



1 Numerical Perturbation Assessment of Multiple Controls on Groundwater Flow 2 and Salinity Transport in Heterogeneous Coastal Delta Aquifers

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18

19 Abstract

20 Coastal-delta groundwater models must represent aquifer heterogeneity,
 21 hydrologic inputs, river–aquifer exchange, and lateral and deep hydraulic connections,
 22 but their relative importance can change with the forecast target. We used an
 23 observation-informed three-dimensional variable-density groundwater-flow and
 24 salinity-transport model of the Pearl River Delta to compare 300 configurations over a
 25 five-year simulation. Eight controls were examined: facies structure, spatial variability
 26 in hydraulic conductivity (K) within a fixed facies structure, recharge, river stage,
 27 riverbed conductance, inland boundaries, coastal boundaries, and model-bottom
 28 elevation. Facies structure produced the largest regional head response, and changes in
 29 hydrogeologic geometry and connectivity exerted a greater influence than within-facies
 30 K variability. Recharge produced widespread responses and the largest changes in
 31 volume-weighted mean total dissolved solids (TDS) and in the volumes of brackish-or-
 32 more-saline and high-salinity groundwater. Coastal boundaries generated the largest
 33 spatial TDS differences, concentrated in estuarine and nearshore aquifers. River-stage
 34 effects exceeded riverbed-conductance effects and followed the distributary network,
 35 whereas inland-boundary effects were concentrated near hydraulically connected
 36 margins. Within-facies K variability produced smaller, spatially dispersed responses,



37 and model-bottom elevation had little influence over five years under the tested bedrock
38 conditions. Model-development priorities depend on the prediction target, area of
39 interest, and spatial and temporal scales. Short-term regional forecasts require reliable
40 initial head and salinity fields, a credible three-dimensional heterogeneous
41 hydrogeologic framework, and well-constrained recharge. Boundary and deep-domain
42 detail become more important near hydraulically connected margins and over longer
43 periods. The perturbation approach and resulting insights are applicable to similar
44 coastal-delta and estuarine aquifers.

45 **1. Introduction**

46 Coastal deltaic aquifers occupy the land–sea transition and commonly contain
47 fluvial, marine, and transitional deposits with contrasting hydraulic properties and
48 complex stratigraphic organization (Barlow and Reichard, 2010; Custodio, 2010).
49 Terrestrial groundwater circulation, river–aquifer exchange, and coastal boundary
50 conditions interact within these systems (Brunner et al., 2009; Winter et al., 1998).
51 Inland recharge and regional hydraulic gradients drive freshwater toward rivers,
52 estuaries, and the sea. Rivers and distributary channels modify local heads and provide
53 pathways for water and solute exchange, whereas coastal water levels, salinity, and
54 density contrasts govern variable-density flow and mixing near the shoreline (Werner
55 et al., 2013). Because large groundwater systems adjust slowly to changes in sea level
56 and freshwater forcing, modern processes often act on salinity distributions that retain
57 the effects of Quaternary transgressions, regressions, and subsequent freshwater
58 flushing (Post et al., 2013; van Engelen et al., 2019, 2021). Regional simulation
59 therefore requires joint consideration of hydrostratigraphic structure, hydrologic
60 forcing, river–aquifer exchange, lateral and deep hydraulic connections, and the
61 inherited salinity field.

62 The internal hydrogeologic framework controls where groundwater can move and
63 where solutes can be stored or redistributed. Topography and the spatial distribution of
64 hydraulic conductivity (K) determine the depth and geometry of regional circulation
65 (Freeze and Witherspoon, 1967; Tóth, 1963). Facies geometry and within-facies K
66 variability define preferential pathways, low- K barriers, and their connectivity (Fogg,
67 1986; Weissmann et al., 1999). Fields with similar lower-order K statistics can produce
68 different flow and transport behavior when the connectivity of high- or low- K zones



69 differs (Renard and Allard, 2013; Zinn and Harvey, 2003). Recent studies further show
70 that multiscale sediment organization and facies interfaces influence plume spreading,
71 mixing, and reaction hotspots (Ren et al., 2022, 2026; Soltanian et al., 2025; Wallace et
72 al., 2021). In coastal and deltaic settings, the scale and arrangement of represented
73 heterogeneity affect salinity distributions, density-driven circulation, and contaminant
74 transport (Michael et al., 2016; Siena and Riva, 2018; Xu et al., 2022; Yu and Michael,
75 2022). Reconstructing this heterogeneity from incomplete observations increasingly
76 combines borehole and geophysical information with geostatistical, process-based, and
77 machine-learning approaches (Koltermann and Gorelick, 1996; Zhan et al., 2022).

78 External forcing and model-domain choices act through this internal framework.
79 Recharge changes freshwater input and regional hydraulic gradients, while river stage,
80 riverbed conductance, bank geometry, and adjacent aquifer structure jointly govern
81 river–aquifer exchange (Brunner et al., 2009; Engdahl et al., 2010; Xian et al., 2021).
82 Lateral boundary formulations represent alternative assumptions about hydraulic
83 connection between the modeled aquifer and surrounding groundwater or surface-water
84 systems, and the preferred mathematical representation depends on the physical
85 boundary and the purpose of the model (Reilly, 2001; Rojas et al., 2008). Model-bottom
86 elevation determines whether deeper flow paths are represented, but its practical
87 relevance depends on bedrock K , recharge, topography, fractures, prediction period, and
88 the output of interest (Cardenas and Jiang, 2010; Frisbee et al., 2017; Goderniaux et al.,
89 2013; Manning et al., 2021). Regional models must therefore decide not only which
90 processes to include, but also how much structural and parameter detail is required for
91 a given prediction.

92 Previous studies establish the relevance of these individual controls, but their
93 results are difficult to compare directly because they use different model geometries,
94 timescales, perturbation ranges, and response variables. Subsurface structures are
95 represented using a growing range of geostatistical, process-based, and data-driven
96 methods (de Marsily et al., 2005; Zhan et al., 2023), while model responses are
97 examined through multi-model comparisons and sensitivity or uncertainty analyses (Ye
98 et al., 2010; Pianosi et al., 2016). Such studies show that the apparent influence of a
99 model component can change with the selected output, spatial domain, and time horizon
100 (Dai et al., 2017; van Engelen et al., 2021). However, it remains difficult to translate
101 these separate findings into model-development priorities for a single observation-
102 informed regional coastal-delta model. In particular, it is unclear how plausible choices



103 in hydrostratigraphic structure, property fields, hydrologic forcing, river exchange,
 104 boundary representation, and domain depth compare within the same model, and how
 105 their effects differ among hydraulic, salinity, volumetric, and spatial prediction targets.

106 The Pearl River Delta provides an observation-informed regional case for this
 107 comparison. Field investigations, borehole logging, and multi-source data integration
 108 provide lithologic, groundwater-head, hydrogeochemical, topographic, and river-
 109 network information (Jiao et al., 2010; Lancia et al., 2020; Wang and Jiao, 2012; Yu et
 110 al., 2023; Sheng et al., 2024). These data support a three-dimensional variable-density
 111 model that represents Quaternary sediments and bedrock, spatially variable hydraulic
 112 properties, river–aquifer exchange, inland lateral connections, coastal water and salt
 113 exchange, and an inherited salinity field. This observational foundation is especially
 114 important in a geologically complex delta, where the credibility of reconstructed
 115 subsurface structures depends on data coverage, geological complexity, and spatially
 116 independent evaluation (Enemark et al., 2019; Zech et al., 2021; Zhan et al., 2026).
 117 Unlike idealized delta models, this regional platform retains the irregular geometry,
 118 distributary network, and observed hydraulic and salinity patterns of an actual coastal
 119 delta. The baseline is used as a consistent, behaviorally acceptable reference for
 120 comparing alternative model configurations.

121 **2. Model Configuration and Methods**

122 **2.1. Hydrogeological setting and observational data**

123 The Pearl River Delta (PRD) plain is a heterogeneous coastal-delta groundwater
 124 system in which inland topographic gradients, a dense distributary river network,
 125 Quaternary aquifer–aquitard deposits, bedrock, and coastal water and salt exchange
 126 occur within the same setting. The model domain extends from mountain-front areas in
 127 the north and northwest to the Pearl River estuary and southern coast, lies within
 128 112.55–114.10° E and 21.99–23.80° N, and spans approximately 165 km × 214.3 km
 129 (Fig. 1). The low-relief plain is underlain by heterogeneous Quaternary fluvial and
 130 marine deposits and is surrounded and locally underlain by bedrock. Regional
 131 groundwater generally moves from inland and mountain-front recharge areas toward
 132 the lower delta, estuary, and coast, while river–aquifer exchange modifies this pattern
 133 locally (Jiao et al., 2010; Lancia et al., 2020).



