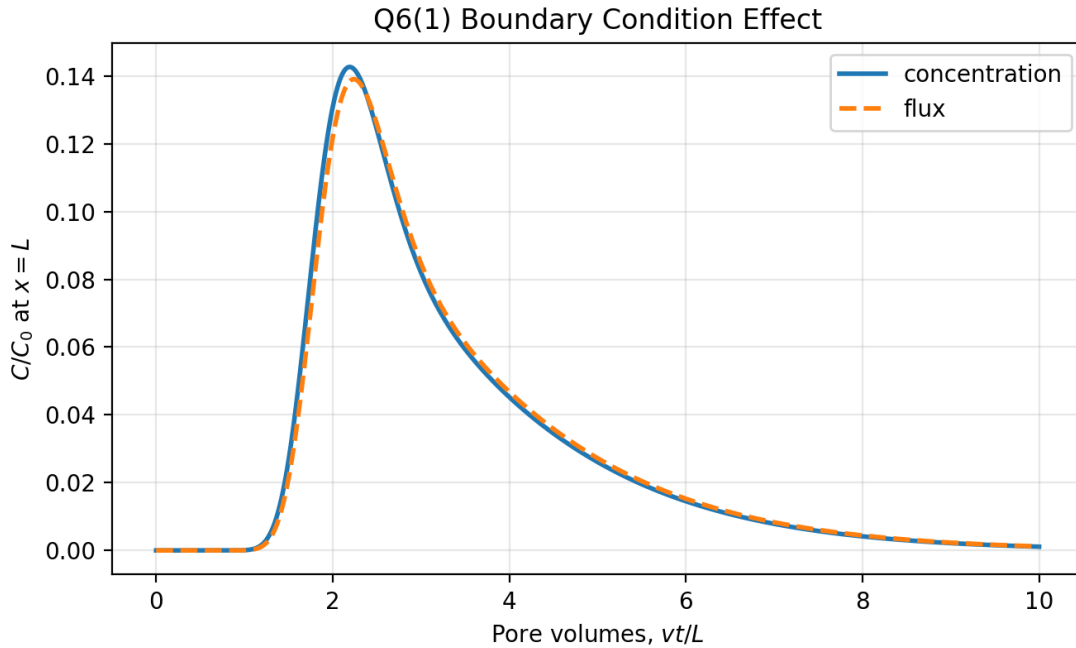
   - (a) (5 points) Baseline and boundary condition effect:
     - Start from the default settings in the notebook.
     - Run one case with `bc_type = 'concentration'` and one case with `bc_type = 'flux'` (all other parameters unchanged).
     - Plot normalized outlet breakthrough curves (C/C_0 at $x = L$) versus pore volumes on the same figure and compare peak concentration and arrival behavior.

   - (b) (5 points) Dispersion sensitivity:
     - Set `sorption_type = 'none'` and `use_two_site = False`.
     - Run at least three dispersion values (for example, low, medium, high D while keeping L and v fixed).
     - Compare how increasing D changes early breakthrough, curve steepness, and tailing at the outlet.

   - (c) (5 points) Equilibrium sorption model comparison:
     - Keep transport parameters fixed and run `sorption_type = 'none'`, `'linear'`, `'freundlich'`, and `'langmuir'` with `use_two_site = False`.
     - On one figure, compare outlet breakthrough curves and rank the four cases by apparent retardation (earliest to latest mean arrival).
     - Briefly explain whether differences are mainly shifts in arrival time, shape changes, or both.

- (d) (5 points) Kinetic two-site effects:
    - Choose one equilibrium isotherm (`'linear'`, `'freundlich'`, or `'langmuir'`) and turn on `use_two_site = True`.
    - Compare at least three kinetic scenarios by changing `F_s` and/or `alpha_s` (including one case close to equilibrium behavior and one strongly kinetic case).
    - Using linear and log-scale BTC plots, explain how kinetic sorption affects late-time tailing and mass release relative to the equilibrium-only case.

Answers:

All the results below were obtained using the finite-domain numerical solution notebook with parameters changed as requested in each sub-part.

