

S1. Multiscale facies-structure realizations

Four material classes were represented: clay-dominated sediment, sand-dominated sediment, weathered bedrock, and unweathered bedrock. The three-dimensional facies structure was generated in three linked stages on the 1 km model grid. Stage 1 used support vector machine (SVM), random forest (RF), multilayer perceptron (MLP), radial basis function (RBF) network, and k-nearest-neighbour (KNN) alternatives with fivefold borehole cross-validation to delineate the sediment–bedrock boundary. Stage 2 applied the same classifier family within the bedrock domain to distinguish weathered from unweathered bedrock. Stage 3 used transition-probability-based conditional geostatistical simulation within the sediment domain to generate clay–sand patterns with the volume proportions and directional mean lengths in Table S1.

The three stages were combined into 100 borehole-conditioned four-class facies realizations. Common random seeds made the generation reproducible. The realizations vary facies volume proportions, directional mean lengths, and learned bedrock-boundary alternatives within the prescribed ranges; they do not represent a probability-weighted or exhaustive distribution of geological histories.

Table S1. Settings used to generate the facies-structure realizations.

Facies class	Quantity	Range or setting
Clay-dominated sediment	Volume proportion	0.64–0.69
Clay-dominated sediment	Horizontal mean length (x and y)	5–30 km
Clay-dominated sediment	Vertical mean length (z)	9–13 m
Sand-dominated sediment	Volume proportion	0.31–0.36
Sand-dominated sediment	Horizontal mean length (x and y)	5–15 km
Sand-dominated sediment	Vertical mean length (z)	6–8.5 m

In the CTRL001 reference model, clay-dominated sediment, sand-dominated sediment, weathered bedrock, and unweathered bedrock occupy 15.3 %, 8.3 %, 5.4 %, and 71.0 % of the active three-dimensional domain, respectively. These whole-domain proportions describe the reference structure and differ from the sediment-domain clay and sand target volume proportions in Table S1.

S2. CTRL001-conditioned within-facies hydraulic-conductivity realizations

One hundred facies-conditioned horizontal hydraulic-conductivity (K_h) fields (KC001–KC100) were generated within the fixed four-class facies structure of CTRL001. All other model inputs were copied from CTRL001. Each active cell was

perturbed around its exact cellwise CTRL001 K_h value in logarithmic space. The class-specific perturbations had zero mean and the target standard deviations in Table S2, preserving the baseline class centers while introducing spatial variability within each class.

Pilot-point locations were randomly offset within the nominal spacings in Table S2. Each class contained at least 32 pilot points and approximately one pilot point per 650 active high-resolution cells when that criterion required more points. Pilot values were interpolated separately within each facies using normalized Gaussian kernels; values were not smoothed across facies boundaries. After vertical projection and aggregation to the MODFLOW grid, each class field was rescaled to a zero-mean, unit-standard-deviation perturbation before the specified class standard deviation was applied. Vertical hydraulic conductivity (K_z) was set to $K_h/10$.

Table S2. Variability and interpolation settings for the within-facies hydraulic-conductivity realizations.

Facies class	Target SD of log10 perturbation	Pilot spacing (y, x, z cells)	Gaussian scale (y, x, z cells)
Clay-dominated sediment	0.080	10, 10, 4	10, 10, 3
Sand-dominated sediment	0.120	8, 8, 4	9, 9, 3
Weathered bedrock	0.125	7, 7, 3	8, 8, 2.5
Unweathered bedrock	0.150	12, 12, 4	12, 12, 3

The perturbation in each cell was defined relative to the exact CTRL001 cellwise K_h ; Table S2 therefore reports the imposed variability rather than replacement class means.

Generation diagnostics for the 100 fields are summarized in Table S3. At the generator grid, all hard pilot values were reproduced exactly. On the MODFLOW grid, the maximum absolute facies mean of the log10 perturbation was 6.4×10^{-17} , and each realized facies standard deviation matched its target to numerical precision.

Table S3. Numerical diagnostics for the 100 CTRL001-conditioned hydraulic-conductivity fields.