Groundwater salinity is spatially heterogeneous, with brackish to saline groundwater extending well inland of the modern shoreline. Hydrogeochemical and isotopic evidence links this distribution to Quaternary marine transgression and subsequent freshening (Wang and Jiao, 2012). Paleo-hydrogeologic reconstructions further show that late-Pleistocene and Holocene boundary changes remain expressed in the present groundwater system (Yu et al., 2023; Sheng et al., 2024). The experiments therefore begin from an observation-informed three-dimensional salinity field and diagnose its redistribution over 2020–2024 under alternative model configurations.

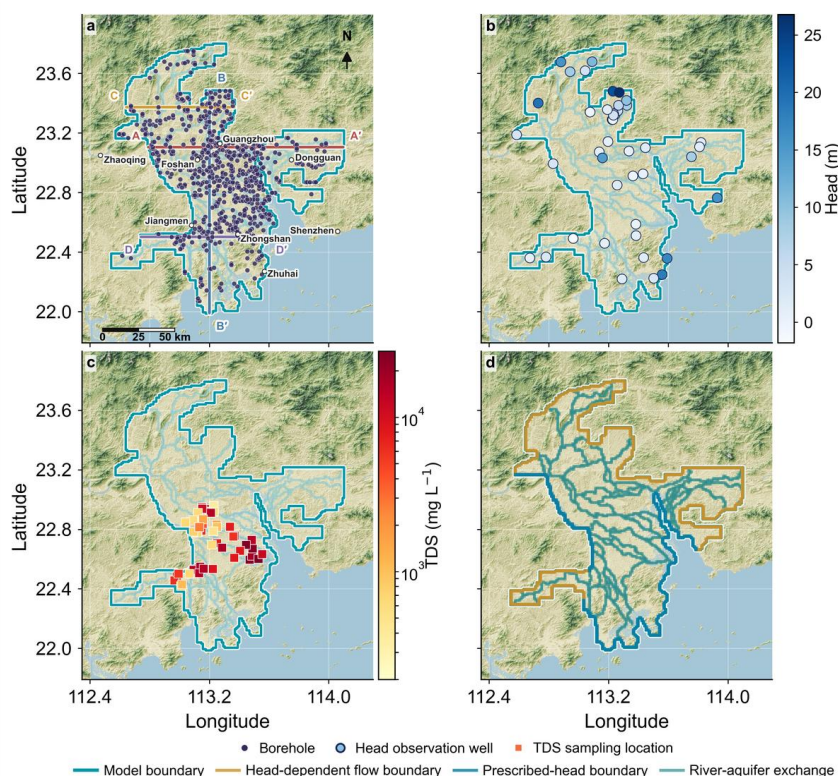


Figure 1. Pearl River Delta model domain, observations, and hydrological boundary representations. The four cross-sections A–A' to D–D' correspond to Fig. 2. Panels show (a) borehole locations and cross-sections, (b) groundwater-head observation wells and observed heads, (c) TDS sampling locations and concentrations, and (d) head-dependent flow boundaries, prescribed-head boundaries, and river–aquifer exchange reaches.

The regional model is constrained by complementary data sets (Fig. 1). Borehole lithologic records were harmonized into four model classes: clay, sand, weathered bedrock, and unweathered bedrock. Groundwater-head observations were used to construct the initial hydraulic field and evaluate the baseline configuration. Total



152 dissolved solids (TDS) observations from one regional sampling campaign were
 153 spatially interpolated to construct the initial three-dimensional TDS field. Topography
 154 and the mapped river network define the model top, river–aquifer exchange reaches,
 155 and the spatial positions of the inland and coastal boundaries. Initial head and TDS
 156 together define the common observation-informed starting state for the simulations.

157 **2.2. Regional model and baseline configuration**

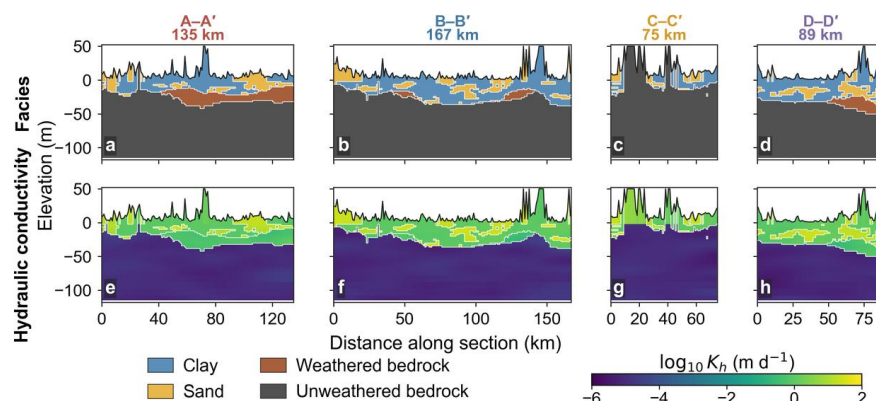
158 The regional model uses a $1\text{ km} \times 1\text{ km}$ structured horizontal grid and contains
 159 275,054 active three-dimensional cells in the global baseline. The model top follows
 160 land-surface topography. The global baseline has 33 layers and a model-bottom
 161 elevation of -115 m . The full baseline discretization and the deeper grids used in the
 162 model-bottom experiments are documented in SI Sect. S3 and Tables S4–S5.

163 The integrated four-class facies structure was constructed through a hierarchical,
 164 scale-aware workflow constrained by borehole data. Ensemble machine learning first
 165 delineated the sediment–bedrock boundary and then partitioned bedrock into weathered
 166 and unweathered classes. Transition-probability-based conditional simulation
 167 generated clay–sand facies within the sediment domain. These stages were combined
 168 on the 1 km model grid; their settings are documented in Sect. S1 and Table S1 of the
 169 Supporting Information. The 100 facies configurations vary facies volume proportions
 170 and directional mean lengths within borehole-constrained ranges. For the facies-
 171 structure experiments, representative horizontal hydraulic conductivities (K_h) were 1,
 172 12, 0.5, and 10^{-5} m d^{-1} for clay, sand, weathered bedrock, and unweathered bedrock,
 173 respectively; vertical hydraulic conductivity (K_z) was set to $K_h/10$. Weathered bedrock
 174 was retained as a separate transition zone to represent its mapped position and
 175 continuity between the sediments and deeper bedrock.

176 The K -field ensemble examines within-facies hydraulic-property variability while
 177 retaining one fixed four-class facies structure. One hundred facies-conditioned pilot-
 178 point realizations vary horizontal hydraulic conductivity (K_h) within the interpreted
 179 classes. Interpolation is performed separately within each facies, preserving the facies
 180 boundaries. The lower row of Fig. 2 therefore preserves the fixed categorical geometry
 181 while displaying spatially continuous within-facies K_h variability. The hierarchical
 182 facies workflow is described in SI Sect. S1 and Table S1; pilot-point spacing, Gaussian-
 183 kernel interpolation scales, facies-specific $\log_{10}(K_h)$ distributions, and realization
 184 diagnostics are reported in SI Sect. S2 and Tables S2–S3. Together, the facies-structure



185 and K -field ensembles examine two hierarchical levels of heterogeneity: the geometry
 186 and continuity of the four classes, and hydraulic-property variation within those classes.



187
 188 **Figure 2. Fixed facies structure and a representative facies-conditioned horizontal hydraulic-**
 189 **conductivity field.** Upper panels (a–d) show clay, sand, weathered bedrock, and unweathered
 190 bedrock along sections A–A' to D–D'. Lower panels (e–h) show cellwise $\log_{10}(K_h)$ for one
 191 reproducibly selected realization on the same grid and sections. The same thin white boundary
 192 network is plotted in both rows, so each lower panel uses the facies geometry shown directly above.
 193 Lower-row colors show continuous K_h values; color variation within a white-bounded region
 194 records within-facies variability, and similar colors can occur in clay and weathered bedrock
 195 because their hydraulic-conductivity ranges overlap. The fixed four-class structure is shared by all
 196 100 K -field configurations; section locations are shown in Fig. 1a.

197 Groundwater flow and TDS transport were simulated using the MODFLOW 6
 198 framework (Hughes et al., 2017) and its tightly coupled Groundwater Flow and
 199 Groundwater Transport (GWF–GWT) models (Langevin et al., 2022). TDS controls
 200 fluid density and viscosity in the flow calculation. The transport formulation represents
 201 advection, mechanical dispersion, molecular diffusion, mass storage, and source–sink
 202 mixing, with TDS used as the salinity variable.

