

Dear Dr. Guo,

Thank you and the three reviewers for the insightful comments and suggestions on our manuscript (Paper # egusphere-2025-2631). The manuscript has been carefully revised by addressing the constructive suggestions. The following is point-point response to all the comments. Notably, the following line numbers in blue are according to the “Manuscript\_text\_Clean”.

**Handling Editor:**

We received comments from three reviewers. All three reviewers recognize that the study addresses an important problem and could make a useful contribution, but the current manuscript requires substantial revisions. In particular, the conceptual description, numerical/physical justifications (especially geometry, mass conservation, and boundary conditions), validation, and novelty positioning will need thorough rework. I encourage the authors to treat the reviewers’ critiques as a roadmap and to submit a point-by-point response with added analyses and clarified text/figures. Given the convergent critiques on (i) conceptual/modeling clarity, (ii) geometry/boundary physics and mass conservation, (iii) validation sufficiency, and (iv) positioning of novelty, I recommend major revision. The manuscript is potentially suitable for HESS after a substantial, well-documented revision that fully addresses the reviewers’ comments.

**Reply:** Thank you for your comments and suggestions! We have thoroughly revised the manuscript, including a comprehensive introduction to the conceptual framework and boundary conditions, see lines 130-179 and 228-267. We have validated the numerical and physical justifications, including the neglect of geometry, mass conservation, and periodic conditions, through additional simulations, see lines 239-254, 266-267 and 433-466. For the validation of our numerical simulation against Wolke et al. (2020), we refined the numerical model parameters to achieve a better fit with the experimental data, see lines 467-508. Additionally, we have supplemented and highlighted the novelty of this study in the Introduction and Model description, see lines 110-121 and 147-159.

Below is a summary of some of the major revision points upon my assessment of the reviewers’

comments (Please refer to the original review comments for a complete list).

1. Reframe and clarify the conceptual model.

Rewrite §2.1 with a precise, self-contained description of the one-domain/multi-variable setup; clearly define layers, interfaces, exchanges, and computational pools; ensure Figure 1 and captions match the text. Address mass conservation explicitly (for water and for all species), with complete boundary condition definitions.

**Reply:** We have revised Section 2.1 to include a precise description of the conceptual model (one-domain/multi-variable domain), clear definitions of the riverbed surface/layer, water exchange, and the computational domain (riverbed sediment), see lines 129-179. We have also revised Figure 1 and its corresponding caption to match the revised text, and added Figure 2 to illustrate the complete boundary conditions for water and all species. Additionally, mass conservation calculations have been performed and incorporated into the revised manuscript, please see lines 266-267.

2. Justify the geometry treatment—or add explicit-geometry tests.

Either (a) incorporate simulations with resolved ripple geometry and compare HEF, mixing fields, shear, and key metrics to the flat-bed surrogate, or (b) provide strong external validation for the simplification (e.g., compare shear/pressure fields against CFD or experimental references) and quantify the induced uncertainty.

**Reply:** As suggested by the Editor, we have conducted additional simulations incorporating ripple geometry and compared their results, including hyporheic flow fields and biogeochemical parameters, with those of the flat-bed model. Both the triangular ripple model and the flat-bed model were used to reproduce the experiment conducted by Wolke et al. (2020), and the successful reproduction of the experimental results confirms the reliability of the flat-bed model, please see the revised Section 3.1 Model validation (lines 433-508). Regarding the influence of neglecting ripple geometry on shear velocity, we have provided robust references to support the rationality of the calculated shear velocity and bedform migration celerity, rather than establishing a CFD model. The revised manuscript explicitly states these limitations, proposes CFD-based validation as future work, and confirms that the empirical approach is appropriate

for the context and objectives of this study, please see lines 730-745.

### 3. Revisit nitrate partitioning and kinetics.

Demonstrate mass conservation with the surface water and groundwater nitrate split under Monod kinetics; specify all boundary conditions for both pools; or adopt an alternative formulation (single nitrate field with provenance diagnostics) and justify the choice.

**Reply:** Based on different nitrate sources, we define stream-borne and groundwater-borne nitrate as two distinct reactants, which participate in denitrification without any differences in reactivity. We have justified our choice of approach, specified all boundary conditions for water and all solutes, and verified the mass conservation of water and solutes through calculations, please see lines 177-179, 229-266, and 266-267.

### 4. Demonstrate novelty and scope vs. the authors' 2022 paper.

Expand the literature review and explicitly delineate what is new here beyond Ping et al. (2022): for example, new physics, regimes, or predictive relationships (e.g., scaling, regime maps) that are generalizable; avoid over-claims (e.g., “first time”) unless defensible.

**Reply:** We have expanded the literature review, highlighted the novelty of this study, and clarified the differences from Ping et al. (2022) in the revised Introduction and Methods sections, please see lines 110-121 and 147-159. New mixing regimes and their impacts on mixing-triggered denitrification reactions have been observed under dynamic bedforms, findings that cannot be derived from previous studies. We have also re-summarized these new findings in the Results and Discussion, please see lines 510-630 and 631-714. Additionally, we avoided using the expression “for the first time” throughout the manuscript.

### 5. Justify and stress-test the new mixing metrics.

Provide a physical/statistical rationale for the 16–84% mixing-zone threshold; include sensitivity to threshold choice, grid resolution, and numerical dispersion; relate your metrics to established measures of mixing.

**Reply:** We have provided a physical rationale for the threshold and performed sensitivities analysis on three alternative thresholds, please see lines 376-387. Sensitivity analysis was also

performed to assess grid resolution, ensuring reliable simulation results with minimal numerical dispersion, see lines 363-368. The mixing-related metrics have also introduced clearly in the revised text, see lines 376-414.

6. Address model idealizations and limits.

Discuss implications of the 2-D, single-wavelength, homogeneous-sediment assumptions; where feasible, add sensitivity tests (e.g., heterogeneity, multiple wavelengths, anisotropy).

**Reply:** We have discussed the limitations and implications of the 2D, single-wavelength, homogeneous-sediment assumptions in the revised text, see lines 715-773.

**Response to Reviewer #1:**

The hyporheic zone plays a vital role in mitigating contaminants through interactions between surface water and groundwater. This study investigates the effects of bedform migration on the mixing dynamics of these waters and the accompanying biogeochemical reactions, particularly under gaining stream conditions, by utilizing a coupled hydrodynamic and reactive transport model. The research focus is meaningful, and the numerical model is well validated. However, I believe the overall clarity and presentation of the manuscript can be further improved. My suggestions are as follows:

**Reply:** Thank you for the comments and suggestions on the manuscript. The manuscript has been carefully revised by addressing all the comments. The following is point-point response to the comments.

Parameter explanations: I strongly recommend that the authors carefully review and expand the explanations of all parameters. Many parameters are currently not well defined, which may reduce accessibility for future readers.

**Reply:** We have thoroughly reviewed the explanations of all parameters across the text, including those in the method, results and notation sections. For parameters that were previously insufficiently defined (e.g.,  $D_{50}$  in line 105,  $dt$  in line 232,  $R_i$  in line 191,  $r$  in line 288 in the revised version), we have expanded their descriptions to include definitions and units.

Writing style: I suggest avoiding the use of "we" throughout the manuscript, as this expression is less common in formal academic writing. Rephrasing such sentences into more objective forms would enhance the manuscript's style.

**Reply:** In the revised version, all sentences originally containing “we” have been rephrased into objective expressions. For instance, statements such as “we only focused on a representative section and constructed a two-dimensional rectangular domain of length 0.2 m and depth 0.16 m for modeling” have been adjusted to “a two-dimensional (2D) rectangular domain is constructed with a length ( $\lambda$ ) of 0.2 m and depth ( $l$ ) of 0.16 m”, “we introduced the dimensionless parameter  $Ur$  to represent ...” has been modified to “the dimensionless parameter  $Ur$  was introduced to represent ...”, and “in this study, we focused on ripples and, more broadly, shorter-wavelength topographic roughness elements that form under low subcritical flow conditions in sandy riverbeds” have been changed to “this study focuses on ripples and, more broadly, shorter-wavelength topographic roughness elements formed under low subcritical flow conditions in sandy riverbeds” etc.

Specific comments:

Line 22: Please consider adding a comma between "migration" and "this" ("incorporates bedform migration this paper" → "incorporates bedform migration, this paper").

**Reply:** We have revised “incorporates bedform migration this paper” to “incorporates bedform migration, this paper” in line 24.

Notation consistency: I recommend keeping nitrate consistently as  $\text{NO}_3^-$  throughout the manuscript (e.g., Line 81 uses  $\text{NO}_3^{-1}$ , while Line 55 uses  $\text{NO}_3$ ).

**Reply:** We have revised “ $\text{NO}_3$ ” to “ $\text{NO}_3^-$ ” in line 60, and checked the overall manuscript to keep nitrate consistently as  $\text{NO}_3^-$ .

Line 100: Please explain  $D_{50}$  here.

**Reply:**  $D_{50}$  is defined as the median grain size of riverbed sediments, see line 105.

Line 114: Since the manuscript refers to "multi-component," I recommend using brackets to

quickly introduce these components.

**Reply:** The specific components (DOC, O<sub>2</sub>, and NO<sub>3</sub><sup>-</sup>) are added after “multi-component”, see lines 122 and 170.

Line 125: Providing the dimensions of parameters (as done in Line 152) would be helpful.

**Reply:** The manuscript has been carefully reviewed to ensure the dimensions of all parameters are provided. The missing dimensions of parameters in line 125 (in the original version) have been added, see lines 137-142 (in the revised version).

Figure 1: The figure is somewhat confusing. Using a different color scheme for the mixing zone would improve clarity, as the current colors resemble a geological layer. Adding a note to indicate that the blue curve represents river elevation would also help. In the caption, I suggest rephrasing as: "NMD reaction = non-mixing-dependent reaction and MD reaction = mixing-dependent reaction."

**Reply:** To improve clarity, we have revised the color of the mixing zone from gray to light yellow and added a label reading “mixing zone”. The blue curve has been removed because stream flow simulation was not included in this model (see Figure 1). In the caption, “NMD reaction=non-mixing-dependent reaction and MD reaction=mixing-dependent reaction” has changed to “NMD reaction = non-mixing-dependent reaction and MD reaction = mixing-dependent reaction”, see lines 167-168.

Line 133: Please revise "and SW out is ..." to "SW out is ...."

**Reply:** We have revised “and SW out is ...” to “SW out is ...”, see line 164.

Line 150: Since the bedform has a nonuniform distribution, would it be possible to consider anisotropic hydraulic conductivity in this study?

**Reply:** The numerical models assume isotropic sediment *K*. In fact, natural riverbeds with small-scale bedforms (e.g., dunes and ripples) commonly exhibit strong anisotropy. For bedforms with flow-transverse crests, pore pathways parallel to the crests are relatively continuous and straight yielding high transverse *K*. In contrast, pathways perpendicular to the

crests are highly tortuous: water here must move upward through erosional, high-porosity troughs and downward over depositional, low-porosity crests. This undulating flow path, combined with flow separation and local energy losses at morphological transitions, substantially increases hydraulic resistance and lowers longitudinal  $K$  (Dallmann et al., 2020; Salehin et al., 2004). Additionally, spatial variability in bedform dimensions (e.g., increasing dune wavelength downstream) enhances this anisotropy by introducing zones of differing flow resistance along the streamwise direction (Venditti et al., 2005). Given that the model is constructed along a longitudinal section with spatially consistent, periodic bedforms, the use of an isotropic hydraulic conductivity assumption is justified. Incorporating anisotropic  $K$  is critical for accurately modeling hyporheic exchange and related biogeochemical processes in three-dimensional models. We have added this paragraph in the Discussion of the revised manuscript, see lines 760-773.

