Response Statement to Community's Comments (CC7)

Wang and Jeng

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The authors thank the reviewer for the valuable comments. The manuscript has been revised by carefully considering all the comments. The changes are highlighted in the marked copy, and detailed responses to the reviewer's comments are provided below.

Comment #CC7:

You model landfill-liner-like consolidation with chemistry. There are some questions with (1) the mechanical model (elastic vs elasto-plastic/creep typical in clays), (2) the lack of reaction-induced porosity/permeability evolution (I know you already acknowledge this which is good, but it reduces interpretability of long-term plume changes), (3) boundary conditions (drainage, injection as fluxes at multiple points) and whether they represent a realistic exposure. Consider adding a short justification for the constitutive law used and explicitly call the case studies "demonstration problems" rather than predictive landfill designs. Add one sentence in the Conclusions about what would change when property feedbacks are included (directional expectation is fine, but label it as expectation).

Also some minor comments below:

(1) In benchmark 2 you say early-time deviations come from transport formulation and boundary representations; please add one sentence indicating which boundary treatment differs (Dirichlet/Neumann/mixed; inlet formulation), and whether refinement improves it.

(2) Consistently distinguish "hydraulic conductivity K" vs "permeability k" (the symbol list emphasises K).

(3) Injection strengths are given as fluxes at J1–J3; ensure it's always explicit whether that is imposed as boundary flux (mol/($m^2 \cdot s$)) and over what area.

(4) Computational performance section: helpful, but reviewers will ask for scaling beyond 4 MPI ranks and/or mesh size dependence. Even a small strong-scaling plot (1,2,4,8,16) on one case would help.

(5) Consider moving the limitations to earlier in the discussion.

Response:

We thank the reviewer for the constructive and insightful comments, which have helped us to better clarify the scope, assumptions, and applicability of the proposed framework. The manuscript has been revised accordingly. Our detailed responses are provided below.

Major comments

1. A justification of the small-strain elastic constitutive assumption has been added to the Conclusions. We now explicitly state that the formulation is intended for scenarios in which deformations remain limited and significant yielding or creep does not occur, and that elasto-plastic or visco-plastic constitutive laws would be required for long-term simulations involving large settlements or time-dependent deformation of clay liners.

2. We have added a statement in the Conclusions clarifying that reaction-induced porosity–permeability feedbacks are not considered in the present study. We further note that incorporating such feedbacks is *expected* to intensify preferential flow and increase the spatial heterogeneity of solute plumes over long time scales. This statement is explicitly framed as a qualitative expectation rather than a quantified prediction.

3. We have clarified that the boundary conditions and source configurations are intended as demonstration problems designed to explore coupled hydro–mechanical–chemical mechanisms, rather than predictive landfill-scale exposure scenarios. In particular, we now explicitly state that the injection patterns represent localised defects or preferential leakage pathways, whereas spatially uniform large-scale leakage is not considered representative of engineered barrier systems. Owing to the absence of site-specific field data, the simulations are therefore framed as scenario-based analyses rather than field-calibrated predictions. This clarification has been added at the end of the boundary-condition subsection.

[Added new content:] *This study presents a multi-dimensional HMC modelling framework by embedding a flexible geochemical module into an existing hydro-mechanical solver, enabling the consistent treatment of multi-component aqueous species and mineral reactions in near-saturated deformable porous media. The formulation is developed for small-strain, predominantly elastic behaviour, applicable to scenarios in which deformations remain limited and the soil skeleton does not undergo significant yielding or creep. For long-term conditions involving large settlements or plastic deformation of soft clays, an elasto-plastic or visco-plastic constitutive description, together with reaction-induced porosity–permeability feedbacks, would be required. Incorporating these effects is expected to intensify preferential flow and increase the spatial heterogeneity of solute plumes over time. These developments, together with quantitative benchmarking against laboratory and field data, will be pursued to further strengthen the predictive capability of the framework.*

[Line 258–259]

[Added new content:] *It is emphasised that the imposed concentration boundary conditions are adopted as controlled demonstration settings to explore the sensitivity of coupled hydro-mechanical–chemical responses to source strength and drainage configuration. The leakage cases considered correspond to localised defects or preferential pathways rather than spatially uniform barrier failure, which is not regarded as realistic for engineered containment systems. In the absence of site-specific investigation data, the present simulations should therefore be interpreted as scenario-based analyses aimed at mechanistic understanding, rather than predictive landfill exposure assessments.*

