Greetings. I have revised the paper entitled 'Real-time Monitoring of Petroleum Hydrocarbons in Groundwater using Hybrid Machine Learning Architectures'. The paper deals with Machine Learning-based approaches to assess the contaminant plume of benzene pollutants and their fate in groundwater. The work is scientifically sound, and its methodology is robust. However, I'm recommending some adjustments before further proceeding down the publication path. Best regards.

- I cannot state the boundary conditions, extensions, and their type in your work. Hence, I cannot fully understand how you tuned your model.
- It is clear that geological (hence facies conductivity) heterogeneity is a key driver in your transport model. However, the methodology lacks supporting equations and a sufficient explanation. Indeed, at lines 91-93, you write "The RTM used in this study is based on the model developed in Wu et al. (2024), implemented in Python using FloPy within a Jupyter Notebook environment. Groundwater flow was simulated using MODFLOW 2005, and contaminant transport was modeled with MT3DMS, incorporating advection and dispersion processes". Therefore, I suggest carving a brief section, maybe before the present section 2.3, to explain governing equations (see also Bedekar et al., 2016). Please incorporate a short section. I would just write a couple of lines for MODFLOW 2005 and then focus on transport:

  "The MT3D model simulates dissolved solute transport in groundwater using the advection–dispersion–reaction equation. In terms of concentration per unit volume of water, the governing mass balance is

$$\frac{\partial C}{\partial t} = \nabla \cdot (\mathbf{D} \nabla C) - \mathbf{v} \cdot \nabla C + \frac{q_s}{\theta}(C_s - C) - \lambda C$$

  where C is solute concentration, θ is porosity, $\mathbf{v} = \mathbf{q}/\theta$ is the seepage velocity derived from the Darcy flux $\mathbf{q}$ (computed by MODFLOW), $\mathbf{D}$ is the hydrodynamic dispersion tensor, q_s and C_s represent fluid sources/sinks and their concentrations, and λ is a first-order decay coefficient.

  When linear equilibrium sorption is included, transport is retarded and the equation becomes

$$R_f \frac{\partial C}{\partial t} = \nabla \cdot (\mathbf{D} \nabla C) - \mathbf{v} \cdot \nabla C - \lambda C$$

  where the retardation factor is

$$R_f = 1 + \frac{\rho_b K_d}{\theta}$$

with ρ_b the bulk density and K_d the distribution coefficient."

- Which numerical schemes were adopted in the transport simulations for the advection, dispersion, and reaction terms? Specifically, which advection solver was used (Upstream finite difference, TVD, MOC/MMOC, or HMOC), and how were dispersion (finite-difference formulation) and reactions handled (explicit or implicit solution)?
- Can you frame your work in the wider Machine-Learning literature? There is a wide class of Genetic Algorithms that perform extremely well and could be adapted to your framework (Rajwar et al., 2023; Schiavo & Pedretti, 2026). I think the paper should deal with this branch of research, explaining (i) why your methodology is better (or not) and (ii) possible employments of metaheuristics-driven approaches.
- Can you highlight the driving parameters for each of your three scenarios, and how they are involved in XGBoost regression? I suggest offering a framework where these parameters are well-highlighted. See e.g. Schiavo & Pedretti, 2026, Figure 1.
- Figures 3 and 4 are very hard to read properly. I suggest, at least for the latter one, employing boxplots to show the MAE.

Suggested References:

Bedekar, V., Morway, E.D., Langevin, C.D., and Tonkin, M., 2016, MT3D-USGS version 1: A U.S. Geological Survey release of MT3DMS updated with new and expanded transport capabilities for use with MODFLOW: U.S. Geological Survey Techniques and Methods 6-A53, 69 p., http://dx.doi.org/10.3133/tm6A53

Rajwar, K., Deep, K., & Das, S. (2023). An exhaustive review of the metaheuristic algorithms for search and optimization: Taxonomy, applications, and open challenges. Artificial Intelligence Review, 56(11), 13187–13257. https://doi.org/10.1007/s10462-023-10470-y

Schiavo, M., & Pedretti, D. (2026). Genetic and Iterative Metaheuristics-Informed Algorithms for Precision Shallow Groundwater Modeling and Drought Inference. *Journal of Geophysical Research: Machine Learning and Computation*, *3*(1), e2025JH000854. https://doi.org/10.1029/2025JH000854