Line 153: As the abbreviation BC first appears here, it should be explained. (Since it also appears in Fig. 1 as line BC, I suggest not using BC as the abbreviation for boundary condition to avoid confusion.) Similarly,  $u_c$  and  $dt$  in Eq. (2) require explanation. Given the large number of parameters, I recommend creating a notation table summarizing all variables with their definitions.

**Reply:** We have added and described the boundaries of the modeled domain in Section 2.1 Model description, see lines 144-146. In equation (2, in the original version),  $u_c$  and  $dt$  represent the ripple migration celerity and a certain timestep in the simulation, respectively. We add their explanation in equation (10, in the revised version), see lines 230 and 232. We have also created a notation table summarizing all variables with their definitions, see line 16.

Line 161: Please clarify whether  $n$  and  $a$  have physical meaning or relationships. This would improve the organization of the manuscript.

**Reply:** There is no physical meaning or inherent relationship between parameters  $n$  and  $a$ ; they are merely constant coefficients, we have stated that clearly in the revised manuscript.

Line 165: Explanation of  $Ri$  is missing.

**Reply:**  $R_i$  [ $M L^{-3}T^{-1}$ ] denotes the biogeochemical rate of reactive components and was added in the revised manuscript text, see lines 191-192.

Line 168: Explanations of  $v_i$  and  $v_j$  are missing. Also, note that  $v$  is a vector in Eq. (4) but a scalar in Eq. (5). Please clarify if they represent the same variable.

**Reply:** Bold  $\mathbf{v}$  denotes the seepage velocity vector, and non-bold  $v$  represents the magnitude of the seepage velocity  $v = |\mathbf{v}|$ ;  $v_i$  and  $v_j$  denote the seepage velocities in the  $i$ -direction and  $j$ -direction, respectively, see lines 196-197. Equations 4 and 5 in the original version have been checked and revised, with the variable  $\mathbf{v}$  formatted in bold uniformly in the revised version, see lines 189 and 194.

Line 171: Emphasizing why the three chemical species were selected would strengthen the manuscript (e.g., due to dominant reactions or research focus).

**Reply:** The reactive transport model considered three chemical species: DOC,  $O_2$ , and  $NO_3^-$ . The biogeochemical reactions, aerobic respiration (AR), non-mixing-dependent, and mixing-dependent denitrification (DN), with DOC as the electron donor and  $O_2$  and  $NO_3^-$  as sequential electron acceptors, capture the primary mechanism of  $NO_3^-$  cycling and are widely used in studies on hyporheic zone nitrogen dynamics (Bardini et al., 2012; Hester et al., 2019; Zheng et al., 2019). Denitrification is the well-recognized critical process for  $NO_3^-$  transformation and reduction in riparian and hyporheic zones. Dissimilatory nitrate reduction to ammonium (DNRA) and anaerobic ammonium oxidation (ANAMMOX) are not included in the model, as these processes play secondary role on nitrogen cycling and require highly specific conditions to occur (Zarnetske et al., 2012). Ammonia ( $NH_4^+$ ) was excluded, as it is unstable in the study environment:  $NH_4^+$  in surface water or groundwater is prone to nitrification (converting  $NH_4^+$  to  $NO_3^-$ ) either within hyporheic flow cells or in upwelling groundwater upon  $O_2$  exposure, leading to relatively low  $NH_4^+$  concentrations (Hester et al., 2014). The context has added in the manuscript text, see lines 202-215.

Line 178: Since Monod kinetics is referenced, I recommend directly citing Monod's original work.

**Reply:** The Monod's original work is cited in line 216.

Line 190: In Line 150, you refer to hydraulic head, while here pressure is mentioned. Are these the same variable? Consistency is important. Additionally, please clarify the physical meaning of applying a periodic boundary condition.

**Reply:** Hydraulic head and pressure are not identical variables but are closely related through fluid mechanics principles ( $h = P/\rho g$ ). In line 229, we used "hydraulic head" to describe the boundary condition for the upper riverbed, as the pressure profile along the riverbed surface drives hyporheic exchange. Here, when mentioning "pressure", we specifically refer to the pressure component ( $P$ ) of the hydraulic head, which is used to characterize the pressure difference across the left and right periodic boundaries. The application of periodic boundary conditions is based on modeling the spatially periodic characteristics of the actual riverbed system, with the following specific physical meanings: 1) A periodic pressure boundary condition simulates recurrent pressure variations induced by periodic undulations of the riverbed surface. Since ripples form periodically along the flow direction, pressure at a given position on one dune crest/trough matches that at the equivalent relative position on an adjacent dune, this setup replicates natural pressure continuity between adjacent periodic riverbed units. 2) A periodic concentration boundary condition is implemented to preserve mass conservation and ensure concentration continuity across adjacent periodic units of the riverbed during solute transport. Within the riverbed domain, the concentration and mass flux at the termination of one periodic topographic unit (e.g., the end of a ripple) remains consistent with those at the initiation of the next adjacent unit. This boundary condition effectively extends the "local" model domain to represent the entire periodic riverbed system. We have added a paragraph in Section 2.2.2 Boundary condition, see lines 237-254.

Line 197: The phrase "a set of criteria" is unclear—are these criteria listed in the manuscript? Figure 2 is also difficult to interpret; more explanation would help.

**Reply:** A comprehensive explanation of the criteria for ripple formation has been included in Supporting Information Text S1. Ripples formation was qualitatively determined using the bedform stability diagram (Figure 3, in the revised version). This diagram is a summarized

reference for examining equilibrium bed configurations in unidirectional flow, derived from a series of flume experiments and field studies (Ashley, 1990). Besides, a series of quantitative criteria (Text S1 in the supporting information: Criteria for ripple migration) was developed to ensure ripple formation under the modeled scenarios and the achievement of dynamic equilibrium. For a specific grain size of streambed sediment ( $D_{50}$ ), particular stream velocities ( $U$ ) satisfying all these criteria are selected and displayed in Figure 3. We have added further explanations for Figure 3 in Section 2.3 Bedform migration of the revised manuscript, see lines 269-279.

Line 260: Just a positive note here—I appreciate how the manuscript justifies parameter values with references or physical reasoning. This strengthens the credibility of the work.

**Reply:** Thank you for your comments!

Figure 3: Including RMSE values (simulation vs. experiment) in each subplot would enhance the validation of the model.

**Reply:** The RMSE values (simulated vs. experimental) for each subplot were calculated and are displayed in Figure 5 (in the revised version).

Conclusion: The conclusion could be further strengthened by including quantitative results that highlight the main findings.

**Reply:** We agree that quantitative results in the conclusion will strengthen the conclusion. We have revised the conclusion section to include the key quantitative results. For example, the mixing proportion of total exchange flux and mixing zone scope also experience significant increases at the onset of migration; as stream velocity further rises, the mixing proportion (~60%) and mixing size (~10–15% of the riverbed) gradually reach plateaus.

### **Response to Reviewer #2:**

Ping X. et al reported a modeling study of the mixing process and mixing-dependent denitrification beneath a moving bed form. The topic is very important, and results are valuable. However, there are several critical issues in conceptual model description, ripple geometry

simplification, nitrate concentration partitioning, shear stress estimation, and model validation. Major issues were summarized below for the authors for consideration. Detailed comments are attached at the end.

**Reply:** Thank you for the comments and suggestions on the manuscript. The manuscript has been carefully revised by addressing the suggestions. The following is point-point response to all the comments.

Major comments:

1. Simplifying ripples as a flat surface need justification. For non-mobile bedform, it is well known that non-uniform pressure distribution applied on the ripple surface cause pressure gradients horizontally and vertically, which further control the complex pressure, velocity, and concentration distributions inside and beneath the bedform. Due to its driving force, it is critical to include the ripple geometry in simulations, which is a common practice in most modeling research for stationary hyporheic zone (HZ) (see Cardenas2007, WRR). For mobile bedform, one of the few experiments on hyporheic zone with mobile bedforms show that the distribution of concentrations is mostly complex inside and near moving ripple (Wolke2020, Water). This also suggests the most important role of ripple geometry in reproducing realistic flow and transport distributions in HZ. Without representing ripple geometry in the model, the exchange flux, concentration distributions, and shear stress on, inside, and beneath the ripple will likely have high uncertainty if they are estimated from existing empirical equations. I suggest the authors justify such assumption by adding a new simulation with ripple geometry and then evaluate how much difference could be in exchange flux, concentration flux, and shear stress from models with and without ripple.

**Reply:** We acknowledge the importance of ripple geometry in HZ modeling and address your concern with supplementary simulations and literature. The idealization of a flat bed and a sinusoidal head variation have the following basis. Firstly, the pressure distribution over the riverbed surface can be approximately by a sinusoidal curve. Secondly, the vertical component of pumping into and out of the bed is retained if the bed becomes flat (while retaining the same pressure distribution over the bed). Thirdly, the flow patterns within the riverbed (especially deeper in the bed) are little affected by the topography. These approximations result in only

minor error (Elliott & Brooks, 1997a; Figure 7) in relation to the case with measured (derived from Fehlman 1985, non-sinusoidal) head applied over triangular bed forms. Further, Rutherford (1994) and Rutherford et al. (1995) also illustrated the similarity of the streamlines for the idealized case as compared with the triangular bed form case.

We have conducted an additional simulation incorporating ripple geometry and compared its results with those of the flat bed model as the reviewer suggested; the two sets of results exhibit similar characteristics in hyporheic flow field and solute plume distributions. Compared with the triangular ripple model, the flat bed model exhibit slightly larger hyporheic exchange flux, mixing flux, and stream-borne nitrate influx. The relative errors are approximately 10%.

Meanwhile, both the mixing-dependent and non-mixing-dependent denitrification rates are higher in the triangular ripple model than in the flat bed model, with relative errors around 20%. Differences in the results of the simulated domain cause subtle changes in flow and transport processes, changes that are acceptable for our intended purposes. Detailed comparisons have been added to in Section 3.1.1 Validation of flat bed model with triangular ripple model (see lines 433-466).

Furthermore, these two models were used to reproduce the experiment by Wolke (2020). Based on the parameter adjustments outlined in the previous manuscript text, we refined the numerical model to achieve a better fit with the experimental data. Both models show good agreement with Wolke et al.'s (2020) experimental data, including hyporheic exchange flux, oxygen influx/outflux and oxygen plume, despite some discrepancies between these two models (see Section 3.1.2). Notably, the flat-bed model successfully captured two critical oxygen plume patterns: (1) a conchoidally shaped oxygen plume beneath the bedform in cases of stationary or slowly migrating bedforms, and (2) a uniform oxygen plume beneath rapidly migrating bedforms. Its adequacy is further supported by our successful reproduction of Wolke's (2020) results, thereby confirming its credibility for addressing the study's objectives (see lines 467-508).