Diagnostic	Result	Interpretation
Number of realizations	100	Fixed exact CTRL001 facies structure
Random seed	20260513	Reproducible realization sequence
Pilot-point count (minimum / median / maximum)	1824 / 1947.5 / 2078	Total across the four classes in each field
Maximum hard-pilot reproduction error	0	Exact at the generator grid
Aggregation fallback groups	0	All model-grid groups used the intended projection
Maximum absolute facies mean of log10 perturbation	6.4×10^{-17}	Numerically zero
Realized facies perturbation SD	0.080 / 0.120 / 0.125 / 0.150	Clay / sand / weathered bedrock / unweathered bedrock

The ensemble is conditional on the fixed CTRL001 facies geometry, the specified class standard deviations, and the selected pilot spacings and Gaussian scales. It quantifies responses within those tested choices; it is not a probability-weighted global sensitivity analysis or a complete geological-uncertainty distribution.

S3. Baseline and model-bottom experimental configurations

CTRL001 is the global baseline for the eight model-development groups. It uses a $1 \text{ km} \times 1 \text{ km}$ structured horizontal grid, 275,054 active three-dimensional cells, 33 layers, a top that follows land surface, and a model-bottom elevation of -115 m . Because land-surface elevation varies, total model thickness is spatially variable. Table S4 gives the baseline vertical discretization.

Table S4. Vertical discretization of CTRL001 and treatment in the model-bottom experiments.

Layer(s)	Elevation range	Layer thickness	Treatment in model-bottom experiments
1	Land surface to -2 m	Approx. 3–52 m	Fixed
2–19	-2 to -38 m	2 m	Fixed
20–29	-38 to -78 m	4 m	Fixed; layer 29 defines the protected lower interface
30–32	-78 to -108 m	10 m	Replaced by geometry-specific deep layers
33	-108 to -115 m	7 m	Lowest layer of CTRL001; replaced in the tested geometries

The model-bottom experiments retain the geometry, facies, hydraulic properties, and observation-informed initial fields of layers 1–29 through the -78 m interface. Below -78 m , the number and thickness of deep layers, active-cell count, and model-bottom elevation change together. Newly represented deep cells are unweathered bedrock. The primary series uses unweathered-bedrock $K_h = 10^{-5} \text{ m d}^{-1}$. Two additional series use $K_h = 10^{-4}$ and 10^{-3} m d^{-1} . In all three series, $K_z = K_h/10$.

Initial heads in newly represented deep cells were copied vertically from the deepest active shared-layer head in each column, and their initial total dissolved solids concentration was 0 mg L⁻¹. Each geometry then underwent its own 10-year warm-up before the common 2020–2024 simulation. Coastal constant-head boundaries and perimeter general-head boundaries were extended or truncated with the active geometry. General-head-boundary conductance was recalculated from K_h , layer thickness, and exposed boundary faces. River constant-head boundaries remained in layer 1; deep general-head-boundary records were restored below the 105 river-boundary columns on the historical perimeter, whereas the other 23 internal river-boundary columns received no deep general-head boundary.

Table S5. Configuration and comparison rules for the model-bottom experiments.

Item	Specification	Role in the experiment
Tested model-bottom elevations	–80, –90, –100, –120, –150, –180, –200, –250, –300, –400, –500, and –650 m	Twelve geometries in each bedrock-conductivity series
Corresponding layer counts	30, 31, 32, 34, 37, 40, 42, 44, 46, 50, 54, and 60	Paired with the elevations in the same order
Unweathered-bedrock K_h	10 ⁻⁵ , 10 ⁻⁴ , and 10 ⁻³ m d ⁻¹	The 10 ⁻⁵ m d ⁻¹ series enters the 300-configuration comparison; the other 24 runs evaluate the interaction with model-bottom elevation
Protected and changed domains	Layers 1–29 fixed; layers 30 and deeper geometry-specific	Separates deep-domain changes from the common shallow and sedimentary system
Initialization and warm-up	Common observation-informed fields in layers 1–29; vertically projected deep head; 0 mg L ⁻¹ deep initial TDS; geometry-specific 10-year warm-up	Provides an internally equilibrated starting state for each geometry
Formal simulation	2020–2024 (1827 d)	Identical forcing period and solver settings
Lateral-boundary treatment	Coastal constant head and perimeter general head follow geometry; river constant head remains in layer 1; general-head conductance is recalculated	Maintains boundary connections as the active depth changes
Response domain and reference	Common active clay and sand cells; each bedrock-conductivity series referenced to its own –120 m case	Excludes added or removed deep-bedrock volume from the salinity-volume response and isolates the effect of model-bottom elevation in Fig. 9

The –115 m CTRL001 model remains the global baseline. The –120 m configurations are used only as within-series references in Fig. 9 because all three unweathered-bedrock K_h series contain that geometry.