203 Along most of the inland perimeter, the baseline uses a head-dependent flow
 204 boundary implemented with the General-Head Boundary (GHB) package. For each
 205 boundary cell, exchange flux equals the cell-specific GHB conductance multiplied by
 206 the difference between the external reference head and the simulated boundary-cell
 207 head. Conductance has units of $L^2 T^{-1}$ and represents hydraulic connection between the
 208 delta aquifer and the adjoining groundwater system. Baseline conductance was
 209 calculated as boundary-cell K_h multiplied by the summed area of exposed lateral faces
 210 and divided by a 500 m external connection distance; values below $0.05 \text{ m}^2 \text{ d}^{-1}$ were
 211 set to $0.05 \text{ m}^2 \text{ d}^{-1}$. GHB conductance represents lateral groundwater connection, and
 212 riverbed conductance represents leakage through the riverbed. The coast and selected



213 surface-water bodies use prescribed-head boundaries implemented with the Constant-
 214 Head Boundary (CHD) package. The river network is represented with the River (RIV)
 215 package; exchange along each reach depends on river stage, groundwater head, and
 216 riverbed conductance, which combines effective exchange area, riverbed hydraulic
 217 conductivity, and riverbed thickness. Surface drainage is represented with the Drain
 218 (DRN) package. Recharge is applied as a spatially distributed net-infiltration field
 219 accounting for precipitation, runoff, and evapotranspiration. Coastal water level and
 220 salinity, mapped river reaches, and the net-infiltration field define the baseline
 221 hydrologic inputs and boundary conditions.

222 Initial groundwater heads were constructed from regional observations, and the
 223 initial TDS field was obtained by three-dimensional interpolation of the sampling data
 224 described in Sect. 2.1. A 10-year warm-up generated a common post-warm-up
 225 hydraulic and salinity state for configurations with fixed geometry. Configurations with
 226 modified model-bottom elevation use the geometry-specific initialization described in
 227 Sect. 2.3. These observation-informed initial states provide the common reference for
 228 the eight model-development components. The 2020–2024 simulations quantify how
 229 each tested configuration redistributes groundwater head and the inherited three-
 230 dimensional TDS field.

231 **2.3. Model-diagnostic perturbation design and reference configurations**

232 The analysis applies a group-wise one-factor-at-a-time perturbation design around
 233 the observation-informed baseline. Eight model-development components are
 234 examined: facies structure, K -field variability within a fixed facies structure, recharge,
 235 river stage, riverbed conductance, inland boundary conditions, coastal boundary
 236 conditions, and model-bottom elevation. The primary ensemble contains the global
 237 baseline and 299 alternative configurations, for a total of 300 configurations (Table 1).
 238 Each component is varied from the same baseline to compare changes in the specified
 239 hydraulic, salinity, volumetric, and spatial response measures.

240 Each model component uses a sampling form matched to the corresponding
 241 model-development decision. Facies structure and K fields use realization ensembles;
 242 recharge, river stage, and conductance use parameter gradients; and boundary and
 243 model-bottom experiments use alternative formulations or geometries. The tested
 244 ranges were selected from available observations, regional hydrogeologic interpretation,
 245 and commonly used boundary formulations to span reasonable adjustments



encountered during construction, refinement, and calibration of the regional model. Group medians and spatial envelopes summarize responses across the corresponding tested configurations.

For recharge, one multiplier is applied to every recharge cell so that the baseline spatial pattern is preserved while recharge magnitude changes. River-stage configurations retain riverbed conductance, and riverbed-conductance configurations retain river stage, allowing the two terms in the head-dependent river-exchange relation to be evaluated separately. The main design varies one model component at a time. A targeted model-bottom series additionally combines three unweathered-bedrock K_h values with the bottom-elevation configurations to evaluate their coupled effect.

Table 1. Model-development components and perturbation forms of the primary experiments.

Model component	Cases	Perturbation form and tested alternatives
Facies structure	100	Structural realizations with varying facies volume proportions and directional mean lengths.
K field (fixed structure)	100	One fixed facies structure with 100 random facies-conditioned pilot-point K realizations.
Recharge	12	Baseline net-infiltration field multiplied by 0.4–1.6.
River stage	12	Uniform offsets from –1.5 to +1.5 m along simulated river reaches.
Riverbed conductance	12	Baseline conductance multiplied by 0.1–5.
Inland boundary	26	Alternative boundary types plus prescribed-flux, external-head, and GHB-conductance gradients.
Coastal boundary	26	Alternative prescribed-head and head-dependent formulations, plus gradients in coastal water level, boundary-water TDS, external reference head, and GHB conductance.
Model-bottom elevation	12	–80, –90, –100, –120, –150, –180, –200, –250, –300, –400, –500, and –650 m.

The inland-boundary group includes both alternative boundary types and continuous parameter gradients. Discrete alternatives replace the baseline head-dependent boundary with prescribed-head, prescribed-flux, or no-flow formulations. Continuous experiments vary prescribed freshwater flux, external reference head, or GHB conductance while retaining the associated boundary form. These cases represent practical choices used to conceptualize groundwater divides, mountain-front inflow, and hydraulic connection to adjoining aquifers.

The coastal-boundary group examines both boundary formulation and boundary parameters. The baseline uses a prescribed-head coastal boundary. Two GHB



alternatives represent coastal exchange using either cell geometry and adjacent-cell K_h or a conductance adjusted to reproduce baseline coastal exchange. Continuous gradients separately vary coastal water level, boundary-water TDS, external reference head, and GHB conductance. Coastal water level regulates groundwater exchange with the sea, boundary-water TDS sets the salinity of inflowing coastal water, and the GHB parameters determine the hydraulic connection between the aquifer and the sea.

Cross-group comparisons and discrete boundary-type replacements are calculated relative to the global baseline. Each continuous boundary-parameter gradient is calculated relative to the unperturbed member of the same boundary formulation: zero head offset, a unit flux multiplier, baseline GHB conductance, baseline external head, or baseline boundary-water TDS. This reference scheme quantifies parameter-driven responses within a fixed boundary formulation.

Model-bottom elevation configurations modify model geometry, active-cell count, layer count, and the vertical extent of lateral boundaries. Interfaces and facies in layers 1–29 remain fixed, and the grid below –78 m changes with bottom elevation. Each geometry is initialized and warmed up using its own active domain before the 2020–2024 simulation. The 12 primary configurations use elevations of –80, –90, –100, –120, –150, –180, –200, –250, –300, –400, –500, and –650 m with unweathered-bedrock $K_h = 10^{-5} \text{ m d}^{-1}$. An additional 24 simulations repeat the same elevation series at $K_h = 10^{-4}$ and 10^{-3} m d^{-1} to evaluate the influence of bedrock conductivity (Fig. 9). The 300-configuration cross-group comparison uses the 12 primary cases. Each bedrock- K_h series is referenced to its own –120 m configuration.

2.4. Response metrics and spatial diagnostics

Responses are evaluated within the PRD sedimentary system, defined as active clay and sand cells across all modeled depths, including aquifer and aquitard units. For each configuration–reference pair, the comparison domain consists of sediment cells that are active in both models, providing a common physical domain for the model–bottom comparisons.

For head and TDS RMSDs, three-dimensional sediment cells are first aggregated vertically to plan-view columns. Column head is weighted by sediment bulk volume, which is equivalent to effective sediment thickness because horizontal cell area is constant. Column TDS is weighted by saturation-adjusted pore-water volume. RMSDs are then calculated across the common horizontal sediment columns with equal weight



per mapped location, yielding plan-view measures of average response across the sedimentary system. Mean TDS and threshold-defined groundwater volumes are calculated directly from the three-dimensional sediment cells.

Spatial differences in head and TDS are summarized by root-mean-square difference (RMSD):

$$R_X = \left[\frac{1}{N} \sum_{j=1}^N (\tilde{X}_j^{(p)} - \tilde{X}_j^{(r)})^2 \right]^{1/2} \quad (1)$$

where RMSD is evaluated for vertically aggregated groundwater head or TDS concentration in each horizontal sediment column; superscripts denote a configuration and its reference; and the summation is over common horizontal sediment columns. Cross-group comparisons use the global baseline, whereas boundary-parameter gradients use the subgroup references described in Sect. 2.3.

The volume-weighted mean TDS concentration of the sedimentary system is

$$\bar{C} = \frac{\sum_{i=1}^N C_i V_i}{\sum_{i=1}^N V_i} \quad (2)$$

where pore-water volume is calculated from cell area, thickness, porosity, and water saturation. Groundwater volume above a specified salinity threshold is

$$V(T) = \sum_{i=1}^N V_i I(C_i \geq T), T \in \{1, 10\} \text{ g L}^{-1} \quad (3)$$

where the indicator function selects cells above threshold T . $T = 1 \text{ g L}^{-1}$ represents brackish-or-more-saline groundwater and $T = 10 \text{ g L}^{-1}$ identifies the high-salinity groundwater body, consistent with PRD concentration classes (Wang and Jiao, 2012). Group summaries report absolute net changes in mean TDS and threshold-defined volumes; signed maps retain the direction of local TDS change.

Each model-development group is summarized by the median response across its tested configurations. Heat-map colors are normalized independently within each response-metric column, and annotations report values in their physical units.

All response metrics in Figs. 4–9 are calculated from the last saved state of the formal simulation at 1827 d, corresponding to the end of 2024. The envelopes in Figs. 6 and 7 are constructed by selecting the largest absolute final-state response across the configurations in each group.