For our model, a fixed frame of reference is physically reasonable for studying the processes of bedform migration. In practice, sediment grain suspension and deposition, the key processes driving the forward migration of ripples, occur exclusively in the upper triangular segment of the bedform, whereas the lower portion of the streambed remains stationary. In fact, nitrate

transport primarily takes places within the immobile riverbed sediment. Additionally, given that the height of the ripples (2 cm) is much smaller than that of the underlying immobile domain (16 cm), the undulated riverbed can be reasonably approximated as a flat bed with temporally varying pressure distributions, which represent the passage of successive triangular ripples. Detailed description has been added to Section 2.1 Model description. In addition, for your concerning shear stress estimation with triangular ripples neglected, please refer to the response to comment 5.

2. The conceptual model presentation and Figure 1 needs improvements to better align with text descriptions, Figure 1 and texts in Section 2.2-2.6. In the current modeling approach for HZ, popular approaches are two-layer and three-layer conceptual model. Figure 1 suggests a two-layer model, i.e., splitting the domain as a surface water layer (regions above ripple top boundary) and groundwater layer (regions below ripple top boundary) with riverbed surface (ripple top boundary) as a permeable interface. However, when reading the details in Section 2.1-2.6, the model is a three-layer structure: surface water layer, riverbed layer (a thick 3D layer instead of a riverbed surface), and groundwater layer. Different from traditional 3-layer structure, this paper does not explicitly solve Navier-Stokes equations for surface water layer and Darcy-equation for groundwater layer. Instead, this work only solves the pressure head and concentration for the riverbed layer with simplified boundary conditions for pressure head/concentrations at the top (boundary BC in Figure 1) and bottom (boundary AD in Figure 1) boundary of the riverbed layer. Further, this paper split the riverbed layer into two pools, i.e., non-mixing dependent reaction pool (blue region in Figure 1) and mixing dependent reaction pool (red region in Figure 1). Note that such “two” pools share the same computational domain (bounded by ABCD). They do not have an internal interface (critical for traditional two-layer or three-layer models) to conserve water and concentration mass. Instead, this work defines two variables ( $c_{\text{s-NO}_3}$  and  $c_{\text{g-NO}_3}$ ) and apply the advection-diffusion-reaction equation (equation 4) twice for these two variables. This means the model is essentially a one-domain multiple-variable model. However, most of this information was not clearly presented in Section 2.1, which is supposed to serve for this purpose. I suggest the authors modify Section 2.1 and relevant texts in Sections 2.2-2.7 to reflect the key conceptual model setups in Section 2.1.

Please be aware that further readers may not be familiar with different conceptual models for modeling HZ. Your precise introduction is critical for them to correctly understand your work.

**Reply:** Actually, this model is a one-domain, multiple-variable model. In the present study, our focus was on porewater dynamics and multi-component solute transport within riverbed sediments, and the modeled domain corresponds to the actual rectangular geometry of the riverbed (bounded by ABCD). Rather than simulating turbulent flow over regular triangular bedforms, we adopted an idealized approach: applying sinusoidal pressure variations to a flatbed (i.e., boundary BC in Figure 1). This methodological choice is justified, and the reasons has been shown in our response to Major Comment 1. For the modeled domain, no further subdivision of the riverbed interior into two pools is made. In the original Figure 1, our primary intention is to illustrate the potential scope and spatial distribution of mixing-dependent (red region in Figure 1) and non-mixing-dependent reactions (blue region in Figure 1). To distinguish between non-mixing-dependent and mixing-dependent denitrification, we defined stream-borne nitrate ( $c_{s-NO_3}$ ) and groundwater-borne nitrate ( $c_{g-NO_3}$ ) as two distinct reactants, rather than partitioning the nitrate pool into two separate fractions. The transport of stream-borne and groundwater-borne nitrate in the porous medium is solved separately using the advection-dispersion-reaction equation. The boundary conditions for the transport of stream-borne nitrate and groundwater-borne nitrate were clearly presented in Section 2.2 Boundary condition in the revised manuscript text, respectively. We have revised Figure 1 to accurately reflect the configurations of our conceptual model and added Figure 2 to display a schematic diagram of the simulated domain and boundary conditions. We have also revised Section 2.1 Model Description in the revised manuscript text: it now explicitly specifies the model type (one-domain, multi-variable), defines the modeled domain (riverbed sediments, i.e., ABCD), clarifies key processes and assumptions (e.g., no simulation of surface water flow, idealized top-boundary pressure), and details the two nitrate variables (including their sources and boundary conditions). Additionally, we systematically cross-checked and revised Sections 2.2-2.6 to ensure full consistency with Section 2.1 (see lines 180-373).

3. It is not clear if mass conversation for pressure head and concentration can be achieved based on the current model descriptions. The boundary BC and DC is fine due to use simple “periodic”

boundary. For boundary BC and AD, it is not clear to me how to guarantee consistent at boundary conditions at BC and AD for pressure head, head gradient (used to further compute exchange flux), and concentration gradient due to unclear boundary condition descriptions.

**Reply:** We have clarified the boundary naming, stated the governing equations, and given the exact boundary conditions used for both porewater flow and reactive solute transport. We also reported quantitative mass-balance checks. These additions were included in the revised manuscript text, see Section 2.1 Model description and Section 2.2 Boundary condition.

1) Clarification of the boundary naming (revised Figure 1): we now state explicitly the rectangular domain has corners A (0, 0), B (0, l), C ( $\lambda$ , l) and D ( $\lambda$ , 0). The lateral boundaries are AB (left,  $x = 0$ ) and CD (right,  $x = \lambda$ ); the top boundary is BC ( $y = l$ ) and the bottom boundary is AD ( $y = 0$ ). The outward unit normal is  $\mathbf{n}$ .

2) Boundary conditions for flow (Figure 2): the lateral boundaries AB and CD are prescribed with periodic conditions, with an additional pressure drop ( $\Delta P$ ) between the upstream and downstream ( $P(0, y, t) = P(\lambda, y, t) - \Delta P$ ). The pressure drop describes the riverbed hydraulic gradient and is calculated by applying the equation  $\Delta P = S\rho g\lambda$ . The top boundary BC is prescribed with a Dirichlet head condition  $h(x, l, t) = h_m \sin m(x - u_c t)$ . The exchange flux across BC is not prescribed, and it is computed from the solution  $q_h(x, t) = -\mathbf{n} \cdot K \nabla h|_{BC}$ . The bottom boundary AD is set as Neumann boundary (specified upward flux  $u_q$ ). The top and bottom-boundary equations are mutually compatible: one boundary prescribes head; the other prescribes normal flux.

3) Boundary conditions for solute transport (Figure 2): the lateral boundaries AB and CD are prescribed with periodic conditions for concentration and its normal derivative:  $c(0, y, t) = c(\lambda, y, t)$ , and  $-\mathbf{n} \cdot (D_{ij} \nabla c_i)|_{x=0} = \mathbf{n} \cdot (D_{ij} \nabla c_i)|_{x=\lambda}$ . For stream-borne nitrate, the top boundary BC is defined as an open boundary, where the flow direction switches between inflow and outflow in accordance with the computed normal Darcy flux  $q_h$ :  $c = c_{ext}$  (Dirichlet) if  $q_h < 0$  (inflow) and  $\mathbf{n} \cdot (-D_{ij} \nabla c_i) = 0$  (outflow condition) if  $q_h \geq 0$  (outflow); and the bottom boundary AD is defined as an outflow boundary. For groundwater-borne nitrate, the bottom boundary AD is set as an open boundary with a constant  $c_{ext}$ , and the top boundary BC is set as an outflow condition. Here  $c_{ext}$  is the external stream-borne or groundwater-borne solute concentration at the inflow boundary.

4) Model conservation calculations were also performed to ensure fluid and solute mass

balance. We verified the fluid and mass balance by calculating the total influx and outflow fluxes across all boundaries over the simulation period for conditions of  $Re = 3000$ ,  $U_b = 0.6$ , and  $D_{50} = 0.15$  mm. The fluid influx and outflux, as well as the solute input and output across various model boundaries, together with internal consumption were quantified and presented in the table below. The influx of fluid is equal to the outflux of fluid. And the solute influx is approximately equal to the sum of solute outflux and consumption. Notably, the relative error remains below the acceptable threshold (less than 5%) for numerical models, effectively confirming the conservation of fluid and solute mass. The context has been added in supporting information, see Text S2.

4. Partitioning the total Nitrate into surface water layer contribution ( $c_{\text{s-NO}_3^-}$ ) and groundwater layer contribution ( $c_{\text{g-NO}_3^-}$ ) maybe problematic due to the involvement of non-linear reaction rate in the Monod kinetics. From equation 7, the reaction rate of denitrification  $R_{\text{DN}}$  is a function of Nitrate concentration, i.e.,  $R_{\text{DN}} = f(\text{NO}_3^-)$ . If simulating the total  $\text{NO}_3^-$  with partitioning, there will be two reaction rate  $R_{\text{DN}}(c_{\text{s-NO}_3^-})$  (equation 8) and  $R_{\text{DN}}(c_{\text{g-NO}_3^-})$  (equation 9). Due to non-linearity of Monod equation  $f$ ,  $R_{\text{DN}}$  does not equal the summation of the reaction rate from two partition components, i.e.,  $f(\text{NO}_3^-) \neq f(\text{sNO}_3^-) + f(\text{gNO}_3^-)$ . This means partition approach is not mass-conservation. Additionally, introducing two concentration variables means need 4 more boundary conditions at top and boundary conditions for  $c_{\text{s-NO}_3^-}$  and  $c_{\text{g-NO}_3^-}$ . This paper does not clearly explain how such boundary conditions are assigned. In short, the current Nitrate concentration approach causes mass conservation issues and needs 4 more boundary conditions data which are not well described. I suggest the authors clarify these issues in the revision.

**Reply:** Based on different nitrate sources, we define stream-borne and groundwater-borne nitrate as two distinct reactants that participate in denitrification with identical reactivity. This definition aims to distinguish between non-mixing-dependent and mixing-dependent denitrification reactions in the model. We separately solve for the transport of these two nitrate fractions in the porous medium using the advection-dispersion-reaction equation. As outlined in our response to Comment 3, each nitrate type, differentiated by its origin, has its own set of boundary conditions. We quantified the inputs and outputs of both stream-borne and

groundwater-borne nitrate, as well as their internal consumption via denitrification. Notably, the relative error remains below the acceptable threshold ( $< 5\%$ ), confirming the conservation of solute mass (see our response to Comment 3 for details). We have added Figure 2 to present a schematic diagram of the simulated domain and its boundary conditions, and revised Section 2.2 to clearly describe these boundary conditions.

5. Estimation of shear stress that drives sand transport is likely not reliable. The estimation of migration velocity  $u_c$  depends on shear velocity and shear stress on the ripple surface. Due to the simplification of ripple into a flat surface, calculation of shear stress/shear velocity is not possible. This paper estimates the shear velocity using the Chezy equation. The Chezy equation usually works well for flat surface with homogenous sediments. In this work, the sand is very small (0.08-0.36 mm) and homogenous. However, the ripple is much bigger (height 0.02 m). The correct shear stress is the one on the surface with both large ripple and small sand. The use of Chezy is likely not adequate to estimate such variables. The most accurate way will be using numerical model to directly compute shear stress with the ripple geometry as the top boundary. If the authors want to use the Chezy equation, it needs to be verified against at least one CFD simulated or observed shear stress to quantify potential uncertainty.

