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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.

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Response to Reviewer' Comments on: https://doi.org/10.5194/hess-2018-222

The authors thank the reviewer for the quick response. The manuscript has been improved substantially based on the constructive comments of the reviewer.

Response to Comments of Reviewer #1

General Comment: 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 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

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Discussion paper

analyses that would include calculations to generate eigenvalues and vectors, matrix computations, and predictive analyses. Response: We agree and have now added a new section in the manuscript that provides a comparison between the running times of the developed ROM and MT3DMS. “Considering the computational costs, the developed nitrate ROM was superior (it ran about ten times faster than MT3DMS). More specifically, the computational time for the predictive MT3DMS model was about 89 seconds. This value reduced to nine seconds when we applied the developed ROM for simulation of nitrate in the aquifer using the same computer. Note that the computational time for running the developed ROM model includes calculations to generate matrix computations, eigenvalues and eigenvectors, and predictive analyses.”

General Comment: 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? Response: We agree and have added a new section in the manuscript that provides useful information about the general applicability, suitability, limitations, and the robustness of the ROM. “Considering the computational costs, the developed nitrate ROM was superior (it ran about ten times faster than MT3DMS). Also, it is noteworthy that the quality of analyses resulting from ROM was as good as the quality of the underlying numerical model. Thus, it can be concluded that the developed ROM model with a simple structure and considerably less running time than MT3DMS appropriately simulated the nitrate concentration in the Karaj Aquifer. Regarding the ROM applications for the future times, all time dependent factors in the aquifer responses, such as hydrometeorological, hydrogeological, and well operation strategies in the simulation period is expressed by temporal component τ(t) in the ROM. Thus, the model is applicable for future prediction of nitrate in the aquifer under conditions that already existed during the simulation period of the modelling process. In other words, the predictive POD model can appropriately memorize historical processes experienced during the simulation period so that the model captures the dominant modes of nitrate variation in the

aquifer. These modes that include space and time dependent terms of nitrate (Θ(x) and τ(t), respectively), clearly represent the spatiotemporal variation (STV) of this pollutant in the aquifer. Thus, the changes in the input concentrations are expressed in the time dependent terms of the developed model extrapolated in the future (i.e. τ(t+n)). By considering these, we used the predictive POD model developed by the first four modes that represent more than 99.99% of system energy to predict nitrate in the aquifer. This means that the developed model conserves more than 99.99% of STV of nitrate in the aquifer. Therefore, it can be concluded that the results of developed model for prediction of nitrate match well the nitrate simulated by MT3DMS. To clearly show this fact, one-year data from April 2012 to March 2013 was employed to compare the developed predictive POD model with the MT3DMS. As described in the manuscript (Section 3.4.2), the absolute error between the developed model and the MT3DMS was less than 0.5 mg/l in the most parts of the aquifer. This clearly shows that the developed model behaves in a similar accuracy as MT3DMS. However, while the developed model is applicable for prediction of nitrate in the future, it cannot be used for evaluation of different scenarios. In fact, inputs used for development of the predictive POD model are Θ(x) and τ(t). Although all time dependent factors (such as hydrometeorological and hydrogeological variables) in the aquifer responses are expressed by τ(t) in the developed predictive POD model, τ(t) doesn't individually include these time dependent factors. Therefore, it is not possible to change these time dependent factors in the predictive POD model individually although they are totally expressed by τ(t). In addition, it is noteworthy that the predictive POD model is developed based on a historic numerical model simulated using MT3DMS and therefore, (1) the quality of analyses resulting from this model is as good as the quality of the underlying numerical model, (2) one needs to have the results of a historic numerical model to develop the predictive POD model although it can be independently applied for the prediction of nitrate." We have now added a section in the manuscript that clearly describes these limitations of the developed POD model."

General Comment: It is noteworthy that the ROM methodology is based on a his-

toric 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. Response: Thanks for the comment. We have now added a new section in the manuscript that provides useful information about the general applicability, suitability, limitations, and the robustness of the ROM. “Also, it is noteworthy that the ROM is developed based on a historic numerical model simulated using MT3DMS and therefore, (1) the quality of analyses resulting from this model is as good as the quality of the underlying numerical model, (2) one needs to have the results of a historic numerical model to develop ROM model although it can be independently applied for the prediction of nitrate.”

Comment: 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. Response: We agree and have deleted it and updated the statement.

Comment: Page 1, line 22: provide some numbers to demonstrate “shorter calculation times”. Response: We have now provided some numbers about the running times of the models.

Comment: 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? Response: Thanks for the comment. We meant the difficult management of large data produced by these models. However, we have now updated this statement.

Comment: 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. Response: Thanks for the comment. We have now deleted this statement entirely.

Comment: 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. Response: In arid and semi-arid regions like Iran, most of rivers are not permanent and the Karaj river is no exception. In our groundwater modeling, recharge of river is a small amount compared to the deep groundwater flow. In addition, it is varied during the year although it is considered indirectly in the model.

Comment: 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. Response: Thanks for the comment. We have now shortened this section.