6(a) Baseline and boundary-condition effect Defaults from the notebook were used ($L = 10$ m, $v = 1$ m/day, $D = 0.2$ m^2/day, $t_p = 3$ day, `sorption_type='linear'`, `use_two_site=True`, etc.) and only `bc_type` was switched.
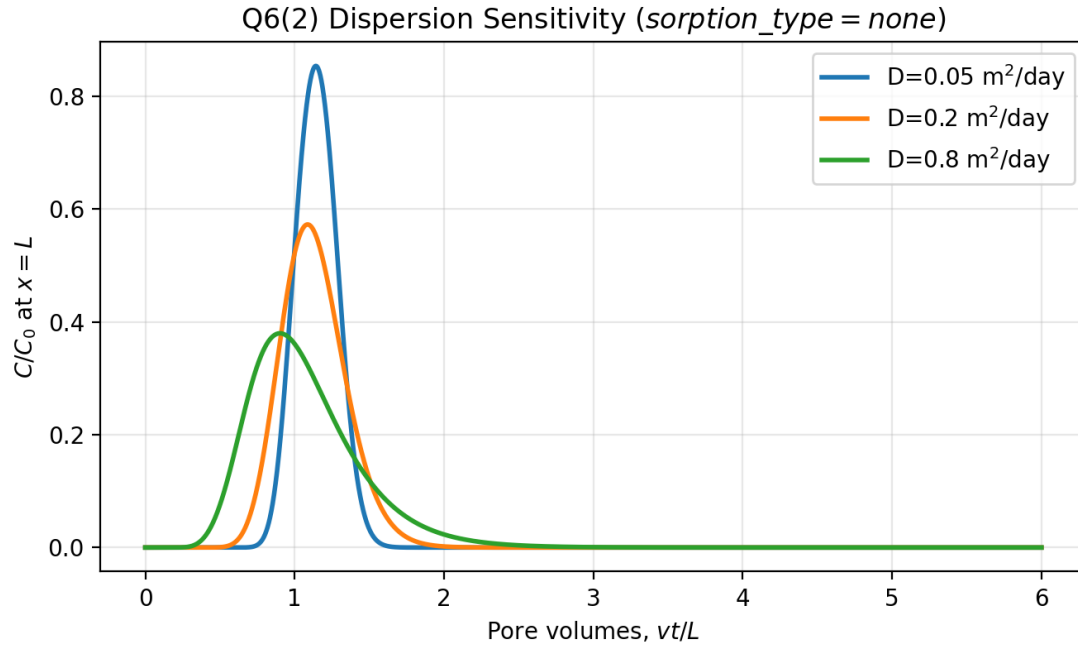

Q6(1) Boundary Condition Effect

Results (outlet BTC at $x = L$):

- `concentration` BC: peak ≈ 0.143 at $PV \approx 2.192$, mean arrival ≈ 3.328 PV.

- `flux` BC: peak ≈ 0.139 at $PV \approx 2.239$, mean arrival ≈ 3.391 PV.