**Reply:** The classical Chezy equation was specifically used to estimate the flatbed shear velocity—a prerequisite for determining incipient sediment motion (i.e., the threshold for ripple initiation). This application aligns with its well-validated scope: homogeneous sediments (0.08–0.36 mm in our study) and flat-bed conditions, where it reliably predicts baseline shear stress for sediment transport initiation.

For quantifying ripple migration celerity post-ripple formation, we did not rely solely on the Chezy-derived shear velocity. Instead, we integrated the empirical relationship by Coleman and Melville (1994), which is explicitly calibrated against extensive flume experiments to account for form drag from periodic bedforms. This two-step framework, using grain resistance for incipient motion and form drag-based empirical models for bedform migration, is widely accepted in bedform migration literature (e.g., Ahmerkamp et al., 2017; Zheng et al., 2019) and has been validated against experimental data, including our successful reproduction of Wolke et al. (2020) results. This confirms the approach’s ability to capture key bedform migration

characteristics relevant to our study.

Our core objective focused on investigating how bedform migration modulates hyporheic solute transport and mixing-dependent denitrification, rather than resolving turbulent flow details or precise shear stress distribution over ripple surfaces. To this end, we employed two complementary simplifications: (1) idealized sinusoidal pressure variations at the sediment-water interface (mimicking ripple-induced periodic pressure fluctuations) and (2) empirically derived bedform migration celerity. These methods prioritize the dynamic effects of bedform migration (the central research question) while balancing computational feasibility.

We fully agree that CFD simulations would provide more precise shear stress profiles and pressure distributions over complex ripple geometries. As highlighted in the revised manuscript, we have explicitly stated this limitation and proposed CFD-based validation as a key direction for future work. This will help quantify potential uncertainties and refine the mechanistic understanding of bedform-hyporheic interactions. These contexts have added in the revised text, please see lines 730-745 in Discussion.

6. What were compared in the model validation is not clear. Figure 5 shows a comparison between model and observation. However, how  $HEF$ ,  $AO$ ,  $F_{in}$ ,  $F_{out}$  were computed is not explained clearly. The model results are distributed data. The authors need to explain how to convert distributed values into single values like  $HEF$ ,  $AO$ ,  $F_{in}$ ,  $F_{out}$ . Second, the oxygen concentration from the model is affected by reaction R1. It is not clear if the experiment also implemented a similar reaction. If the model has a reaction R1 and the experiment does not, then it is not reasonable to compare model predicted  $RO$  with experiment observed  $RO$ . Please add more information about the details of model validation. Especially, please clarify if the model setup is consistent with the experiment setup, especially the reaction part.

**Reply:** We have added a detailed descriptions of the experimental measurement methods and simulated calculation methods in the key metrics, including  $HEF$ ,  $AO$ ,  $F_{in}$  and  $F_{out}$ . This added content can be found in Section 3.1.2 Validation of numerical models with laboratory experiments (see lines 468-508). In the numerical model,  $HEF$  was calculated by integrating the volumetric flux over the inflow zones along the sediment-water interface. Oxygen transport was governed by the advection-dispersion-reaction equation, where oxygen consumption occurred

through aerobic respiration following the Monod kinetics described by Equation (8). The  $F_{in}$  and  $F_{out}$  were then computed by multiplying the  $HEF$  by the oxygen concentration in the surface water and the oxygen concentration over the outflow zones along the sediment-water interface, respectively. The oxygenated area  $A_o$  was calculated by integrating the riverbed portions where oxygen saturation exceeds 15%. For oxygen consumption, Wolke et al. (2020) did recognize and observe that oxygen is consumed in riverbed sediments, yet they did not clarify which specific process is responsible for this consumption. However, aerobic respiration by microbial biomass is widely recognized as the dominant process driving oxygen consumption in such environments (Ahmerkamp et al., 2017; Reeder et al., 2018). Therefore, oxygen transport was governed by the advection-dispersion-reaction equation, where oxygen consumption occurred through aerobic respiration following the Monod kinetics (R1) in our modeling. The experimentally observed RO is calculated using oxygen influx/outflux and the mean oxygen penetration depth, and it represents the volumetric oxygen consumption rate across the entire domain. The good agreement between the simulated and measured  $F_{in}$  and  $F_{out}$ , coupled with the spatial distribution of oxygen plumes, ensures minimal discrepancy in this RO-derived rate. Additionally, RO differs in meaning from R1 within the model: the latter specifically refers to the reaction rate per unit pore volume. Therefore, we did not compare the model-predicted R1 with the experimentally observed RO.

7. The validation result from Figure 5 suggests model prediction for HEF and concentration flux may be reliable (if potential issues in Comment 5 get clarified). However, simulation for concentration distribution (which could be used to compute AO in Figure 5b) shows much larger uncertainty. Because this work focuses on analyzing denitrification that depends on accurate prediction of nitrate concentration. I am concerned that the prediction for Nitrate may have similar uncertainty level as the RO shown in Figure 5b. I suggest the authors provide additional information to verify if the prediction uncertainty for nitrate is negligible for your analysis. If lab experiment is not available. A potential solution is to run your model with the ripple geometry explicitly represented by mesh and compute the difference of Nitration distribution with and without ripple geometry. According to Line 349, the authors seem to acknowledge that the larger error in RO shown in Figure 5b could be caused by the exclusion of the ripple

geometry. Such additional modeling work will help to explain Figure 5b and enhance the prediction reliability for nitrate distribution.

**Reply:** As suggested by the reviewer, we conducted an additional simulation incorporating ripple geometry and compared its results with those of the flatbed model; both models were used to reproduce Wolke et al. (2020) experiment. For a more detailed response, please refer to our response to Major Comment 1. The supplementary content has been added in Sections 3.1.1 Validation of flatbed model with triangular ripple model (see lines 433-466) and 3.1.2 Validation of numerical models with laboratory experiments (see lines 467-508) of the revised manuscript.

This work has several figures (e.g., figures 1-4) and most equations similar to the Ping X. 2022 (10.1029/2022WR033258), please highlight major novelty in this paper compared to the existing paper.

**Reply:** This work is relevant to that of Ping et al. (2022) but with significant differences. While certain basic figures (e.g., figures 1-4 in the original version) and equations share similarities with their study, these correspondences arise because they describe fundamental hyporheic and biogeochemical processes. Actually, this study is quite different from Ping et al. (2022) because: 1) Firstly, in this study, we focus on downstream section of rivers under gaining conditions firstly to simulate surface water-groundwater mixing processes under dynamic bedforms, while Ping et al. (2022) focused on hyporheic exchange processes in the headwater to midstream sections of rivers under neutral conditions. Therefore, the research focus is quite different for these two studies. 2) Secondly, the mixing process has been considered in this study. As far as we know, this process has not been thoroughly investigated in the migrating ripple model (Jiang et al., 2022; Zheng et al., 2019; Kessler et al., 2015). It is notable that the bedform migration affect mixing process significantly. 3) Thirdly, Ping et al. (2022) only considered the reduction and removal of stream-borne solutes via non-mixing dependent reactions, while in this study we evaluate and quantify the self-purification ability of the hyporheic zone for groundwater-borne contaminant. We have supplemented and highlighted the novelty in this study in the Introduction and Model description, see lines 110-121 and 147-159.

Other minor comments are listed below for reference:

Line 22: missing a comma between “migration” and “this”.

**Reply:** The comma was added between “migration” and “this”, see line 24.

Line 123: Riverbed and riverbed surface mean different things. If the “Riverbed” at this sentence means “the top surface of the riverbed”, it is better to use “riverbed surface”.

**Reply:** We have revised “riverbed” to “riverbed surface” to clarify that ripples develop and migrate downstream on the riverbed surface as a result of bedload transport, see line 132.

Figure 1: Figure 1 looks very similar to Figure 2 in Ping2022 (10.1029/2022WR033258). The ripple shapes are the same in two papers. I guess this figure is modified from Figure 2 in Ping 2022. In this scenario, please add the following information in figure caption: [Figure is modified from Figure 2 in Ping 2022, permission has granted from Wiley]

**Reply:** We have revised the caption of Figure 1 to include the required attribution: “This figure is modified from Figure 2 in Ping et al. (2022), with permission granted by Wiley”, see lines 168-169. We have successfully applied for and obtained the image usage permission.

Figure 1: Because HZ is a complex system, it involves concepts such as domain, layer, surface, interface, flux on surface, in from domain/surface, out from domain/surface. I suggest the authors modifying the Figure 1 and captions to carefully choose vocabularies to “concisely” describe such concepts. For example, riverbed could mean riverbed surface or riverbed layer. Clearly selecting words will help readability of the paper. This comment is also related to Major comment 2.

**Reply:** We have revised Figure 1 and captions to describe these concepts more clearly. In the manuscript text, we have also eliminated the use of the general term “riverbed” without specific qualification; instead, we explicitly refer to the “riverbed surface” when describing the top surface of the riverbed, and the “riverbed layer” when referring to the subsurface immobile sediment domain.

Line 144: I am not quite agree with this. From Elliot1997 paper, the size of ripple heights is 1-2.5 cm, and surface water depth is of 3-7 cm, which means ripple heights are 15-20% of the

water depth. In Cardenas2007 CFD simulation paper (10.1016/j.advwatres.2006.06.009), dune height is 5 cm and water depth is 45 cm. Their ratio is 10% (Figure 2 Cardenas2007). At line 144, I don't see the actual size for ripple and depth, so it is reasonable to say ripple heights are negligible. Such negligible assumption will lead to the simplification of "triangular ripple" into a "flat" surface. From both Elliot1997 and Cardenas 2007 paper, they do not simplify the ripple/dune into flat surface. Instead, Elliot1997 shows the pressure varies sinusously along the surface of the ripple. In Cardenas 2007, it shows that pressure head variations are affected by Reynolds number. The sinusoidal function reported in Elliot1997 is valid only at low Reynolds number and such match is applied only half of the region along the ripple surface (see Figure 9 in Cardenas 2007 10.1016/j.advwatres.2006.06.009). Therefore, whether you can simplify the ripple as flat surface (which will affect how you design the computational domain) and using a sinusoidal function (depending on your Reynolds number) requires more justification. This comment is also related to Major comment 1.

**Reply:** In our model, the ripple height is set to 2 cm, the stream water depth to 10 cm, and the riverbed layer height to 16 cm. This results in a ripple height that accounts for 20% of the stream water depth and is significantly smaller than the riverbed layer depth (1/8), see lines 136-140. Section 4.2 of Cardenas (2007) discussed discrepancies between the pressure distribution on the riverbed surface and Fehlman's measured pressure profiles. As  $Re$  increases, the distance between the pressure separation and reattachment points of water vortices contracts: the minimum pressure point persists at the crest, while the maximum pressure point progressively migrates toward the crest from the trough. These conclusions were derived by Cardenas under laminar flow conditions ( $Re < 3000$ ). When the river flow regime transitions from laminar to transitional/turbulent flow ( $Re = 3000-50,000$ ), observational and computational findings from multiple studies demonstrate that the riverbed surface pressure distribution aligns with Fehlman's measured pressure curves (Mendoza & Shen, 1990; Yoon & Patel, 1996). For laminar flow, the pressure profile exhibits high sensitivity to the Reynolds number (Figures 4 and 9); in contrast, the pressure profile for turbulent flow is anticipated to display substantially diminished sensitivity to  $Re$  (Fehlman, 1985; Shen et al., 1990; Cardenas & Wilson, 2007). Thus, simplifying the sinusoidal pressure distribution to a flat-bed approximation is reasonable, given that the  $Re$  in this study ranges from 2000 to 6000. To validate the simplification the triangular

ripple geometry to flat riverbed surface, we evaluated the effects of the triangular ripple model and flatbed model on our simulation results using two distinct simulation approaches. Based on these evaluations, we consider this simplification reasonable, with the resulting computational deviations being acceptable. For detailed explanations of these revisions and validations, please refer to our response to Major Comment 1.