For the 299 positive-response non-baseline configurations, head and TDS RMSDs are transformed to base-10 logarithms and independently scaled using their 5th and 95th percentiles:

$$h^* = \text{clip}\left(\frac{\log_{10} R_h - q_{h,0.05}}{q_{h,0.95} - q_{h,0.05}}, 0, 1\right), C^* = \text{clip}\left(\frac{\log_{10} R_C - q_{C,0.05}}{q_{C,0.95} - q_{C,0.05}}, 0, 1\right) \quad (4)$$



331 The normalized hydraulic–salinity response contrast, D , is
 332
$$D = C^* - h^* \quad (5)$$

333 where the lower and upper bounds are the 5th and 95th percentiles of the log-
 334 transformed head response, with analogous definitions for TDS; clipping truncates
 335 normalized values to $[0, 1]$. Positive D indicates a larger normalized TDS response, and
 336 negative D indicates a larger normalized head response. The zero-RMSD global
 337 baseline is assigned $D = 0$. The index provides a relative comparison of normalized
 338 hydraulic and salinity responses across the present configuration sets.

339 For spatial figures, each configuration is first aggregated vertically to plan view:
 340 head uses effective-sediment-thickness weighting and TDS uses saturation-adjusted
 341 pore-volume weighting. At each horizontal location, the envelope for a model
 342 component retains the response with the largest absolute value among configurations
 343 in that group, together with its sign:

$$344 \quad \Delta X^*(x, y) = \Delta X_{k^*}(x, y), k^* = \underset{k}{\operatorname{argmax}} |\Delta X_k(x, y)| \quad (6)$$

345 Because the selected configuration can differ among grid cells, each map
 346 combines local maximum responses from multiple configurations into a signed
 347 maximum-response envelope. Head maps use a common zero-centered linear scale, and
 348 TDS maps use a common symmetric-log scale to retain the sign of responses spanning
 349 several orders of magnitude.

350 **3. Results**

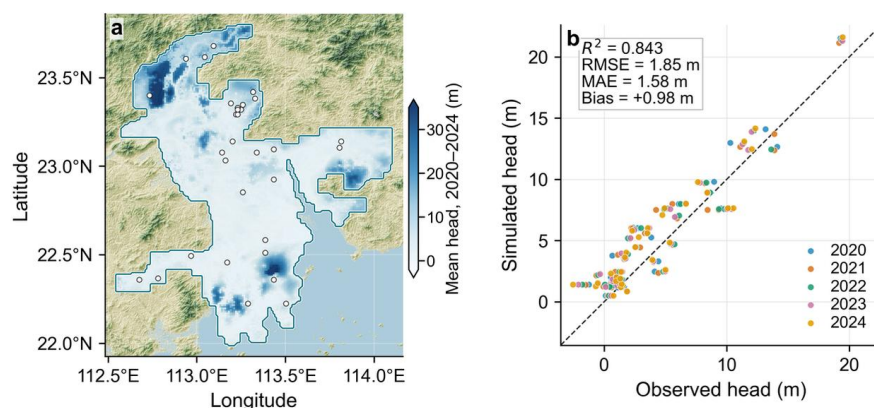
351 **3.1. Baseline groundwater-head conditions and performance**

352 The mean of the five year-end head states for 2020–2024 shows a clear regional
 353 hydraulic pattern across the PRD (Fig. 3a). Heads are highest along the northern and
 354 northwestern mountain front, where several zones exceed 30 m, and decline across the
 355 central plain toward the estuary and southern coast. Secondary high-head zones occur
 356 in the eastern and southern parts of the domain, while low heads occupy most of the
 357 central plain and estuarine areas. The simulated field therefore retains the first-order
 358 inland-to-coastal hydraulic gradient expected for the regional system.

359 Baseline hydraulic performance was evaluated using 34 monitoring wells and 170
 360 observed–simulated well-year pairs for 2020–2024 (Fig. 3b). Simulated heads were
 361 extracted from model layers corresponding to the monitored intervals. Annual point
 362 clouds largely overlap and follow the 1:1 relation across the monitored range. The



363 pooled comparison gives a coefficient of determination (R^2) of 0.843, RMSE = 1.85 m,
 364 MAE = 1.58 m, and bias = +0.98 m. These statistics show that the baseline captures the
 365 regional head pattern with modest overall overprediction and provides a consistent
 366 reference for the perturbation experiments.



367
 368 **Figure 3. Baseline groundwater head and comparison with observations for 2020–2024.** Panel
 369 (a) shows the mean of five year-end head states and locations of the 34 monitoring wells. Panel (b)
 370 compares 170 observed–simulated well-year pairs; colors denote years and the dashed line is the
 371 1:1 relation. Reported statistics are $R^2 = 0.843$, RMSE = 1.85 m, MAE = 1.58 m, and bias = +0.98
 372 m.

373 3.2. Responses across tested model-development configurations

374 The eight model-development groups produced distinct median responses across
 375 the five metrics (Fig. 4). Within the tested configuration sets, median head RMSD was
 376 largest for facies structure (0.905 m), followed by recharge (0.506 m), the inland
 377 boundary (0.397 m), river stage (0.278 m), the K field (0.236 m), and the coastal
 378 boundary (0.174 m). Riverbed conductance produced 0.00775 m, and model-bottom
 379 elevation produced 6.92×10^{-6} m. The facies-structure head RMSD median was
 380 approximately 3.8 times the K -field median, indicating that the tested changes in
 381 geometry and connectivity had a larger effect on the regional hydraulic state than the
 382 tested within-facies K variability.

383 The ordering changed for spatial TDS response. The coastal boundary produced
 384 the largest median TDS RMSD (0.230 g L^{-1}), followed by recharge (0.144 g L^{-1}), facies
 385 structure (0.126 g L^{-1}), and river stage (0.0819 g L^{-1}). The K field produced 0.0363 g
 386 L^{-1} , slightly above the inland boundary (0.0270 g L^{-1}), while riverbed conductance and
 387 model-bottom elevation produced 0.00222 and $5.54 \times 10^{-5} \text{ g L}^{-1}$, respectively.

388 Recharge produced the largest median absolute change in volume-weighted mean
 389 TDS (0.0999 g L^{-1}). Corresponding medians were 0.0261 g L^{-1} for the coastal boundary,



0.0162 g L⁻¹ for facies structure, 0.00633 g L⁻¹ for river stage, 0.00595 g L⁻¹ for the inland boundary, and 0.00362 g L⁻¹ for the *K* field; riverbed conductance and model-bottom elevation were below 10⁻⁴ g L⁻¹. For groundwater with TDS ≥ 1 g L⁻¹, recharge also produced the largest median volume change (0.139 km³), followed by facies structure (0.115 km³), river stage (0.0599 km³), the inland boundary (0.0351 km³), the coastal boundary (0.0189 km³), and the *K* field (0.0138 km³). The recharge response represents approximately 0.34% of the baseline volume of 41.50 km³.

For groundwater with TDS ≥ 10 g L⁻¹, recharge produced a median volume change of 0.157 km³, approximately 1.0% of the baseline volume of 15.61 km³. Facies structure and river stage produced similar secondary responses of 0.0318 and 0.0300 km³. The coastal boundary, *K* field, riverbed conductance, and inland boundary produced 0.0124, 0.00741, 0.00175, and 0.00148 km³, respectively; model-bottom elevation remained below 10⁻⁶ km³. The coastal boundary therefore combined the largest median TDS RMSD with modest threshold-volume changes, whereas recharge led all three bulk salinity metrics. River-stage responses exceeded riverbed-conductance responses for all metrics.

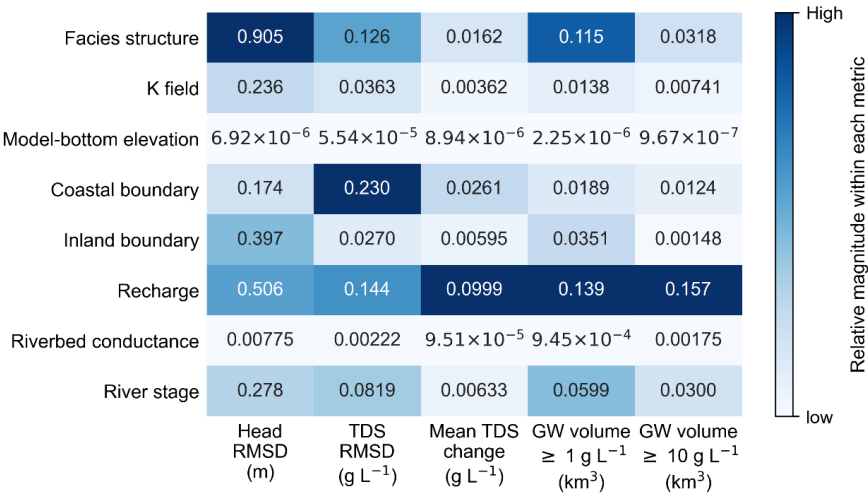


Figure 4. Median responses across 300 model configurations in eight model-development groups. The primary ensemble contains 299 nonbaseline configurations plus the global baseline. For display, the zero-response baseline is included in the Facies structure group (*n* = 100) but is excluded from group-median calculations. Cell annotations report absolute median responses in the physical units shown. Color intensity is normalized within each metric column and does not indicate relative importance across metrics.