[Line 258–259]

Minor comments:

1. We thank the reviewer for this comment. In Benchmark #2, both the reference solver and the present framework prescribe inlet concentration using fixedValue (Dirichlet-type) boundary conditions. However, the effective advective boundary fluxes differ because the reference implementation evaluates advection using the face-based volumetric flux ϕ, whereas the present model employs a cell-centred Darcy-based velocity field that is interpolated to the boundaries. This structural difference leads to irreducible early-time discrepancies that cannot be eliminated by mesh or time-step refinement.

2. This has now been corrected throughout the manuscript.

3. We have clarified that J_1–J_3 are imposed as prescribed boundary mass fluxes with units of $\mathrm{mol\,m^{-2}\,s^{-1}}$ over the corresponding inlet areas along the top boundary. The description of the top boundary conditions has been revised accordingly.

4. We agree that this would strengthen the manuscript. A strong-scaling test (1, 2, 4, 8 and 16 MPI ranks) has now been added for a representative case, and the results are reported in the revised computational performance section.

5. The limitations associated with the elastic constitutive law and the absence of reaction-induced property feedbacks are now discussed in the opening paragraph of the Conclusions to ensure that the scope and applicability of the model are clearly stated before the main findings are summarised.

[Added new content:] *Along the top boundary, three contaminant inlets (depicted by blue arrows) are prescribed as boundary molar fluxes J_1–J_3 with units of* $\mathrm{mol/(m^2 \cdot s)}$*. Each inlet is applied uniformly over a top-boundary patch of width* 4 m *(i.e., an inlet area* $A_i = 4\ \mathrm{m} \times 0.02\ \mathrm{m}$*, where* 0.02 m *is the out-of-plane thickness of the quasi-2D OpenFOAM model). The intervening top-boundary segments are assigned zero solute flux. The entire top surface is subjected to a uniform mechanical load.*

[Line 258–259]

[Added new content:] *To evaluate the parallel efficiency of the developed solver, the wall time required for a five-year simulation is analysed as a function of the number of MPI processes. Figure 1 presents the measured wall time together with the corresponding speedup, which is defined relative to the baseline case with two MPI processes as Speedup* $= T_2/T_N$.

As the number of MPI processes increases from 2 to 16, the wall time decreases substantially from approximately 3.5×10^4 s *to below* 5×10^3 s*, demonstrating a marked improvement in computational efficiency. The speedup increases monotonically over the same range and remains close to linear scaling, indicating that the developed solver is well parallelised and can effectively exploit distributed-memory computing for the problem size considered. Overall, these results confirm satisfactory strong-scaling performance up to 16 MPI processes for the five-year simulation.*

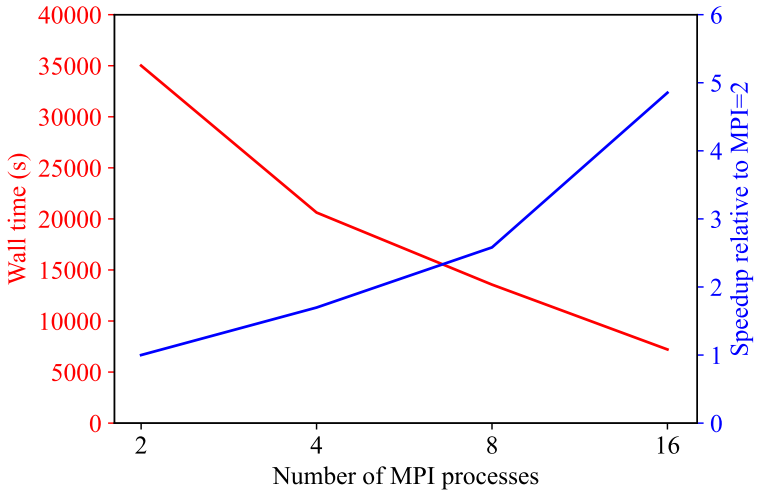

Figure 1: Wall time and speedup versus number of MPI processes.

[Line 258–259]