Line 142: show lambda on Figure 1. Also please visualize ripple height in Figure 1.

**Reply:** We have revised Figure 1 to explicitly visualize the height of the ripple.

Line 146: A periodic morphological feature does not mean periodic conditions for pressure, velocity, and concentration. Previous work shows that the flow in upstream of ripple influences flow downstream (see Sinha2017 WRR, 10.1002/2016WR019662). Due to this issue, numerical simulation will need to use at least two ripples to minimize impacts of upstream (see Cardenas2007, 10.1016/j.advwatres.2006.06.009). In this work, a period boundary is applied at the location B and C (see Figure 1) where pressure and velocity are not periodic (see Figure 2 in Cardenas2007). However, all the information mentioned above is for stationary ripple/dune. For the moving ripple, whether you should/should not use a periodic boundary may be different but requires further justification.

**Reply:** Compared to Cardenas (2007) (Figure 2), even with the application of periodic boundary conditions at the left and right vertical boundaries, pressure and velocity do not exhibit periodicity in their flow field when  $Re < 1124$ . In our study, however,  $Re$  ranges from 2000 to 6000, and pressure and velocity display periodic characteristics. The use of periodic boundaries at AB and DC (Figure 1) is not intended to enforce periodicity of flow variables, but rather to replicate the repetitive geometric constraints of the streambed. This is a well-established practice in hyporheic exchange modeling, as it minimizes edge effects without the need for computationally intensive full-scale simulations of multiple consecutive bedforms. This approach is supported by Cardenas & Wilson (2007), who illustrated that periodic boundaries can effectively approximate the hydrological behavior of repetitive bedforms when paired with reasonable pressure-gradient assumptions. To further validate this simplification, we simulated three consecutive ripples, focusing on the middle one to compare its pressure and solute

concentration along these vertical boundaries with results from the single-ripple model (which uses periodic boundaries). Moderate differences in right and left boundary pressure were detected between the two simulation results; however, such differences had minimal effects on reactive solute transport. This context was added in the revised manuscript text (see lines 237-254) and Supporting Information (see Text S2), and we consider the use of periodic boundaries to be reasonable for moving ripples.

Line 153: Is this "BC" the top edge of the blue region in Figure 1? In this work, the 'BC' is a flat surface. However, equation 2 is usually applied to the top surface of the ripple which is not a flat surface. Please justify if such simplification affects results (e.g., exchange flux and distribution of nitrate in the computational domain).

**Reply:** This “BC” represents the riverbed surface. The influence of the simplification on the simulated results has been evaluated; please refer to our response to Major Comment 1.

Line 154: equation 2 was first introduced in Boano2013. It is better to cite correct references.

**Reply:** We have corrected the reference citation for equation 10, see line 231.

Line 163: For equation 4/5, you use bold ( $\mathbf{v}$ ), non-bold  $v$ ,  $v_i$ ,  $v_j$ , and  $|v|$ . In general, bold ( $\mathbf{v}$ ) means vector. For non-bold  $v$ , there is no definition. Also, no definition for  $v_i$ ,  $v_j$ . Please correct such variables to make sure they are consistent and mathematically correct.

**Reply:** Bold  $\mathbf{v}$  denotes the seepage velocity vector, and non-bold  $v$  represents the magnitude of the seepage velocity  $v = |\mathbf{v}|$ ;  $v_i$  and  $v_j$  denote the seepage velocities in the  $i$ -direction and  $j$ -direction, respectively, see lines 196-197. Equations 2 and 3 (in the revised version) have been checked and revised, with the variable  $\mathbf{v}$  formatted in bold uniformly in the revised version, see lines 189 and 194.

Line 164 equation 4: gradient  $\mathbf{v}\cdot\mathbf{c}_i$  should be gradient dot ( $\mathbf{v}\cdot\mathbf{c}_i$ ).

**Reply:** We have revised the equation 2 (in the revised version): 
$$\frac{\partial c_i}{\partial t} - \nabla \cdot (D_{ij} \nabla c_i) + \nabla \mathbf{v} \cdot \mathbf{c}_i = R_i$$

Line 173: Does this sentence mean you solved both  $c_{\{sNO_3\}}$  and  $c_{\{gNO_3\}}$ ? Note that most previous work does not distinguish which portion of nitrate from surface water and which portion is from groundwater, which means they only solve for one concentration for  $NO_3$ . From this sentence, it seems you are solving both concentrations of Nitrate. Please confirm if this is the case. Also, for models that solve for one concentration for  $NO_3$ , you only need to assign two boundary condition for  $NO_3$ , one is at the top boundary (BC) and one is for the lower boundary (AD). But if you are solving for two concentrations for  $NO_3$ , you need to assign 4 boundary conditions. You need boundary conditions at both BC and AD for both  $c_{\{sNO_3\}}$  and  $c_{\{gNO_3\}}$ . Please clarify how each of these boundary conditions is determined.

**Reply:** We defined stream-borne nitrate ( $c_{s-NO_3}$ ) and groundwater-borne nitrate ( $c_{g-NO_3}$ ) as two distinct reactants, rather than partitioning the nitrate pool into two separate fractions. The transport of stream-borne and groundwater-borne nitrate in porous medium are solved separately using the advection-dispersion-reaction equation. Detailed explanations can be found in our responses to Major Comments 2 and 3.

Line 176 equation R1/R2: it is better to add a citation for equations R1 and R2. It is also important to add a justification for why you choose such a reaction. Note that in lab or field experiments, the reaction network is quite complex, which is much different than the equation R1/R2 used here. R1/R2 is a kind of idealized or conceptualized reaction, which could be used as qualitative understating. However, to compare the results to experiment or field observation, you may need to add more information regarding how the assumed reaction R1/R2 is consistent with lab/field reaction network.

**Reply:** Equations R1 and R2, with DOC as the electron donor and  $O_2$  and  $NO_3^-$  as sequential electron acceptors, capture the primary mechanism of  $NO_3^-$  cycling and are widely used in studies on hyporheic zone nitrogen dynamics (Bardini et al., 2012; Hester et al., 2019; Zheng et al., 2019). Denitrification is the well-recognized critical process for  $NO_3^-$  transformation and reduction in riparian and hyporheic zones. The reaction stoichiometry and electron acceptor utilization order in R1 and R2 match well-established principles from lab incubations and field investigations (Hedin et al., 1998; Liu et al., 2017; Zarnetske et al., 2011a, 2011b). Dissimilatory

nitrate reduction to ammonium (DNRA) and anaerobic ammonium oxidation (ANAMMOX) are not included in the model, as these processes play secondary role on nitrogen cycling and require highly specific conditions to occur (Zarnetske et al., 2012). Ammonia ( $\text{NH}_4^+$ ) was excluded, as it is unstable in the study environment:  $\text{NH}_4^+$  in surface water or groundwater is prone to nitrification (converting  $\text{NH}_4^+$  to  $\text{NO}_3^-$ ) either within hyporheic flow cells or in upwelling groundwater upon  $\text{O}_2$  exposure, leading to relatively low  $\text{NH}_4^+$  concentrations (Hester et al., 2014). The citation and explanation have been added in the manuscript text, see lines 202-215.

Line 180 equation 7: I am not quite sure the meaning of  $C_{\text{/g-NO}_3}$ . Does this mean the summation of  $C_{\text{/s-NO}_3}$  and  $C_{\text{/g-NO}_3}$ ? Or it means  $C_{\text{/s-NO}_3}$  or  $C_{\text{/g-NO}_3}$ ? I also have doubts about the mass balance issue caused by this equation. Please see my major comment 3 for details.

**Reply:** The notation of  $c_{\text{/g-NO}_3}$  represents either  $c_{\text{/s-NO}_3}$  or  $c_{\text{/g-NO}_3}$ . This is because we defined stream-borne nitrate ( $c_{\text{/s-NO}_3}$ ) and groundwater-borne nitrate ( $c_{\text{/g-NO}_3}$ ) as two distinct reactants, where  $c_{\text{/s-NO}_3}$  and  $c_{\text{/g-NO}_3}$  participate in non-mixing-dependent and mixing-dependent denitrification, respectively. We have revised equation 7 to

$$R_{DN} = V_{DN} \times X_{DN} \times \frac{c_{\text{NO}_3^-}}{c_{\text{NO}_3^-} + K_{\text{NO}_3^-}} \times \frac{c_{\text{DOC}}}{c_{\text{DOC}} + K_{\text{DOC}}} \frac{K_{inh}}{K_{inh} + c_{\text{O}_2}}, \text{ to avoid any potential}$$

misunderstanding. Detailed explanations are provided in our responses to Major Comments 2 and 3.

Line 190: the period boundary ab AB and DC need more justification. From previous work (Cardenas2007 Figure 2 10.1016/j.advwatres.2006.06.009), the distribution of pressure at AB and DC could be quite different depending on Reynolds number. A better way is to use two ripples and apply period at the beginning of the first ripple and the end of the second ripple. Please justify the current setup.

**Reply:** We conducted a comparison by simulating three consecutive ripples, focusing on the middle one to compare its pressure and solute concentration along the vertical boundaries, as well as the hyporheic flow field and solute plumes, with results from the single-ripple model

(which uses periodic boundaries). Minor differences in pressure at the left and right boundaries were observed between the two simulation results; however, such differences had negligible effects on reactive solute transport. This analysis has been added to the revised manuscript (see lines 237-254) and the Supporting Information (Text S2).

Line 190: If  $P(0) = P(\lambda) + \Delta P$ , this is not called period boundary. You can just use the mathematical formula to describe it, but do not call it "periodic". Also, equation 1 means you are solving for pressure head  $h$ , but no pressure  $P$ . You need to assign the boundary for  $h$ , but not  $P$ .

**Reply:** We have revised the labels in Figure 2 (in the revised version) and added the corresponding mathematical formula in Figure 2 and Section 2.2 Boundary condition.

Specifically, the relationship between head ( $h$ ) and pressure ( $P$ ) can be expressed as  $h = P/(\rho g)$ , where  $\rho$  denotes fluid density and  $g$  represents gravitational acceleration, see lines 246-247.

Line 193: How do you determine the concentrations at boundary BC? For pressure head  $h$ , it is determined by the sinusoidal function from previous work, but for concentration, how do you get it.

**Reply:** The concentrations of DOC, O<sub>2</sub>, and s-NO<sub>3</sub><sup>-</sup> in stream were specified as 30 mg/L, 8 mg/L, and 5 mg/L. This configuration represents a pristine stream characterized by moderate nutrient levels. See lines 343-345 in manuscript text.

Line 195: What is the boundary condition for  $h$  at AD boundary?