With all else fixed, the concentration BC gives slightly earlier/higher breakthrough; flux BC is slightly more damped and delayed.
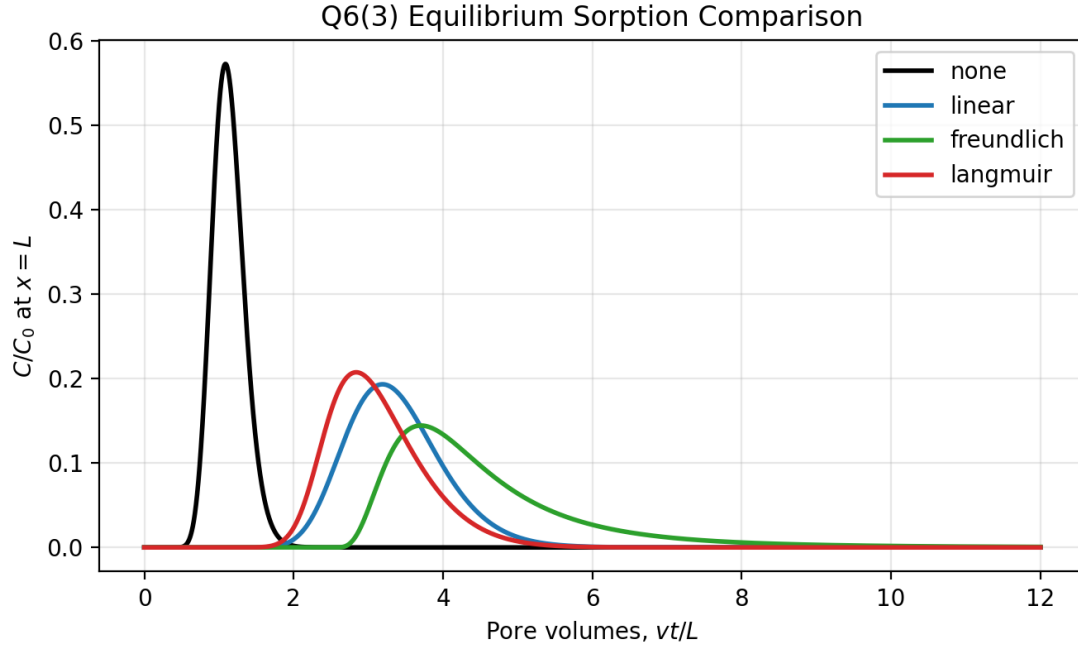
6(b) Dispersion sensitivity Set `sorption_type='none'` and `use_two_site=False`. Ran $D = 0.05$, 0.2, and 0.8 m^2/day (with $L = 10$ m, $v = 1$ m/day fixed).

Q6(2) Dispersion Sensitivity (*sorption_type = none*)

Comparison:

- Larger D gives stronger early breakthrough (e.g., at 0.8 PV: $C/C_0 \approx 0.022$, 0.179, 0.355 for $D = 0.05$, 0.2, 0.8).

- BTC fronts become less steep as D increases.

- Tailing/spreading increases with D.