3.3. Relative head and TDS responses

Across the 299 nonbaseline configurations, sedimentary-system head and TDS RMSDs span several orders of magnitude and occupy distinct but partly overlapping regions of response space (Fig. 5a). Facies-structure configurations occupy the high-head, moderate-to-high-TDS region. Recharge and river-stage configurations show intermediate responses in both variables. *K*-field configurations occupy mainly intermediate head and low-to-moderate TDS ranges, with a wider spread than their medians alone indicate. Riverbed-conductance configurations remain in the lower response range, and model-bottom configurations occupy the lowest end of both axes.

Inland and coastal boundary groups show the clearest contrast. Inland-boundary configurations commonly combine moderate-to-large head RMSDs with smaller TDS RMSDs. Coastal-boundary configurations cover a wider TDS range, including cases with large TDS changes and limited head response and cases that affect both variables. The range reflects separate perturbations of coastal water level, boundary-water TDS, external head, GHB conductance, and boundary representation. Section 3.5 resolves these responses by parameter gradient and boundary type.

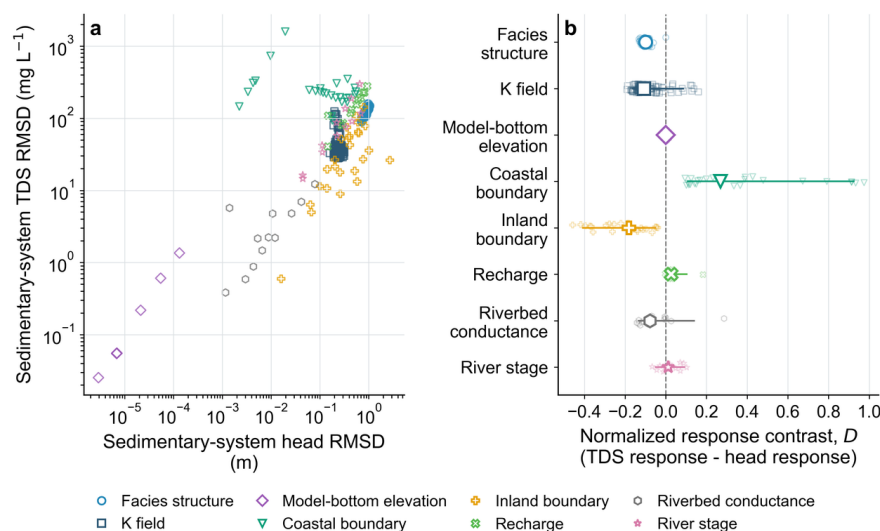


Figure 5. Hydraulic–salinity response contrast for the eight model-development groups. Panel (a) shows 299 nonbaseline configurations relative to the global baseline; the baseline itself is the zero-response origin and is not shown on logarithmic axes. Panel (b) reports *D*, calculated by independently scaling the log₁₀-transformed head and TDS RMSDs to their 5th–95th percentile ranges across the 299 nonbaseline configurations and subtracting normalized head response from normalized TDS response. The baseline is shown at *D* = 0 only as a visual reference.



436 The normalized contrast D summarizes these relative hydraulic and salinity
437 characteristics (Fig. 5b). The coastal-boundary group has the largest positive median
438 and widest positive range. Recharge and river stage have slightly positive medians.
439 Facies structure, the K field, riverbed conductance, and the inland boundary have
440 negative medians; the inland boundary has the most negative median and therefore the
441 clearest relative emphasis on head response. The K -field median is also negative,
442 indicating a larger normalized head response than TDS response within that group. The
443 model-bottom median is near zero because both normalized responses remain near their
444 lower limits. Because D is calculated from percentile-normalized head and TDS
445 RMSDs, the positions and spread in Fig. 5b describe the relative balance of the two
446 responses across the 299 nonbaseline configurations; the physical response magnitudes
447 are reported in Fig. 4.

448 **3.4. Spatial distributions of head and TDS responses**

449 Signed maximum head-response envelopes differ markedly among model
450 components (Fig. 6). Facies structure produces the broadest high-amplitude mosaic of
451 positive and negative change, with prominent clusters along the northern and
452 northwestern mountain front and across parts of the southern lower delta. The K -field
453 envelope is also spatially distributed but lower in amplitude; its strongest clusters occur
454 in the northwestern mountain-front zone and the southern lower delta, with weaker
455 patchy responses across the central plain. This contrast is consistent with the larger
456 domain-wide head RMSD of the facies-structure ensemble.

457 Recharge produces a broad and comparatively continuous head response. Most
458 cells in its envelope are selected from the 0.4-times-recharge configuration, which
459 lowers heads across much of the delta and produces the largest declines in the central
460 and southern domain. River-stage responses trace the distributary network. Coastal-
461 boundary responses remain around the estuary and southern coast, whereas inland-
462 boundary responses follow northern, western, and locally eastern connected zones.
463 Riverbed-conductance responses are smaller in magnitude and restricted to individual
464 reaches. Model-bottom-elevation responses remain close to the color corresponding to
465 zero across almost the entire sedimentary domain on the common -3 to $+3$ m scale. The
466 group-median head RMSD is only 6.92×10^{-6} m, and the head RMSDs in the dedicated
467 bottom-elevation experiments of Sect. 3.6 remain below 0.17 mm, leaving only very
468 faint local changes visible in Fig. 6.

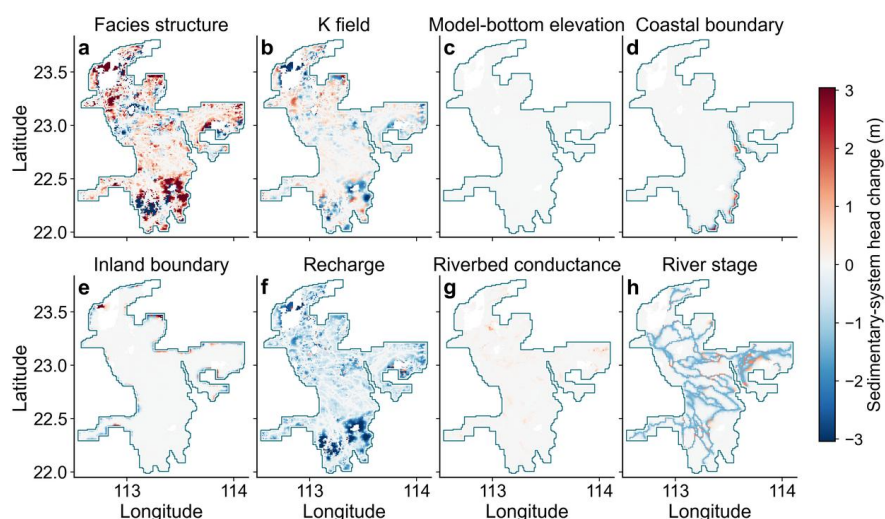


Figure 6. Signed maximum groundwater-head response envelopes in the sedimentary system for the eight model-development groups. At each horizontal grid cell, the response with the largest absolute head change among configurations in that group is retained with its sign. Head is vertically aggregated using effective sediment thickness. All panels use a common zero-centered linear color scale.

TDS-response envelopes are concentrated farther south than the corresponding head responses (Fig. 7). Facies structure generates extensive alternating positive and negative changes from the central plain through the lower delta, estuary, and southern coast. The *K*-field envelope occupies much of the same fresh–saline transition zone but has lower amplitudes and a less extensive high-response area. Recharge produces the broadest coherent TDS response; its envelope is controlled mainly by the 0.4-times-recharge configuration, under which TDS increases across much of the central and southern delta and decreases locally around parts of the estuarine river network.

River-stage perturbations produce branching positive and negative TDS responses along the river network, particularly in the central and lower delta. The coastal-boundary envelope forms narrow bands along the estuary and coastline. Inland-boundary effects are sparse and occur near selected margins and a small number of connected interior locations. Riverbed-conductance effects remain near individual reaches, and model-bottom elevation produces only faint local changes. At the common plotting scale, facies structure and recharge dominate the regional TDS patterns, while *K*-field variability introduces smaller, spatially distributed contrasts within the fixed architecture. Head responses extend farther north than TDS responses, whereas salinity changes concentrate around the inherited central and southern fresh–saline transition.