**Reply:** The AD boundary is defined as a constant-flux boundary, designed to mimic upward groundwater flux. Unlike constant-head boundaries, where head ( $h$ ) is assigned a fixed pre-defined value, the head at constant-flux boundaries is not pre-specified. Instead, the head at the AD boundary is derived from the model simulated flow field results. Detailed descriptions of the model boundary conditions have been added to Section 2.2 of the revised manuscript.

Line 213: using the Chezy equation to estimate shear stress seems not reliable. Please see my major comment 4 for details.

**Reply:** Please refer to our response to Major comment 5 for details.

Line 215: How do you calculate the  $\tau_{cr}$ ?

**Reply:**  $\tau_{cr}$  is calculated by the critical Shield parameter  $\tau_{cr}^*$  ( $\tau_{cr}^* = \tau_{cr} / g (\rho_s - \rho) D_{50}$ ).

Specifically, the critical Shield parameter represents the threshold for the initialization of motion, and it is determined by the dimensionless particle parameter  $D^*$  (Zheng et al., 2019):

$$\tau_{cr}^* = \frac{0.3}{1 + 1.2D^*} + 0.055 \left[ 1 - \exp(-0.02D^*) \right]$$

where  $D^* = D_{50} \cdot (rg/v^2)^{1/3}$  and  $r$  denotes submerged specific gravity of sediment ( $r = (\rho_s - \rho) / \rho$ ),  $\rho_s$  and  $\rho$  are the density of sediment and water. We have added an introduction to the calculation of  $\tau_{cr}$  and  $\tau_{cr}^*$  in revised manuscript, see lines 285-294.

Line 217: what is  $r$  in the equation used for computing shields number at line 217?

**Reply:**  $r$  denotes submerged specific gravity of sediment ( $r = (\rho_s - \rho) / \rho$ ),  $\rho_s$  and  $\rho$  are the density of sediment and water, see line 288.

Line 231: Is the  $S$  at line 231 the same  $S$  at line 212? Do you define  $K$  somewhere? Do you provide the value for  $K$ ?

**Reply:** The symbol  $S$  at line 231 is consistent with that at line 212 (in the origin version), where both denote the combined slope of the stream and streambed. The definition of  $K$  has been added in line 184 and the value of  $K$  is calculated from  $k$  (the permeability of riverbed). In this study,  $k$  is determined by the medium grain size of sediment and calculated using the empirical relation  $k = Da' \times 735 \times 10^6 \times D_{50}^2$  (where  $Da' = 9.869 \times 10^{-13}$  is the conversion factor for unit Darcy to  $m^2$ ), see lines 340-342 in the manuscript text.

Line 241: Is  $u_q$  upwelling groundwater flux? How do you decide this value?

**Reply:** Yes, the symbol  $u_q$  denotes the upwelling groundwater flux, whose magnitude ranges from 30% to 70% of the hyporheic exchange flux driven by bedforms. An upward flux exceeding 90% of the hyporheic flux would eliminate the entire hyporheic flow cell; thus, the maximum boundary flux was set slightly below this threshold. Meanwhile, a minimum of 20% of the hyporheic flux ensures that upwelling groundwater still mixes with surface water, with

only minor influences on the hyporheic flow cell, see lines 357-361.

Line 264: Is the  $Da$  at line 264 the same as the  $Da$  in equation 18? If not, please use a different variable.

**Reply:** The symbol  $Da$  at line 264 differs from  $Da$  in equation 18 of the original version. Specifically,  $Da$  in equation 18 denotes the dimensionless Damköhler number, defined as the ratio of the characteristic transport timescale to the reaction timescale. In contrast,  $Da'$  at line 264 represents a unit conversion factor (for converting Darcy to  $m^2$ ) in the calculation of riverbed layer permeability. These two parameters have been clearly distinguished using  $Da$  and  $Da'$  in the revised version.

Line 266: How are these values estimated? Are these assumed values? Please provide a justification for why you choose such values.

**Reply:** These values are assumed values. Dissolved organic carbon (DOC), oxygen ( $O_2$ ), and nitrate ( $NO_3^-$ ) were assigned concentrations of 30 mg/L, 8 mg/L, and 5 mg/L, respectively. This boundary setup mimics a pristine stream with moderate nutrient concentrations, which are consistent with the range of measurements from natural field rivers (Briody et al., 2016; Ocampo et al., 2006). See lines 343-345 in the revised version.

Table 1: Please visualize  $l$ ,  $l_c$ ,  $\lambda$ ,  $H_d$ ,  $H$  in Figure 1. What is the difference between ripple crest and height of ripple crest. In Figure 1, the ripple height is clearly visualized, but the ripple crest is not visualized. Please describe their difference.

**Reply:** We have added labels for all the required parameters in Figure 1, including the ripple wavelength ( $\lambda$ ), riverbed depth ( $l$ ), the position of ripple crest ( $\lambda_c$ ), and ripple height ( $H_d$ ). The ripple height ( $H_d$ ) is the vertical distance between the ripple crest and the ripple trough (that is the flat riverbed layer). The position of ripple crest ( $l_c$  in the original version) refers to the horizontal distance between the ripple trough and the ripple crest; this parameter is consistent with the “ripple crest ( $\lambda_c$ ; in the revised version)” listed in Table 1. The stream water depth ( $H$ ) is not included in Figure 1, as the stream flow was not incorporated into our model.

Tabel 1: Provide citation for porosity, longitudinal and transverse dispersivity or any justification to use such values.

**Reply:** The porosity used in this study is 0.38, which falls within the typical range (0.30–0.40) of porosities for sandy riverbed sediments reported in previous literature (Ahmerkamp et al., 2015; Huettel et al., 2014). For anisotropic dispersion in dunes, Gelhar et al. (1992) demonstrated that longitudinal dispersivities can be reliably estimated as 0.01–0.1 times the transport distance, while transverse dispersivities are 1 to 2 orders of magnitude smaller than longitudinal dispersivities over these distances. Consistent with prior research, our model incorporates two key dispersivity assumptions: a constant transverse-to-longitudinal dispersivity ratio ( $\alpha_T/\alpha_L$ ) of 0.1, and a longitudinal dispersivity ( $\alpha_L$ ) of 0.01 m. This parameterization is consistent with dispersivity settings in earlier studies focusing on streambed topography-driven hyporheic exchange (Bardini et al., 2012; Cardenas et al., 2008). These citations have been added to the footnote of Table 1.

Line 283: Does COMSOL solve the equations 1-11? Do you develop your own COMSOL solver using equations 1-11 or you use the default equations in COMSOL? Is the COMSOL setup and data available in public data repository?

**Reply:** COMSOL was used to solve Equations 1-11 with the default settings. The relevant COMSOL configuration files and associated data are available from the first author upon request.

Line 291: I am confused by the term "surface water". From Figure 1, your computational domain is the region bounded by ABCD. The whole region is beneath the surface (or stream) water. This means the model framework does not solve anything related to surface water that is not governed by Darcy flow. Please clarify this.

**Reply:** We did not directly simulate surface water flow over the bedforms. Instead, we focused on the infiltration of surface water into riverbed sediments and its interaction with groundwater, which is driven by hyporheic exchange processes—specifically pumping and turnover. Pumping refers to the process where pressure variations at the sediment-water interface, induced by bedforms, drive the interstitial flow of stream water through the sediments. Additionally,

turnover, triggered by bedform migration, further facilitates surface water-groundwater exchange: as bedforms migrate, sand grain erosion on the stoss side releases pore water, while sediment deposition on the lee side traps surface water from the water column. Equation 10 describes the driving forces behind these two processes, and within the riverbed, surface water-groundwater interaction and mixing do occur.

Line 301: Is bottom boundary AD and streambed surface BC?

**Reply:** Yes. Boundary AD functions as the bottom boundary, and Boundary BC corresponds to the streambed surface, both of which have been clearly labeled in Figure 2 (in the revised version).

Line 302: Is “streambed surface” the "surface water layer" (a layer with pure water)?

**Reply:** The streambed surface refers to the flat riverbed surface, i.e., the top boundary of the riverbed layer. To avoid the potential confusion caused by the term “stream water”, we have removed it from Figure 1, as it is not included in the conceptualization and establishment of the model.

Line 303: more accurate description: surface water enters riverbed layer.

**Reply:** The sentence “surface water enters the bed” has been revised to “surface water enters the riverbed layer” in the manuscript, see line 393.

Line 304-305: From Figure 1, the groundwater is separated from the surface water layer by "the sediment layer", it seems groundwater cannot be directly transported to the surface water layer. When you use "groundwater discharged to stream", are you trying to identify which portion of water is from groundwater when such groundwater is first "up-welled" to the sediment layer and further "up-welled" to the surface water layer? If this is the case, you may need to explicitly describe this purpose. And you may add a sentence that "such identification could be achieved using tracer or different color/size of tracer".

**Reply:** Groundwater is not separated by a sediment layer. The gray band represents the surface water-groundwater mixing zone (now changed to yellow) rather than a sediment layer.

Upwelling groundwater infiltrates the sediments: some mixes with surface water that has infiltrated via hyporheic exchange (blue arrows) before discharging into the stream (green arrows), while some discharges directly into the stream (red arrows). Our objective was to identify the portion of groundwater that mixes with surface water (blue arrows). To prevent potential misunderstanding, we have revised Figure 1 by removing the distinct color zones and adding arrows of different colors to distinguish between the various water sources. Such identification is achieved by adding conservation tracer in groundwater, see lines 388-407.

Line 317: Where is the ripple surface? Is ripple surface the boundary BC? How do you compute  $F_{swi}$ ?

**Reply:** Boundary BC represents the riverbed surface.  $F_{SWI}$  [ $L T^{-1}$ ] was deleted in the revised manuscript text. Instead, we calculate the total influx (including advection and dispersion flux) of nitrate using equation 25, see lines 419-420.

Line 322: Is this streambed "boundary BC"?

**Reply:**  $L_{top}$  refers to the boundary BC and  $L_{bottom}$  denotes the boundary AD. The content has added in manuscript text, see lines 421-422.

Figure 3b: From Wolke2019, the oxic zone occurs mainly inside the dune (the triangular region as shown in Figure 1). However, in this paper, the computational domain is a rectangular shape, and the triangular shape is "neglected". How do you compare the oxic zone as reported in the Wolke2019 paper? From Figure 3b, the uncertainty for AO between model and experiment is much larger than the rest 3 variables, could this larger error be caused by the over-simplification of the ripple to a flat surface? Also see major comment 6.

**Reply:** Please refer to our responses to Major Comment 6 and 7.

Figure 3: Is this the average upwelling flux at the boundary BC? If not, please clarify where and how the HEF is computed. From the numerical, the flux is a distribution, it is necessary to clarify how you get a single value from a distribution. See also major comment 5.

**Reply:** The hyporheic exchange flux (HEF) refers to the total inward stream flux that infiltrates

through boundary BC and is calculated by integrating the volumetric flux over the inflow zone of the riverbed surface in numerical simulations. A detailed response to this issue can be found in Major Comment 5.

Line 345: From Figure 3b, the relative error between model and experiments could be up to 100%. The statement of "slightly lower" is not consistent with the data. Please compute the relative error between model results and observation and then make a more accurate conclusion for the accuracy using the computed data.

**Reply:** We performed additional parameter refinement to enhance the agreement between simulated results and experimental data. The root mean square error (RMSE) between experimental data and simulated results was computed, and the RMSE values (simulated vs. experimental) for each subplot are shown in Figure 5 of the revised manuscript. The model parameters used and adjusted are summarized in Supporting Information Text S3: Model Calibration.