6(c) Equilibrium sorption model comparison Kept transport parameters fixed and ran `none`, `linear`, `freundlich`, and `langmuir` with `use_two_site=False`.
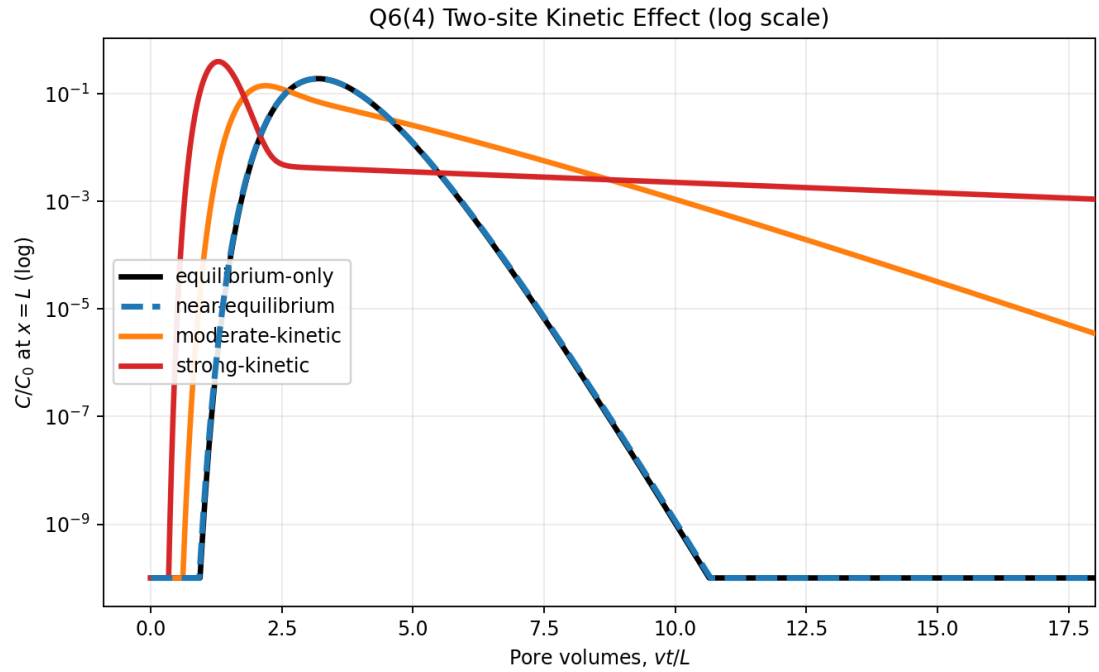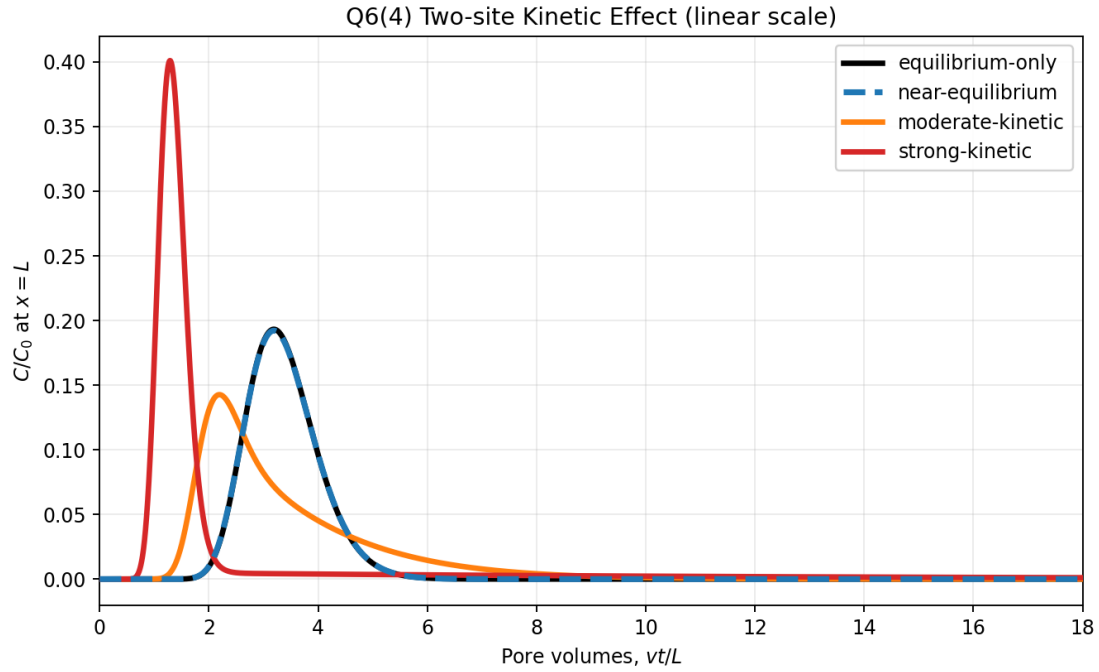
Q6(3) Equilibrium Sorption Comparison

Ranking by apparent retardation (earliest to latest mean arrival):

$$\text{none} < \text{langmuir} < \text{linear} < \text{freundlich}.$$

Interpretation:

- `none`: earliest arrival, least retardation.

- `linear`: mostly a time shift with comparatively limited distortion.

- `langmuir` and `freundlich`: both show shape changes because retardation is concentration-dependent.

- `freundlich` (with $N < 1$ here) shows the strongest late-time persistence among these runs.

6(d) Kinetic two-site effects Assuming `sorption_type='linear'`, compare: - near-equilibrium: `F_s=0.95`, `alpha_s=5.0` - moderate kinetic: `F_s=0.50`, `alpha_s=0.1` - strong kinetic: `F_s=0.10`, `alpha_s=0.01` plus an equilibrium-only reference (`use_two_site=False`).

Q6(4) Two-site Kinetic Effect (linear scale)

Q6(4) Two-site Kinetic Effect (log scale)

Observed behavior:

- Near-equilibrium almost overlaps equilibrium-only.

- Moderate/strong kinetic cases show stronger nonequilibrium signatures: earlier breakthrough and enhanced late-time tailing on log scale.

- Example tail indicator at 8 PV: equilibrium-only ≈ 0, moderate-kinetic $\approx 4.1 \times 10^{-3}$, strong-kinetic $\approx 2.7 \times 10^{-3}$.

Decreasing equilibrium fraction and/or slowing mass-transfer kinetics increases persistence of late-time release relative to the equilibrium-only case.