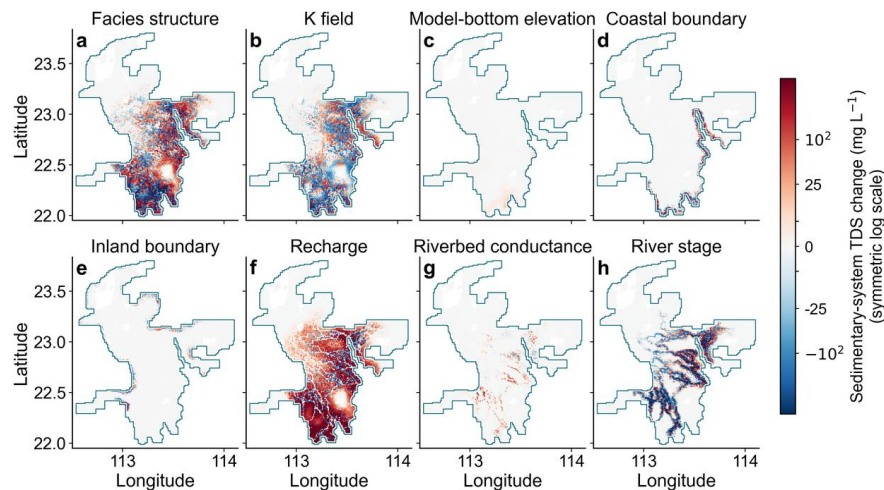
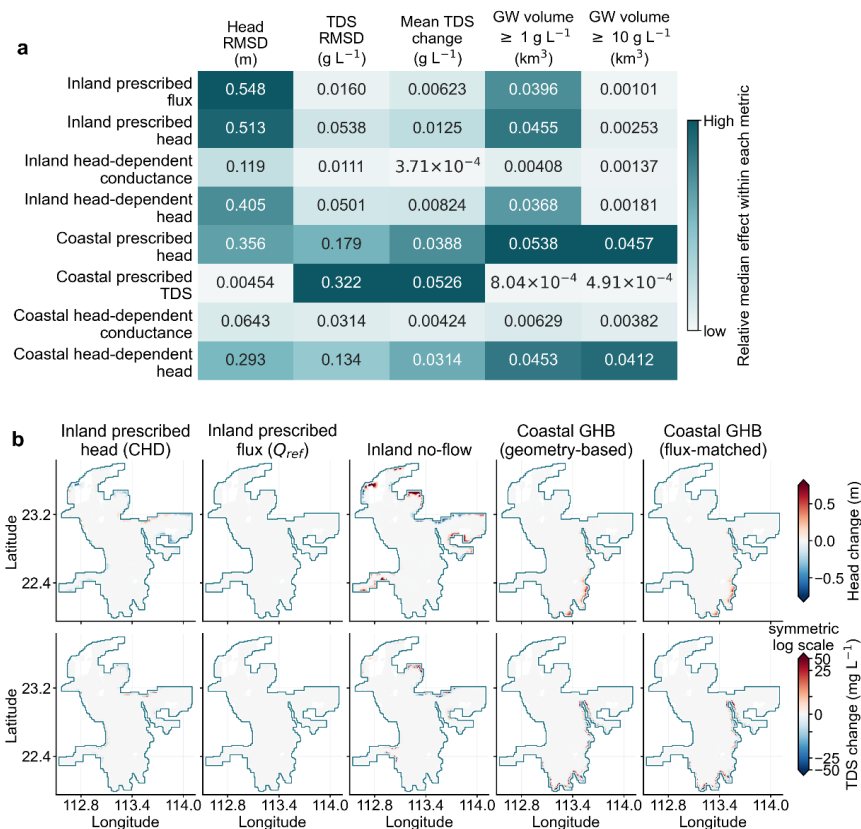


Figure 7. Signed maximum TDS response envelopes in the sedimentary system for the eight model-development groups. The same group-specific maximum-envelope rule as in Fig. 6 is used. TDS is vertically aggregated using saturation-adjusted groundwater volume, and all panels use a common symmetric-log color scale.

3.5. Boundary-parameter gradients and alternative representations

Inland-boundary experiments compare prescribed-flux, prescribed-head, and head-dependent formulations (Fig. 8a). Reducing prescribed freshwater inflow lowers heads in boundary-connected zones, while increasing inflow raises heads and propagates the response along connected pathways; associated TDS changes remain comparatively small. Prescribed-head changes produce corresponding local head adjustment and measurable TDS redistribution. Within the inland GHB formulation, external-head changes generate larger median head and TDS RMSDs than conductance changes. Thus, the tested external hydraulic forcing matters more than conductance refinement for this boundary formulation.

Coastal-boundary experiments separately examine prescribed coastal water level, prescribed boundary-water TDS, and external head and conductance under coastal GHB formulations (Fig. 8a). Changing coastal water level modifies the nearshore hydraulic gradient and salinity distribution and produces clear changes in threshold-defined groundwater volumes. Changing boundary-water TDS mainly alters concentrations near the estuary and coast, with limited head response and small threshold-volume changes. Within coastal GHB formulations, external-head changes again produce larger head and TDS responses than conductance changes.



517

518 **Figure 8. Boundary-parameter and boundary-type replacements.** Panel (a) summarizes eight
519 parameter gradients, each containing six configurations, using subgroup references; annotations
520 report physical responses. In panel (a), color intensity is normalized within each metric column
521 and does not indicate relative importance across metrics. Panel (b) maps signed head and TDS changes
522 for five boundary-type replacements relative to the global baseline: inland prescribed head,
523 prescribed flux matched to baseline lateral exchange, inland no-flow, and geometry-based and flux-
524 matched coastal GHB representations. Together the panels account for all 52 unique boundary
525 perturbations; the flux-matched inland case appears in both panels but represents one simulation.

526 Alternative boundary representations reinforce these contrasts (Fig. 8b). Replacing
527 the inland GHB with prescribed head concentrates response in a few northern and
528 eastern connected zones. A prescribed-flux boundary matched to baseline lateral
529 exchange produces still more localized differences. The no-flow inland boundary
530 generates the broadest inland response, with head changes along northern, eastern, and
531 southwestern margins and selected interior pathways. Geometry-based and flux-
532 matched coastal GHB formulations both produce continuous head and TDS bands along
533 the estuary and southern coast; their regional extents are similar, with local amplitude
534 differences along inner-estuary and southern coastal reaches.



3.6. Effects of model-bottom elevation

The response to model-bottom elevation depends on unweathered-bedrock K_h (Fig. 9). Configurations above the -120 m reference elevation truncate the active domain. At -80 m, head RMSD ranges from approximately 0.135 to 0.169 mm across the three K_h values, and TDS RMSD ranges from 1.38 to 1.90 mg L $^{-1}$. Both responses decline sharply as the model bottom is lowered from -80 to -120 m.

For model-bottom elevations below -120 m, the three K_h series diverge. At $K_h = 10^{-5}$ m d $^{-1}$, head and TDS RMSDs remain near 0.004 mm and 0.03 mg L $^{-1}$ from -150 to -650 m. At $K_h = 10^{-4}$ m d $^{-1}$, responses increase as the bottom is lowered to approximately -250 to -300 m and then approach plateaus near 0.061 mm and 0.63 mg L $^{-1}$. At $K_h = 10^{-3}$ m d $^{-1}$, head RMSD increases from approximately 0.041 mm at -150 m to 0.126 mm at -300 m and 0.151 mm at -500 m; TDS RMSD increases from approximately 0.40 to 1.08 and 1.21 mg L $^{-1}$.

Only small additional changes occur as the bottom is lowered from -500 to -650 m at $K_h = 10^{-3}$ m d $^{-1}$, where head and TDS RMSDs reach approximately 0.154 mm and 1.23 mg L $^{-1}$. The elevation at which the curves approach a plateau becomes lower as bedrock K_h increases, but head RMSD remains below 0.17 mm and TDS RMSD below 2 mg L $^{-1}$ for every tested combination. Model-bottom elevation therefore has negligible practical influence on the 2020–2024 sedimentary-system predictions within the tested bedrock- K range.

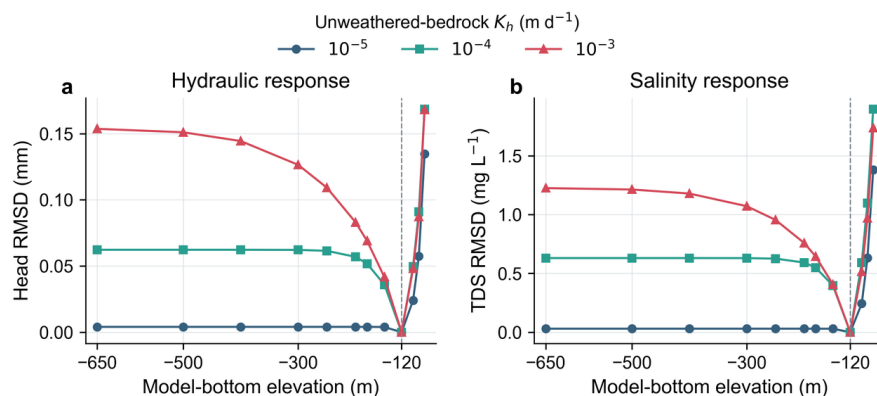


Figure 9. Effects of model-bottom elevation at different unweathered-bedrock horizontal hydraulic conductivities. Each curve is referenced to the -120 m model-bottom configuration within the same bedrock- K group, separating elevation effects from the bedrock- K main effect.