Line 349: This is related to my major comment 1 and 6. As suggested by the author, the missing of the mobile (triangular ripple) can cause significant error for estimating the total area of the oxygen zone. As the rest of the paper is to study the denitrification which will use data of concentrations of nitrate. My guess is that the missing of the triangular ripple zone (mobile zone) will also significantly affect the accuracy of nitration concentration prediction (could be similar uncertainty of oxygen as shown in Figure 3b). I suggest the authors clarify how much impact will be by simplifying the mobile ripple as flat surface.

**Reply:** A detailed explanation of this issue has already been included in our responses to the major comments; please refer to the responses to Major comment 1 and comment 6.

Line 375 and Figure 4: This is something uncleaned at lower left corner of Figure 4.

**Reply:** That is the line number blocked by the Figure 4.

Line 474: This paper has a lot of similarity to Ping 2022 (10.1029/2022WR033258). It may be over statement to use "first time" due to the existing of Xue2022 paper.

**Reply:** We avoided using the expression “the first time” in the revised manuscript.

Line 852: citation year is not correct.

**Reply:** The year in the citation has been corrected from 2019 to 2020.

**Response to Reviewer #3:**

This study investigates the effects of migrating bedforms on surface-groundwater mixing and denitrification in a gaining stream reach. The authors employ a numerical model that couples Darcy flow with a translating sinusoidal head boundary and a multi-species reactive transport model. While the paper introduces new metrics such as “mixing flux,” “mixing fraction,” and “mixing-zone area,” my primary concern is the substantial overlap with the authors' previous work (2022). The modeling framework, numerical implementation, and validation appear nearly identical.

**Reply:** We thank this reviewer for the constructive comments on our manuscript. Actually, this study is quite different from Ping et al. (2022) because: 1) Firstly, in this study, we focus on downstream section of rivers under gaining conditions firstly to simulate surface water-groundwater mixing processes under dynamic bedforms, while Ping et al. (2022) focused on hyporheic exchange processes in the headwater to midstream sections of rivers under neutral conditions. Therefore, the research focus is quite different for these two studies. 2) Secondly, the mixing process has been considered in this study. As far as we know, this process has not been thoroughly investigated in the migrating ripple model (Jiang et al., 2022; Zheng et al., 2019; Kessler et al., 2015). It is notable that the bedform migration affect mixing process significantly. 3) Thirdly, Ping et al. (2022) only considered the reduction and removal of stream-borne solutes via non-mixing dependent reactions, while in this study we evaluate and quantify the self-purification ability of the hyporheic zone for groundwater-borne contaminant. We have further highlighted the novelty of this study and clarified the difference with Ping et al. (2022) in the introduction and method, see lines 113-124 and 147-159.

Concerning model validation, this study offers far more comprehensive validation than the Ping et al. (2022) publication. Firstly, we conducted an additional simulation incorporating ripple geometry and compared the numerical results with those from the flat-bed model in this study.

This was done to evaluate the reliability of the established model and the differences in simulation results induced by the neglect of triangular ripples. Detailed comparisons have been added to in Section 3.1.1 Validation of flat bed model with triangular ripple model (see lines 433-466). Secondly, these two models were used to reproduce the experiment by Wolke et al. (2020). Beyond comparing the spatial shape and size of oxygen plumes in riverbed sediments, a critical validation step in the 2022 model, we supplemented the validation process with a fitting analysis between experimentally measured and numerically simulated hyporheic parameters, including hyporheic exchange flux and oxygen influx/outflux. Detailed comparisons have been added to in Section 3.1.2 Validation of numerical models with laboratory experiments (see lines 467-508).

The claimed novelty rests on applying the existing model to a different scenario and introducing new diagnostic metrics. However, the justification for these metrics is insufficient, and their introduction does not lead to the discovery of new physical mechanisms. Furthermore, the main conclusion: bedform migration shortens residence times and thereby reduces denitrification—reiterates, is a key finding from the 2022 paper (<https://doi.org/10.1029/2022WR033258>). The manuscript reads more as an incremental application of prior work rather than a standalone scientific article with a distinct and significant contribution.

**Reply:** In fact, we have obtained several novel findings in this study that cannot be derived from Ping et al. (2022), which can be summarized as follows: 1) Bedform migration reshapes the patterns of the surface water-groundwater mixing zone and mixing-triggered biogeochemical zones; these zones progressively transition from crescent-shaped to uniform band-like configurations as bedforms migrate. 2) At slow to moderate migration rates, bedform migration expands the surface water-groundwater mixing zone, increases the mixing fraction in hyporheic flux, and elevates the mixing-dependent denitrification rate; 3) The onset of bedform migration enhances the nitrate removal efficiency of groundwater-borne nitrate, whereas moderate to large migration celerities restrict this removal process, thereby weakening the hyporheic zone's function as a natural barrier against groundwater contaminants. We have re-summarized the new recognitions in the Results and Discussion.

The primary reason for introducing these metrics is to address a gap in the 2022 study: they

quantify surface water-groundwater mixing and assess its effects on both mixing-dependent denitrification rates and groundwater-borne nitrate reduction efficiency. Mixing flux and mixing zone describe the magnitude and scope of mixing, respectively, and their calculation follows the methods outlined in Hester et al. (2013, 2014). These metrics are critical factors governing the occurrence of mixing-induced biogeochemical reactions. As you noted, while these metrics do not reveal “new physical mechanisms”, they enable a quantitative mechanistic explanation that was previously unavailable. For instance, we now demonstrate that in gaining reaches, bedform migration, at slow to moderate celerities, increases mixing-dependent denitrification rates and enhances groundwater-borne nitrate removal efficiency. This phenomenon is driven by elevated mixing flux and expanded mixing zones, despite shortened residence times. This represents a key insight unavailable in the 2022 study and offers actionable guidance for stream remediation (e.g., targeting mixing enhancement alongside residence time extension).

1. The literature review should be expanded to include a more thorough discussion of numerical model development in this field. Critically, this section must clearly and explicitly state how this study's model and objectives differ from and advance upon the 2022 paper. The work appears to be a case study applying a previously established model. It does not introduce a new mechanistic framework, a dimensionless parameter space map, or any analytical/scaling relationships that would constitute an independent and generalizable scientific contribution.

**Reply:** We have thoroughly discussed the development of the numerical model and highlighted the novelty of this study in the Introduction (see lines 113-124). Additionally, a comparison and contrast between the present work and the 2022 study have been added to the Model Description section (see lines 147-159). Rather than introducing a new mechanistic framework, we extended the existing mechanistic framework proposed by Ping et al. (2022) and focused on a substantially different scenario from that of Ping et al. (2022). In this study, we first focus on the downstream sections of rivers under gaining conditions to simulate surface water-groundwater mixing and the associated biogeochemical processes triggered by such mixing, under dynamic bedform conditions. To the best of our knowledge, this process has not been thoroughly investigated in migrating ripple models (Jiang et al., 2022; Zheng et al., 2019; Kessler et al., 2015). The metrics and parameters employed in this study provide a quantitative mechanistic

explanation for how bedform migration influences surface water-groundwater mixing and the mixing-dependent denitrification rate, results that cannot be derived from previous studies. For further details, please see our response to the aforementioned main comment.

2. Thresholds used to define the mixing zone (e.g., 16%–84% concentration range) are presented without a clear physical or statistical basis. The robustness of the results is questionable without a sensitivity analysis of these thresholds, as well as the numerical dispersion and grid resolution. Furthermore, the newly proposed metrics are not validated against any established, well-accepted measures of mixing from the fluid dynamics or hydrology literature, making their utility and interpretation difficult to assess.

**Reply:** Actually, there is no standard for the threshold of the mixing zone; however, it is generally accepted that the mixing zone ranges from 10% to 90% in terms of groundwater proportion (Hester et al., 2013; Woessner et al., 2000). This interval effectively distinguishes the mixing zone, where groundwater and surface water interact dynamically, from the two endmembers: pure groundwater (>90%) and pure surface water (<10%). In this study, we selected the 16–84% range, which corresponds to the  $\pm 1\sigma$  interval of a normal distribution, as proposed by Santizo et al. (2020). To assess how threshold variations influence results, we perform a sensitivity analysis that tests three alternative concentration ranges: 10%–90% (wider interval), 16%–84%, and 20%–80% (narrower range), see lines 376–387. While these groundwater fraction thresholds determine both the flux and extent of mixing, they do not alter the influence of migration celerity on these mixing patterns. The comparative results have been incorporated into the manuscript text (see lines 582–591), and the simulated results along with detailed comparisons are provided in Supporting Information Text S4.

Numerical dispersion and grid resolution can influence solute transport and mixing results. We tested three grid sizes to assess the impacts of spatial discretization: the baseline grid (original resolution), a fine grid, and a coarse grid. Critical parameters (including hyporheic exchange flux, mixing flux, mixing zone, and denitrifying zone) were compared across all grids. This analysis confirms that the baseline grid is sufficiently resolved to capture small-scale mixing dynamics and minimize numerical dispersion. The content was added in the manuscript text, see lines 363–368, and Supporting Information Text S2.

The calculations of mixing metrics in this study follow the methods outlined by Hester et al. (2013, 2014). These metrics are not newly proposed by this study; instead, they have been widely applied and validated in previous studies (Santizo et al., 2020, 2022; Nogueira et al., 2022; Woessner et al., 2000), the evidence that supports their rationality. We have expanded the introduction of these metrics in revised manuscript, see lines 376-414.

3. The model's idealizations limit the generalizability of its findings. Key simplifications include: (a) representing bedform migration as a simple translating sinusoidal head, which neglects morphodynamic feedbacks; (b) using a 2-D domain with a single bedform wavelength and amplitude; and (c) omitting sediment heterogeneity, such as grain size variations or layering, which are known to strongly influence hyporheic exchange.

**Reply:** (a) We have conducted an additional simulation incorporating ripple geometry and compared its results with those of the flat bed model; this was done to evaluate the reliability of the proposed model and the differences in simulation results induced by the neglect of triangular ripples. The two sets of results exhibit similar characteristics in hyporheic flow field and solute plume distributions. Compared with the triangular ripple model, the flat bed model exhibit slightly larger hyporheic exchange flux, mixing flux, and stream-borne nitrate influx. The relative errors are approximately 10%. Meanwhile, both the mixing-dependent and non-mixing-dependent denitrification rates are higher in the triangular ripple model than in the flat bed model, with relative errors around 20%. Differences in the results of the simulated domain cause subtle changes in flow and transport processes, changes that are acceptable for our intended purposes. Detailed comparisons have been added to in Section 3.1.1 Validation of flat bed model with triangular ripple model (see lines 433-466). Furthermore, these two models were used to reproduce the experiment by Wolke (2020). Based on the parameter adjustments outlined in the previous manuscript text, we refined the numerical model to achieve a better fit with the experimental data. Both models show good agreement with Wolke et al.'s (2020) experimental data, including hyporheic exchange flux, oxygen influx/outflux and oxygen plume, despite some discrepancies between these two models (see Section 3.1.2 Validation of numerical models with laboratory experiments). Its adequacy is further supported by our successful reproduction of Wolke's (2020) results, thereby confirming its credibility for addressing the study objectives

(see lines 467-508).

