

#CC1

The manuscript presents a 3D variably saturated flow and multi-component reactive transport model (PFLOTTRAN) to evaluate the long-term impacts of managed aquifer recharge (MAR) on groundwater recovery and nitrate mitigation in the Xiong'an depression, North China Plain. You explicitly separate the contributions of dilution and denitrification and explore the role of geological heterogeneity using T-PROGS-based realizations.

The topic is timely and important, the study area is of high practical relevance, and using a regional 3D reactive transport model for long-term MAR evaluation is scientifically interesting. The overall narrative is clear and the paper is generally well organized. I recommend publication after considering these comments:

Response:

Thank you for your encouraging feedback on the value of this work. We greatly appreciate your insights and recommendations, which have significantly improved the clarity and depth of our research. In response to your comments, we have made the necessary revisions. Below, we provide a point-by-point response to each comment in the revised manuscript.

1. The TPROGS-based heterogeneous fields are central to the conclusions, but the conditioning data (only 14 boreholes), transition probabilities, variograms, and convergence of 20 realizations are not sufficiently documented. Please add a dedicated subsection describing the limitations of representing heterogeneity with such sparse conditioning.

Response:

We thank the commenter for bringing this vital point to our attention. We agree that the limited conditioning data constrain the TPROGS-based heterogeneous fields. In the revised manuscript, we explicitly acknowledge that the TPROGS realizations should be regarded as plausible but non-unique representations of heterogeneity, used primarily to explore the sensitivity of regional MAR performance to facies connectivity rather than to provide deterministic cell-scale predictions. We will highlight this limitation when interpreting heterogeneity-related results.

Revisions have been made in line 380:

“The geological heterogeneity was characterized based on a sparse borehole dataset, inevitably introducing structural uncertainty in the delineation of localized contaminant migration, although its impact is partially mitigated through stochastic ensemble simulations.”

2. The description of pumping, irrigation returns, and lateral boundary conditions is quite brief relative to their importance, and there is no explicit groundwater or nitrate mass balance. Please provide a brief summary in the paper.

Response:

We thank the commenter for this suggestion. These boundary conditions were already described in lines 146–155 of the original manuscript, and we elaborate on them here for clarity.

Groundwater pumping rates were primarily compiled from public datasets and were further calibrated against observed water-level variations in regional monitoring wells to better represent the actual extraction stress in the Xiong'an New Area. Because the study area is predominantly agricultural, irrigation return flows were estimated based on published regional studies. For lateral boundaries, the western boundary was prescribed as a specified-head (Dirichlet) boundary using the initial potentiometric surface, while the southern boundary adjacent to Baiyangdian Lake was treated as a constant-head boundary. The eastern boundary was prescribed as a recharge (flux) boundary, with fluxes constrained using observed discharge data from nearby surface-water gauging stations. A groundwater water-balance summary is provided in the Supplementary Information (Table S4).

Revisions have been made in line 190:

“A domain-wide groundwater budget was computed to support the interpretation of simulated flow dynamics, and the major inflow and outflow components are summarized in the Supplementary Information (Table S4).”

Table S4. Groundwater water-budget

mass (kg)	Storage change	Pre	Irrigation	western	southern	eastern	Total pumping
$T_{end} - T_{initial}$	1.69×10^{11}	5.22×10^{11}	1.43×10^{11}	5.04×10^{11}	5.02×10^{11}	3.98×10^{11}	-1.9×10^{12}

3. The introduction outlines gaps but does not clearly state what this work adds beyond existing MAR–nitrate modeling in the NCP and globally. Please sharpen the problem statement, explicitly contrast your framework and findings with key prior regional-scale MAR studies, and clearly articulate the unique methodological and management contributions in the last paragraph of the Introduction. I strongly recommend to consider "Assimilation of sentinel-based leaf area index for modeling surface-ground water interactions in irrigation districts"

Response:

We thank the commenter for this insightful suggestion. We agree that, in its current form, the Introduction does not yet clearly convey what our study adds beyond existing MAR–nitrate modeling work in the North China Plain and globally. In the revised manuscript, we will sharpen the problem statement and more explicitly contrast our framework with key regional-scale MAR studies, emphasizing that our work (i) develops a fully 3D variably saturated flow and multi-component reactive transport model for a large groundwater depression cone, (ii) explicitly quantifies the relative roles of dilution and denitrification using domain-integrated nitrate mole balances, and (iii) evaluates the impact of geological heterogeneity through ensembles of T-PROGS realizations. We will also consider and cite the recommended study on assimilation of Sentinel-based leaf area index for modeling surface–groundwater interactions in irrigation districts, and position our work as complementary to that line of research.

Revisions have been made in line 62:

“This paper is organized as follows. First, we describe the hydrogeological setting, water budget, and

groundwater quality of the study area. We then present and justify the modeling framework (calibrated flow, reactive transport for nitrate, and T-PROGS–based heterogeneity), followed by the scenario results. Finally, we discuss management implications for MAR, key limitations, and the transferability of the approach to other overexploited aquifer systems.”

4. The conclusion that ~91% of nitrate reduction is due to dilution is based primarily on domain-average concentration differences between scenarios. Please support this attribution with explicit nitrate mass-balance terms (advective–dispersive fluxes vs. reaction sinks).

Response:

We thank the commenter for this insightful suggestion. To address this concern, we conducted a full-domain nitrate mass balance analysis between the initial and final simulation states and explicitly quantified the contributions of advective–dispersive transport (dilution) and biogeochemical reactions. Table R2 summarizes the nitrate mass balance over the simulation period. The total change in nitrate mass within the domain is -8.723×10^7 mol. This net reduction can be decomposed into three components: (i) nitrate inflow associated with recharge and boundary fluxes ($+1.254 \times 10^9$ mol), (ii) nitrate outflow through groundwater discharge and pumping (1.333×10^9 mol), and (iii) nitrate removal via denitrification reactions (-8.25×10^6 mol).

Based on this explicit mass balance, advective–dispersive transport processes account for approximately 91% of the total nitrate reduction, while denitrification contributes only about 9%. This quantitative result is fully consistent with the concentration-based analysis presented in the main text, but provides a more rigorous and physically grounded attribution of nitrate attenuation mechanisms.

Table R1. Nitrate mass balance between initial and final simulation states

ΔNO_3^- mass (mol)	Global	Inflow	Outflow	Reaction
$T_{\text{end}} - T_{\text{initial}}$	-8.723×10^7	1.254×10^9	-1.333×10^9	-8.25×10^6

Revisions have been made in line 339:

“To rigorously verify the mechanisms driving these reductions, a domain-wide mass balance was computed, revealing a net nitrate storage change of -8.723×10^7 mol. This budget is dominated by transport fluxes (Inflow: 1.254×10^9 mol; Outflow: -1.333×10^9 mol), whereas biological removal via denitrification accounts for only -8.25×10^6 mol.”