559 4. Discussion

560 4.1. Prediction-specific response contrasts and spatial footprints

561 The 300 model configurations reveal three complementary dimensions of regional
 562 groundwater-model behavior: reorganization of the regional flow system, evolution of
 563 the inherited fresh–saline distribution, and changes in the spatial extent of groundwater
 564 within different salinity classes. The model component producing the largest response
 565 differs among these prediction dimensions. Facies structure produced the largest
 566 median head RMSD (0.905 m), coastal-boundary configurations produced the largest
 567 median TDS RMSD (0.230 g L⁻¹), and recharge produced the largest median changes
 568 in volume-weighted mean TDS and in groundwater volumes with TDS ≥ 1 and ≥ 10 g
 569 L⁻¹. The median head response of facies structure was approximately 3.8 times that of
 570 the *K*-field group, showing that changes in the geometry and connectivity of the
 571 represented heterogeneous framework altered the regional hydraulic state more than
 572 spatial *K* variability within the mapped hydrogeologic units.

573 Figures 6 and 7 show that response location is as important as domain-wide
 574 magnitude. Facies structure and recharge affected broad parts of the delta; *K*-field
 575 variability produced lower-amplitude but spatially dispersed changes; river-stage
 576 responses followed the distributary network; inland-boundary responses extended
 577 inward from northern, western, and locally eastern connected margins; and coastal-
 578 boundary responses remained concentrated around the estuary and southern coast.
 579 Configurations with comparable RMSDs can therefore affect different parts of the
 580 groundwater system. The spatial footprints identify where additional structural detail,
 581 parameter refinement, or monitoring data are most likely to change a selected forecast.

582 The concentration of TDS responses in the central and southern delta reflects the
 583 inherited three-dimensional salinity field. Hydrochemical, isotopic, and paleo-
 584 hydrogeologic studies show that brackish and saline groundwater extends far inland of
 585 the modern shoreline and was formed mainly by seawater emplaced during the
 586 Holocene transgression, followed by incomplete freshwater flushing (Wang and Jiao,
 587 2012; Yu et al., 2023; Sheng et al., 2024). Deltaic and shelf aquifers can preserve this
 588 history for thousands of years because salinity adjusts slowly to shoreline migration
 589 and changes in freshwater input (Post et al., 2013; van Engelen et al., 2021). In the five-
 590 year simulations, present-day coastal changes produced their clearest effects in the
 591 estuary and nearshore aquifer. Sustained changes in coastal water level or salinity can



592 propagate farther inland over longer periods, particularly through hydraulically
593 connected aquifer pathways. The limited inland reach over 2020–2024, together with
594 the independent field evidence, supports a predominantly paleo-marine origin for the
595 widespread saline groundwater in the PRD; modern seawater intrusion mainly modifies
596 the estuary and nearshore aquifer over the five-year period.

597 The coastal-boundary experiments further distinguish the roles of coastal water
598 level and boundary-water TDS. Boundary-water TDS directly controls the salinity of
599 water entering from the estuary and coast and mainly changes concentrations close to
600 the boundary. Coastal water level changes the head difference and groundwater
601 exchange across the land–sea interface, so its influence extends across a broader
602 nearshore area and produces larger changes in the volumes of groundwater within the
603 selected salinity classes. Coastal models therefore require separate observations of
604 water level and salinity, together with monitoring of how both vary through time
605 (Werner et al., 2013).

606 TDS RMSD and threshold-defined groundwater volumes describe the intensity
607 and spatial extent of salinity change, respectively. A large concentration change within
608 groundwater that remains above 10 g L^{-1} increases TDS RMSD but produces little
609 change in the high-salinity volume. A smaller change distributed across groundwater
610 close to 1 g L^{-1} can shift a broad transition zone into a different salinity class and
611 produce a larger volume response. This behavior explains why the coastal boundary
612 generated the largest spatial TDS RMSD but only modest threshold-volume changes,
613 whereas recharge produced the largest changes in volume-weighted mean TDS and in
614 both threshold-defined groundwater volumes.

615 Recharge modifies freshwater input, regional hydraulic gradients, saline-water
616 displacement, and dilution across a large part of the model domain. The geometry and
617 connectivity of the regional heterogeneous hydrogeologic framework determine how
618 these changes propagate through aquifers, aquitards, transition zones, and connected
619 pathways, while spatial K variability within the mapped units adjusts local flow rates
620 and gradients along those pathways. The different response magnitudes and spatial
621 footprints therefore link each prediction target to a different combination of structural,
622 hydraulic, and observational requirements.



4.2. Roles of heterogeneous hydrogeologic structure, hydraulic conductivity, recharge, and river conditions

The larger regional response of the facies-structure group highlights the role of the three-dimensional heterogeneous hydrogeologic framework in establishing the principal groundwater pathways and hydraulic barriers. Assigning representative horizontal hydraulic conductivity (K_h) values to the mapped hydrogeologic units translates this framework into groundwater-flow properties: relatively transmissive and connected units carry most regional flow, whereas low- K units restrict lateral or vertical exchange. In the PRD model, sedimentary aquifers and aquitards, weathered bedrock, and low- K unweathered bedrock collectively define the main pathways between the delta plain, river network, coast, and deeper system. The geometry and connectivity of these units determine where regional pathways and barriers occur; spatial K variability within a unit further modifies local flow rates, hydraulic gradients, and exchange locations.

Previous studies show that K fields with similar mean values and overall variability can produce different flow and transport when high- and low- K zones have different spatial connections (Renard and Allard, 2013; Zinn and Harvey, 2003). Multiscale sediment organization and facies interfaces also influence plume spreading, mixing, and reaction hotspots (Ren et al., 2022; Soltanian et al., 2025; Wallace et al., 2021), while coastal simulations demonstrate that the represented scale and arrangement of heterogeneity change salinity distributions and density-driven circulation (Michael et al., 2016; Yu and Michael, 2022). In the PRD simulations, the facies-structure medians were 3.5–8.3 times the corresponding K -field medians across the five metrics. Regional model development should therefore prioritize the three-dimensional heterogeneous framework, including the geometry and connectivity of major aquifers, aquitards, transition zones, and any hydraulically connected bedrock. Detailed K fields within individual units become most useful for local hydraulic gradients, river–aquifer exchange, and transport along particular pathways.

The effects of recharge and river conditions depend on the three-dimensional arrangement and connectivity of relatively high- and low-hydraulic-conductivity units represented by the heterogeneous hydrogeologic model. Recharge acts across the land surface and changes freshwater input and the regional inland-to-coastal gradient, producing broad head and TDS responses. River stage changes the river–aquifer head



656 difference simultaneously along many reaches, whereas riverbed conductance regulates
 657 the exchange rate produced by the existing head difference at each reach. River-stage
 658 changes consequently produced larger responses than riverbed-conductance changes
 659 for all five metrics. Regional river–aquifer predictions should first be constrained by
 660 observed river stage, adjacent groundwater head, and streamflow; detailed riverbed-
 661 conductance estimation can then focus on reaches where exchange flux is a specific
 662 prediction target. Aquifer heterogeneity near a river can still produce different leakage
 663 estimates among models with comparable head fits (Engdahl et al., 2010).

664 Recharge and river stage transmit water and salinity changes through different
 665 parts of the regional heterogeneous hydrogeologic framework. Recharge modifies the
 666 regional freshwater balance over the plain, while river-stage changes are channelized
 667 by the distributary network. Their influence on salinity becomes greatest where
 668 hydraulically connected groundwater pathways intersect the inherited fresh–saline
 669 transition. The different spatial pathways of recharge and river-stage effects indicate
 670 whether a particular forecast requires better information on subsurface heterogeneity,
 671 hydraulic-property measurements, recharge, or river conditions.

672 **4.3. Lateral boundaries and model-bottom elevation**

673 Inland-boundary representation produced a meaningful regional head response. Its
 674 median head RMSD was 0.397 m, close to the recharge response of 0.506 m and larger
 675 than the *K*-field response of 0.236 m. The corresponding median TDS RMSD was much
 676 smaller (0.0270 g L⁻¹). The response maps show that inland-boundary changes mainly
 677 affect the model perimeter and connected pathways extending into the delta. Accurate
 678 boundary type, external head, and lateral inflow are therefore important for regional
 679 head forecasts and for local flow near mountain-front connections, while their five-year
 680 influence on the broad salinity distribution is more limited.

681 The inland-boundary response patterns support a segmented representation of the
 682 model perimeter. Groundwater divides and poorly connected bedrock segments can use
 683 no-flow boundaries; segments with independently estimated lateral recharge can use
 684 prescribed flux; and locations connected to an external aquifer can use head-dependent
 685 boundaries. Heads measured near the boundary, groundwater-flow directions,
 686 hydrochemical contrasts, and environmental tracers can identify the appropriate
 687 connection and constrain external head or flux values (Doyle et al., 2015; Reilly, 2001).



688 Coastal-boundary representation requires comparable attention for salinity
689 prediction. The coastal group produced the largest median TDS RMSD, and the
690 response bands followed the estuary and southern coast. Water-level records constrain
691 groundwater exchange across the coast, while coastal and estuarine salinity records
692 constrain the concentration of incoming water. Longer prediction periods, sustained
693 sea-level change, or pumping near the coast increase the need to represent connected
694 coastal pathways farther inland (Werner et al., 2013).

