Response Statement to Community's Comments (CC5)

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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 #CC5:

At minimum, include: (1) The PHREEQC database used, the key input blocks (KINETICS/EQUILIBRIUM PHASES/etc.), and where they are provided (supplement/Git repo). (2) OpenFOAM discretisation choices for transport (schemes, limiters), linear solvers/preconditioners, coupling tolerances, and convergence criteria (you mention a prescribed tolerance but not what it is). (3) Use a public repository plus archived case files. Without this, the ChemWindow contribution especially will be hard to credit.

Response:

We thank the reviewer for highlighting the importance of reproducibility and transparency. The manuscript has been revised accordingly as follows.

1. **PHREEQC database and input blocks.** We now explicitly state that the thermodynamic database used is `phreeqc.dat` obtained from the official USGS PHREEQC distribution. The conventional PHREEQC input blocks (e.g. `SOLUTION`, `EQUILIBRIUM_PHASES`, and `KINETICS`) are encoded in OpenFOAM chemistry dictionaries specified by the entry `PhreeqcInputFile "phreeqcInput"`, following the `porousMedia4Foam` framework. A detailed description of the OpenFOAM–PHREEQC mapping and representative configuration options is now provided in Appendix C.

2. **OpenFOAM discretisation and solver settings.** A concise description of the discretisation schemes for solute transport, the linear solvers and preconditioners, and the coupling tolerances and convergence criteria has been added to Section 3.3. This includes the convective and diffusive schemes, the solver types and

preconditioners for the pressure, displacement and concentration equations, and the absolute and relative tolerances used to advance the HMC system.

3. **Public repository and archived case files.** A public repository containing the ChemWindow implementation, representative OpenFOAM chemistry dictionaries, and minimal working cases is currently being prepared and will be released upon acceptance of the manuscript. The repository will provide all configuration files and scripts required to reproduce the numerical results reported in this study.

[Added new content:] *Within the OpenFOAM framework adopted in this study, the governing equations were discretised using the finite volume method. Diffusive and dispersive fluxes were evaluated using the Gauss linear scheme, while the advective term of solute transport was discretised using a Gauss limitedLinear scheme with a limiter coefficient of 1 in order to suppress spurious oscillations. Temporal integration was performed using the implicit Euler method. The pressure, displacement and concentration equations were solved using the GAMG solver with a DILU preconditioner, with absolute and relative tolerances of* 10^{-9} *and zero, respectively. The coupled HMC system was advanced using a segregated outer-iteration strategy, and convergence was achieved when the residuals of all primary variables dropped below* 10^{-6}*. Further implementation details are provided in the companion paper (Wang and Jeng, 2025).*

[Line 76–80]

Geochemical reactions are executed through PHREEQC using the PhreeqcRM interface. In contrast to conventional PHREEQC workflows based on standalone input scripts, the present solver introduces a dictionary-based configuration layer within OpenFOAM. Keywords such as `PhreeqcDataBase` *and* `PhreeqcInputFile` *are parsed at runtime and directly mapped to the corresponding PhreeqcRM function calls. Consequently, all reaction systems are fully configurable at runtime and no recompilation of the solver is required when modifying geochemical databases or reaction settings. This design establishes the solver as a configurable reactive-transport computing platform rather than a case-specific implementation.*

Database binding and runtime mapping

The thermodynamic database is specified by the keyword `PhreeqcDataBase`*, which is passed directly to the PhreeqcRM initialisation routine. Similarly, the entry* `PhreeqcInputFile` *defines an OpenFOAM dictionary that encodes the aqueous solution composition using standard PHREEQC* `SOLUTION` *syntax. At runtime, the PhreeqcRM interface converts the dictionary entries into the corresponding PHREEQC command strings and executes them internally via PhreeqcRM, ensuring full compatibility with the official PHREEQC syntax.*

Reaction model configuration

Phase equilibrium and kinetic reactions are configured through the boolean flag `activatePhaseEquilibrium`*. When enabled, mineral reactions are treated as equilibrium phases; otherwise, they are processed as kinetic reactions, reproducing the functionality of the PHREEQC blocks* `EQUILIBRIUM_PHASES` *and* `KINETICS`*. Time integration of kinetic reactions is controlled through the options* `cvODE` *and* `cvODETol`*, which activate the CVODE integrator and prescribe its relative tolerance, respectively. The keyword* `setComponentH2O` *determines whether water is treated as an explicit geochemical component.*

Extensibility

All chemistry-related options are defined exclusively in OpenFOAM dictionaries and are translated to PhreeqcRM calls at runtime. Therefore, new reaction systems, databases, and kinetic models can be introduced by editing configuration files only, without any modification or recompilation of the solver source code.

[Line 76–80]

[Line 258–259]

References

Wang, B.L., Jeng, D.S., 2025. Three-dimensional model for consolidation-induced solute transport in a nearly saturated porous medium. International Journal for Numerical and Analytical Methods in Geomechanics 49, 4436–4464. doi:https://doi.org/10.1002/nag.70070.