(b) To contextualize the generalizability of our 2D findings, we added a discussion in the revised manuscript noting that our conclusions apply most directly to straight, low-curvature streams with periodic bedform distributions. In such stream systems, hyporheic exchange is dominated by streamwise-vertical flow cells, with lateral (cross-stream) hyporheic flux accounting for a small fraction of total exchange (Hu et al., 2014; Naranjo et al., 2015). Importantly, straight, low-curvature streams are prevalent in agricultural and urban downstream gaining reaches, which are characterized by relatively homogeneous sediment types (e.g., fine sands). This is consistent with the focus of our study, as these reaches often face nitrate pollution challenges and depend on natural attenuation to maintain water quality (Hester et al., 2014; Trauth et al., 2017). For highly meandering streams or those with heterogeneous bedforms, 3D modeling would be necessary; however, our 2D results also serve as a critical reference for understanding the dominant process. See lines 715-729 and 746-759.

(c) We omitted this factor in the current study to prioritize isolating the effects of bedform migration. This work specifically targets downstream gaining reaches characterized by fine sand beds: a relatively homogeneous sediment type widely observed in lowland stream systems (Ahmerkamp et al., 2017; Harvey et al., 2012). In practice, sediment heterogeneity creates spatial variability in hydraulic conductivity, which can modify surface water-groundwater mixing dynamics and disrupt solute plume distributions. We have included a discussion that explicitly outlines the implications of sediment heterogeneity, and suggested incorporating stochastic K fields to explore how sediment heterogeneity interacts with bedform migration, specifically, whether high-K hotspots enhance or reduce migration-driven mixing, see lines 726-729.

## Reference

- Ahmerkamp, S., Winter, C., Janssen, F., Kuypers, M., & Holtappels, M. (2017). The impact of bedform migration on benthic oxygen fluxes. *Journal of Geophysical Research: Biogeosciences*, 120(11), 2229-2242.
- Ashley, G. M., (1990). Classification of large-scale subaqueous bedforms: A new look at an old problem-SEPM bedforms and bedding structures. *Journal of Sedimentary Research*, 60(1),

160–172.

- Bardini, L., Boano, F., Cardenas, M. B., Revelli, R., & Ridolfi, L. (2012). Nutrient cycling in bedform induced hyporheic zones. *Geochimica et Cosmochimica Acta*, 84, 47-61.
- Briody, A. C., Cardenas, M. B., Shuai, P., Knappett, P. S. K., & Bennett, P. C. (2016). Groundwater flow, nutrient, and stable isotope dynamics in the parafluvial hyporheic zone of the regulated Lower Colorado River (Texas, USA) over the course of a small flood. *Hydrobiological Journal*, 24(4), 923-935.
- Cardenas, M. B., & J. L. Wilson (2007), Dunes, turbulent eddies, and interfacial exchange with permeable sediments. *Water Resources Research*, 43, W08412.
- Cardenas, M., Wilson, J. L., & Haggerty, R. (2008). Residence time of bedform-driven hyporheic exchange. *Advances in Water Resources*, 31, 1382-1386.
- Coleman, S. E., & Melville, B. W. (1994). Bed-form development. *Journal of Hydraulic Engineering*, 120(5), 544-560.
- Dallmann, J., Phillips, C. B., Teitelbaum, Y., Sund, N., Schumer, R., Arnon, S., & Packman, A. I., (2020). Impacts of suspended clay particle deposition on sand-bed morphodynamics. *Water Resources Research*, 56(8), e2019WR027010.
- Elliott, A. H., & Brooks, N. H. (1997a). Transfer of nonsorbing solutes to a streambed with bed forms: Laboratory experiments. *Water Resources Research*, 33(1), 137-151.
- Elliott, A. H., & Brooks, N. H. (1997b). Transfer of nonsorbing solutes to a streambed with bed forms: Theory. *Water Resources Research*, 33(1), 123-136.
- Eylers, H. (1994). Transport of adsorbing metal ions between stream water and sediment bed in a laboratory flume. WM Keck Laboratory of Hydraulics and Water Resources, Division of Engineering and Applied Science, California Institute of Technology.
- Fehlman, H. M. (1985), Resistance components and velocity distributions of open channel flows over bedforms, M. S. Thesis, Colorado State University, Fort Collins, CO.
- Gelhar, L.W., Welty, C., & Rehfeldt, K.R. (1992). A critical review of data on field-scale dispersion in aquifers. *Water Resources Research*, 28, 1955-1974.
- Harvey, J. W., Drummond, J. D., Martin, R. L., McPhillips, L. E., Packman, A. I., Jerolmack, D. J., ... & Tobias, C. R. (2012). Hydrogeomorphology of the hyporheic zone: Stream solute and fine particle interactions with a dynamic streambed. *Journal of Geophysical Research*:

- Biogeosciences, 117(G4).
- Hedin, L. O., Von Fischer, J. C., Ostrom, N. E., Kennedy, B. P., Brown, M. G., & Robertson, G. P. (1998). Thermodynamic constraints on nitrogen transformations and other biogeochemical processes at soil-stream interfaces. *Ecology*, 79(2), 684-703.
- Hester, E. T., Eastes, L. A., & Widdowson, M. A. (2019). Effect of surface water stage fluctuation on mixing-dependent hyporheic denitrification in riverbed dunes. *Water Resources Research*, 55(6), 4668-4687.
- Hester, E. T., Young, K. I., & Widdowson, M. A. (2013). Mixing of surface and groundwater induced by riverbed dunes: Implications for hyporheic zone definitions and pollutant reactions. *Water Resources Research*, 49(9), 5221-5237.
- Hester, E. T., Young, K. I., & Widdowson, M. A. (2014). Controls on mixing-dependent denitrification in hyporheic zones induced by riverbed dunes: A steady state modeling study. *Water Resources Research*, 50(11), 9048-9066.
- Hu, H., Binley, A., Heppell, C. M., Lansdown, K., & Mao, X. (2014). Impact of microforms on nitrate transport at the groundwater–surface water interface in gaining streams. *Advances in Water Resources*, 73, 185-197.
- Huettel, M., Berg, P., & Kostka, J. E. (2014). Benthic exchange and biogeochemical cycling in permeable sediments. *Annual Review of Marine Science*, 6(1), 23.
- Jiang, Q., Liu, D., Jin, G., Tang, H., Wei, Q., & Xu, J. (2022). N<sub>2</sub>O dynamics in the hyporheic zone due to ripple migration. *Journal of Hydrology*, 610, 127891.
- Kessler, A. J., Cardenas, M. B., & Cook, P. L. (2015). The negligible effect of bed form migration on denitrification in hyporheic zones of permeable sediments. *Journal of Geophysical Research: Biogeosciences*, 120(3), 538-548.
- Liu, Y., Liu, C., Nelson, W. C., Shi, L., Xu, F., Liu, Y., ... & Zachara, J. M. (2017). Effect of water chemistry and hydrodynamics on nitrogen transformation activity and microbial community functional potential in hyporheic zone sediment columns. *Environmental Science & Technology*, 51(9), 4877-4886.
- Mendoza, C., & Wen Shen, H. (1990). Investigation of turbulent flow over dunes. *Journal of Hydraulic Engineering*, 116(4), 459-477.
- Naranjo, R. C., Niswonger, R. G., & Davis, C. J. (2015). Mixing effects on nitrogen and oxygen

- concentrations and the relationship to mean residence time in a hyporheic zone of a riffle-pool sequence. *Water Resources Research*, 51(9), 7202-7217.
- Nogueira, G. E. H., Schmidt, C., Partington, D., Brunner, P., & Fleckenstein, J. H. (2022). Spatiotemporal variations in water sources and mixing spots in a riparian zone, *Hydrology and Earth System Science*, 26, 1883-1905.
- Ocampo, C. J., C. E. Oldham, & M. Sivapalan (2006). Nitrate attenuation in agricultural catchments: Shifting balances between transport and reaction. *Water Resources Research*, 42, W01408.
- Ping, X., Xian, Y., & Jin, M. (2022). Influence of bedform migration on nitrate reduction in hyporheic zones of heterogeneous sediments. *Water Resources Research*, 58(11), e2022WR033258.
- Rutherford, J. C., Boyle, J., Elliott, A. H., Hatherell, T. V. J., & Chiu, T. W. (1995). Modeling benthic oxygen uptake by pumping. *Journal of Environmental Engineering*, 121(1), 84-95.
- Rutherford, J. C., Latimer, G. J., & Smith, R. K. (1993). Bedform mobility and benthic oxygen uptake. *Water Research*, 27(10), 1545-1558.
- Salehin, M., Packman, A. I., & Paradis, M., (2004). Hyporheic exchange with heterogeneous streambeds: Laboratory experiments and modeling. *Water Resources Research*, 40, W11504.
- Santizo, K. Y., Widdowson, M. A., & Hester, E. T. (2020). Abiotic mixing-dependent reaction in a laboratory simulated hyporheic zone. *Water Resources Research*, 56(9), e2020WR027090.
- Santizo, Katherine Y., Widdowson, Mark A., & Hester, Erich T. (2022). Numerical modeling of an abiotic hyporheic mixing-dependent reaction: Chemical evolution of mixing and reactant production zones. *Journal of Contaminant Hydrology*, 251, 104066.
- Shen, H. W., Fehلمان, H. M., & Mendoza, C. (1990). Bed form resistances in open channel flows. *Journal of Hydraulic Engineering*, 116(6), 799-815.
- Trauth, N., & Fleckenstein, J. H. (2017). Single discharge events increase reactive efficiency of the hyporheic zone. *Water Resources Research*, 53(1), 779-798.
- Venditti, J. G., Church, M., & Bennett, S. J., (2005). Morphodynamics of small-scale superimposed sand waves over migrating dune bed forms. *Water Resources Research*,

41(10), W10423.

Woessner, W. W. (2000). Stream and fluvial plain ground water interactions: Rescaling hydrogeologic thought. *Groundwater*, 38(3), 423-429.

Wolke, P., Teitelbaum, Y., Deng, C., Lewandowski, J., & Arnon, S. (2020). Impact of bed form celerity on oxygen dynamics in the hyporheic zone. *Water*, 12(1), 62.

Yoon, J. Y., & Patel, V. C. (1996). Numerical model of turbulent flow over sand dune. *Journal of Hydraulic Engineering*, 122(1), 10-18.

Zarnetske, J. P., Haggerty, R., Wondzell, S. M., & Baker, M. A. (2011a). Dynamics of nitrate production and removal as a function of residence time in the hyporheic zone. *Journal of Geophysical Research*, 116(G1), G01025.

Zarnetske, J. P., Haggerty, R., Wondzell, S. M., & Baker, M. A. (2011b). Labile dissolved organic carbon supply limits hyporheic denitrification. *Journal of Geophysical Research*, 116(G4), G04036.

Zarnetske, J. P., Haggerty, R., Wondzell, S. M., Bokil, V. A., & González-Pinzón, R., (2012). Coupled transport and reaction kinetics control the nitrate source-sink function of hyporheic zones. *Water Resources Research*, 48 (11), 1-15.

Zheng, L., Cardenas, M. B., Wang, L., & Mohrig, D. (2019). Ripple effects: Bed form morphodynamics cascading into hyporheic zone biogeochemistry. *Water Resources Research*, 55(8), 7320-7342.