695 Model-bottom elevation produced a different result. Across all tested bottom
696 elevations and unweathered-bedrock K values, head and TDS responses in the
697 sedimentary system remained below 0.17 mm and 2 mg L⁻¹. The small response reflects
698 the low-conductivity, weakly connected deep bedrock represented in the model and the
699 five-year prediction period. Regional borehole data are currently too sparse to map
700 permeable bedrock aquifers and fracture networks in three dimensions. Deep boreholes,
701 hydraulic testing, environmental tracers, and geophysical surveys should therefore
702 establish whether such connections exist before additional model depth is assigned
703 detailed layers and parameters. For the present regional head and salinity targets, a
704 model bottom near -120 m captures the simulated sedimentary-system response;
705 deeper domains become important when field evidence indicates conductive bedrock
706 pathways or when the prediction concerns long-term circulation, deep exchange, or
707 groundwater residence time (Cardenas and Jiang, 2010; Frisbee et al., 2017;
708 Goderniaux et al., 2013; Manning et al., 2021).

709 **4.4. Prediction-specific priorities for model development and observation design**

710 The five-year PRD simulations show that the initial head and TDS fields anchor
711 the regional spatial pattern. The largest median changes generated by the tested model
712 components were 0.905 m for head and 0.230 g L⁻¹ for TDS. These changes modify
713 local gradients, concentrations, and transition-zone positions within a system that
714 already contains an inland-to-coastal head difference exceeding 30 m and an inherited
715 three-dimensional fresh-saline distribution. Accurate initial conditions are therefore
716 fundamental for short-term regional prediction of both groundwater level and salinity.

717 Initial head and salinity fields in coastal-delta and estuarine aquifer systems should
718 be constructed from long-term and multilevel monitoring. Long-term groundwater-
719 level records define seasonal and interannual variation and allow the initial head field
720 to be matched to the simulation start date. Multilevel head measurements define vertical



721 gradients between aquifer units, while depth-discrete TDS measurements delineate the
722 vertical and horizontal position of the fresh–saline transition. Repeated salinity
723 sampling through time distinguishes actual redistribution from differences caused by
724 sparse spatial coverage. Multilevel monitoring should be widely deployed across
725 coastal-delta and estuarine aquifer systems, with denser vertical profiles across fresh–
726 saline transition zones, inland recharge and lateral-connection areas, major river
727 corridors, estuaries, and coastlines.

728 The response hierarchy also clarifies how subsurface detail should be allocated.
729 The geometry and connectivity of the regional three-dimensional heterogeneous
730 framework require early attention because facies-structure changes produced the largest
731 regional head response and broad salinity changes. At the 1 km regional scale, assigning
732 representative *K* values to the mapped hydrogeologic units captured the principal
733 regional flow pathways. Additional *K* detail within individual units improves local
734 gradients, exchange fluxes, and pathway-specific transport, but its effect on the regional
735 response metrics was smaller than that of changing the heterogeneous framework.
736 Local *K* characterization can therefore concentrate on river corridors, transition-zone
737 pathways, pumping centers, and other locations where the forecast depends on meter-
738 to kilometer-scale flow connections.

739 Net recharge is a comparable regional priority because it generated broad
740 hydraulic and salinity responses and the largest changes in the three bulk salinity
741 measures. Recharge estimation should integrate precipitation, evapotranspiration, land
742 cover, soil properties, runoff, and infiltration or recharge coefficients. Long-term
743 groundwater-level records and regional water-balance estimates provide independent
744 checks on the magnitude and spatial pattern of the recharge field. Boundary
745 observations remain important at the same stage: inland heads and lateral-flow
746 estimates constrain the regional hydraulic gradient, and coastal water level and salinity
747 constrain nearshore groundwater exchange and salt input.

748 Hydrogeophysical surveys can extend the point information from boreholes and
749 monitoring wells. Electrical-resistivity and airborne electromagnetic surveys provide
750 spatial constraints on the distribution and continuity of relatively high- and low-
751 hydraulic-conductivity units and on groundwater salinity, while time-lapse resistivity
752 or other suitable hydrogeophysical measurements can help identify water-table and
753 saturation changes. Seismic-reflection data can delineate sedimentary and bedrock
754 geometry in cross-section and complement the regional coverage of airborne



755 electromagnetic surveys (Marker et al., 2015; Meyer et al., 2019; Oldenborger et al.,
756 2016). Interpretation together with borehole logs, groundwater heads, and water-quality
757 profiles can directly improve the representation of three-dimensional heterogeneity and
758 the head and salinity fields used to initialize and evaluate the numerical model (Day-
759 Lewis et al., 2005).

760 The practical model-development priorities can be stated for four prediction
761 classes. Five-year regional head forecasts require the most detailed constraints on the
762 initial head field, the geometry and connectivity of the regional three-dimensional
763 heterogeneous framework, net recharge, and hydraulically connected inland-boundary
764 segments. Regional salinity patterns and saline-groundwater volumes require a depth-
765 resolved initial TDS field, connected transport pathways within the heterogeneous
766 framework, recharge, and separate coastal water-level and salinity records. River-
767 aquifer exchange and pathway-scale transport require paired river-stage, groundwater-
768 head, and streamflow observations, followed by local riverbed-conductance and K
769 refinement within the relevant hydrogeologic units. Deep-flow and long-term forecasts
770 require direct evidence for bedrock aquifers and fracture connectivity before model-
771 bottom depth and deep hydraulic properties receive detailed representation. This
772 allocation ties model complexity and data collection directly to the forecast quantity,
773 spatial scale, and prediction period.

774 **5. Conclusions**

775 Numerical perturbation analysis of controls on groundwater flow and salinity
776 transport in the Pearl River Delta shows that model-development priorities in
777 heterogeneous coastal-delta and estuarine aquifers depend on the forecast variable, area
778 of interest, and spatial and temporal scales. For five-year regional forecasts, the initial
779 head field determines the starting hydraulic gradients and early head adjustment, while
780 a depth-resolved initial salinity field preserves the freshwater-saline configuration
781 inherited from long-term system evolution; together, they establish the basic spatial
782 state of the short-term simulation. The three-dimensional heterogeneous hydrogeologic
783 framework controls major flow paths, barriers, and routes of salinity redistribution,
784 whereas recharge continually regulates regional freshwater input, hydraulic gradients,
785 and salinity balance. Both therefore require priority representation in regional
786 predictions over different timescales. In the present model, further refinement of



787 hydraulic conductivity within the established heterogeneous framework produced
788 smaller regional changes and was most valuable for resolving local gradients, river–
789 aquifer exchange, and specific transport pathways.

790 Boundary conditions and model depth show a stronger dependence on spatial and
791 temporal scale. Over the five-year simulation, responses to inland and coastal
792 boundaries are concentrated mainly in mountain-front, estuarine, and nearshore areas
793 that are hydraulically connected to those boundaries; boundary type, external head, and
794 boundary-water salinity become critical when forecasts target these locations. Under
795 the low-conductivity bedrock settings tested here, model-bottom elevation has little
796 effect on five-year predictions for the sedimentary system. The limited inland
797 propagation of modern coastal water-level and salinity changes over this period,
798 together with the inherited freshwater–saline distribution, further supports a
799 predominantly paleo-marine origin for widespread inland saline groundwater in the
800 Pearl River Delta, while modern seawater intrusion mainly modifies estuarine and
801 nearshore aquifers. Over much longer geologic timescales, such as 10^4 – 10^5 years,
802 cumulative changes in sea level, shoreline position, coastal salinity, and lateral
803 hydraulic conditions may extend across a much larger groundwater system, and model-
804 bottom elevation, bedrock aquifers, and fracture connectivity may become increasingly
805 important. Model detail, calibration priorities, and monitoring design should therefore
806 be selected jointly according to the forecast variable, target area, and time horizon.
807 These scale-dependent relationships, together with the observation-informed
808 perturbation approach, are transferable to other coastal-delta and estuarine aquifers with
809 comparable depositional heterogeneity, river–coast hydraulic connections, and
810 paleoenvironmental histories.

811 **Code and data availability**

812 The MODFLOW 6 software used for the simulations is available from the U.S.
813 Geological Survey (USGS) at [https://www.usgs.gov/software/modflow-6-usgs-](https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic-model)
814 modular-hydrologic-model. The code used to construct the multiscale heterogeneous
815 structures is available on Zenodo at <https://zenodo.org/records/20772683>. Borehole
816 records obtained from the GeoCloud database of the China Geological Survey are
817 subject to the data-access conditions of the original platform



818 (<https://geocloud.cgs.gov.cn/>). The MODFLOW 6 model configuration is described in
 819 the manuscript.

820 **Author contributions**

821 CZ: Conceptualization, Methodology, Software, Formal analysis, Data curation,
 822 Visualization, Writing – original draft. JJJ: Supervision, Project administration,
 823 Funding acquisition, Writing – review and editing. ZD: Methodology, Funding
 824 acquisition, Writing – review and editing. MRS: Methodology, Writing – review and
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