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Hydrology and Earth System Sciences
Discussions

Interactive comment on "A novel model for simulation of nitrate in aquifers" *by* Roohollah Noori et al.

Anonymous Referee #1

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Review of "A novel model for simulation of nitrate in aquifers"

Summary: The manuscript presents a reduced order modeling (ROM) methodology to make predictive model analyses for subsurface solute transport of nitrate. The reduced order model is first developed based on results from a numerical flow and solute transport model simulated using MODFLOW and MT3DMS. The manuscript then compares predictive results generated using the proposed ROM methodology with the predictive results of MT3DMS.

General Comments

The main point of the manuscript is the computational efficiency of the proposed ROM methodology. It is claimed to be computationally more efficient than simulating

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MT3DMS, however, the manuscript does not provide any comparison of computation time. An appropriate comparison between computing time would include time required for the predictive MT3DMS model, versus time required for ROM analyses that would include calculations to generate eigen values and vectors, matrix computations, and predictive analyses.

It would be beneficial to the reader to also include in the manuscript a discussion about the general applicability and suitability of the ROM methodology, limitations, and the robustness of the ROM predictions. For example, is ROM suitable for predictive scenarios to examine remediation options by adding pumping wells?

It is noteworthy that the ROM methodology is based on a historic numerical model simulated using MT3DMS and therefore, the quality of analyses resulting from ROM is expected to be just as good as the quality of the underlying numerical model, based on which eigen vectors are generated for ROM calculations.

Specific Comments (individual scientific questions/issues)

Below is a list of specific comments that would need to be addressed: - Page 1, line 22: the “simpler structure” of ROM computation is based on matrix calculations but the results are primarily based on MT3DMS computations. I suggest deleting “simpler structure” from the text as that description is misleading.

- Page 1, line 22: provide some numbers to demonstrate “shorter calculation times”.

- Page 2, line 9: “information produced by the models is confusing”, is an inappropriate statement. It is the modeler’s job to understand the meaning of the output that a model generates. Again, the numerical model output is what is used for ROM, which makes it further “confusing”, doesn’t it?

- Page 2, line 31: “complex mathematical form” and “complex solving methods” for numerical models is presented as a limitation, however, ROM is based on the output from these very “complex” numerical models; ROM, in my opinion adds one more layer

of mathematical complexity to the system. If complexity of numerical models is being criticized, ROM stands to be criticized even more. I suggest deleting this line entirely.

- Page 5, line 1: the impact of river recharge is not seen in the head contours; may be the recharge amount is small? I am only stating an observation, this need not be addressed in the manuscript.

- Page 5, line 30: calibration is discussed in detail. My suggestion would be to either shorten the calibration discussion as the focus of the manuscript is the ROM methodology, or include a plot showing the goodness of fit, comparing observed values and simulated results using a scatter plot one for heads and one for concentrations, to complete the calibration discussion.

- Page 6, line 4: incorrect statement, TVD scheme is not a combination of four other methods. I suggest modifying this statement.

- Page 7, line 8-14: the explanation seems unclear. This paragraph is the main feature of this manuscript and needs to be explained better.

- Page 7, line 28: there are several aspects to examine before calling the model well calibrated. It also depends on the objective of the model. In this case, since solute transport is important, getting the gradients and velocities correct becomes important. I am simply pointing this out and the authors may have already examined this aspect but not reported it. This point need not be addressed in the manuscript.

- Page 8, line 5: looking at only the difference can be misleading. Examining time-series is also important to assess trends.

- Page 8, line 8: Nitrate distribution seems locally contained? Is it because the movement is slow with respect to the simulation period? Again, just an observation. This point need not be addressed in the manuscript.

- Page 10, line 4: the limitations of numerical models listed in the manuscript are arbitrary, as pointed out in some of my previous comments. The only relevant limitation

of numerical models, in context of this manuscript, could be the computation time, but that analyses is not presented in the manuscript.

- Page 10, line 15: the claim that “ROM was superior than MT3DMS” is incorrect. ROM is based on the results generated by MT3DMS. How would that make ROM superior than MT3DMS in terms of quality of results? I suggest deleting this line from the manuscript.

Technical Corrections

Below is list of my technical corrections/suggestions:

- Page 1, line 13: delete “Please”, the first word in the Abstract.

- Page 1, line 13: high computational cost is a result of long simulation times, not the other way around.

- Page 1, line 16: replace “presents a solution for the problem in ROMs” with “was”.

- Page 1, line 20: insert code or program or simulator before “(MT3DMS)”.

- Page 1, line 26: consider rearranging the sentence as: “. . . and activities have resulted in spreading pollution in the aquifers that result in groundwater quality deterioration.”

- Page 1, line 28: nitrate is not “often the main concern”, but is one of the common contaminants.

- Page 1, line 31: abstract uses GQM, not GQSM. Search the remainder of manuscript and use a consistent acronym.

- Page 3, line 11: “annual evaporation” or “annual potential evaporation”?

- Page 3, line 28: in equation 1, “∂” is missing in the denominator in 2 places.

- Page 4, line 22: “distribution of hydraulic”, the word ‘of’ is missing.

- Page 4, line 24: consider replacing “are” with “were”.

- Page 5, line 11: consider replacing “including” with “the availability of”.

- Page 5, line 16: what is the difference between gridded network and mesh dimension? Consider clarifying in the text.

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