Comment: Page 6, line 4: incorrect statement, TVD scheme is not a combination of four other methods. I suggest modifying this statement. Response: Thanks for the comment. We have now modified this statement.

Comment: Page 7, line 8-14: the explanation seems unclear. This paragraph is the main feature of this manuscript and needs to be explained better. Response: We have now updated this paragraph. Noted all steps for the introduced methodology are given in Figure 2. However, we did our best to properly describe this section by referring to Figure 2 in the revised manuscript. Note that if the ROM developed by few first selected modes (Eq. (8)) didn't satisfy the defined criteria for evaluating the model performance (such as RMSE and MAE), one need to increase the number of modes so that to reach the defined criteria. This procedure is properly shown in Figure 2.

However, Eq. (8) has a simple structure with a few modes. Thus, one needs the few first significant modes developed based on simulated historic nitrate concentrations using MT3DMS to regenerate this pollutant in the aquifer. In other words, the ROM is applicable for regeneration of nitrate on the solution domain of MT3DMS and it is not applicable to make prediction in the future. In this study, we aimed to enhance the ROM to make predictions into the future, for time steps with no nitrate simulations from the MT3DMS model. This step is shown in subsection "Model Verification" of Fig. 2. For this purpose, we developed a methodology that enables the ROM to independently simulate nitrate concentrations. According to this, it is necessary to calculate both the spatiotemporal components Θ(x) and τ(t) for the future time interval (t + n). Since the component Θ is a function of space, it does not change in time. Therefore, it is necessary to calculate τ for future time steps. For this purpose, a regression equation was used to estimate the time variation of this component (τ(t+n)). Having τ(t+n), the nitrate concentration for future time steps t+n can be calculated by Eq. (9): Eq. (9) simulates the nitrate concentration in different parts of the aquifer for future time t+n using the first few significant modes. According to Fig. 2, if the ROM developed didn't satisfy the defined criteria for evaluating the model performance, one need to increase the number of modes by estimating the trend of more numbers of the time dependent components so that the developed ROM satisfies the defined criteria.

Comment: 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. Response: Thanks for the comment. Due to main focus of this submission is solute transport, we have ignored to provide more discussion on the model calibration.

Comment: Page 8, line 5: looking at only the difference can be misleading. Examining timeseries is also important to assess trends. Response: We agree and have now

added the trends of measured nitrate concentrations and simulated ones by MT3DMS model. We have also added another figure that properly shows the trends of RMSE and MAE averaged over the study area during the calibration period.

Comment: 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. Response: Thanks for the comment. Yes.

Comment: 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. Response: Thanks for the comment. We have now added a new section in the manuscript that provides useful information about the running times of the models, i.e. ROM and MT3DMS. "Considering the computational costs, the developed nitrate ROM was superior where it was run about ten times faster than MT3DMS. More specifically, the computational time for the predictive MT3DMS model was about 89 seconds. This value reduced to nine seconds when we applied the developed ROM for simulation of nitrate in the aquifer using the same computer. Note that the computational time for running the developed ROM model includes calculations to generate matrix computations, eigenvalues and eigenvectors, and predictive analyses."

Comment: 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. Response: Thanks for the comment. We have now deleted the mentioned line.

Comment: Page 1, line 13: delete "Please", the first word in the Abstract. Response: Thanks for the comment. Agreed and amended.

Comment: Page 1, line 13: high computational cost is a result of long simulation times, not the other way around. Response: Thanks for the comment. We have now updated this statement.

Comment: Page 1, line 16: replace “presents a solution for the problem in ROMs” with “was. Response: Thanks for the comment. We have now updated this statement.

Comment: Page 1, line 20: insert code or program or simulator before “(MT3DMS)”. Response: Thanks for the comment. We have now updated this statement.

Comment: 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.”. Response: Thanks for the comment. We have now updated this statement.

Comment: Page 1, line 28: nitrate is not “often the main concern”, but is one of the common contaminants. Response: Thanks for the comment. We have now updated this statement.

Comment: Page 1, line 31: abstract uses GQM, not GQSM. Search the remainder of manuscript and use a consistent acronym. Response: Thanks for the comment. We have now check all text of manuscript and corrected this acronym.

Comment: Page 3, line 11: “annual evaporation” or “annual potential evaporation”? Response: Thanks for the comment. We have now updated this statement.

Comment: Page 3, line 28: in equation 1, “∂” is missing in the denominator in 2 places. Response: Thanks for the comment. We have now corrected this equation.

Comment: Page 4, line 22: “distribution of hydraulic”, the word ‘of’ is missing. Response: Thanks for the comment. We have now updated this statement.

Comment: Page 4, line 24: consider replacing “are” with “were”. Response: Thanks for the comment. We have now updated this statement.

Comment: Page 5, line 11: consider replacing “including” with “the availability of”. Response: Thanks for the comment. We have now updated this statement.

Comment: Page 5, line 16: what is the difference between gridded network and mesh dimension? Consider clarifying in the text. Response: Thanks for the comment. It was a typos error. We have now updated this statement.

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