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Interactive comment on "Machine Learning Deciphers CO_2 Sequestration and Subsurface Flowpaths from Stream Chemistry" *by* Andrew R. Shaughnessy et al.

Anonymous Referee #2

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Review of "Machine Learning Deciphers CO2 Sequestration and Subsurface Flowpaths from Stream Chemistry" by Andrew R. Shaughnessy, Xin Gu, Tao Wen, and Susan L. Brantley

This study focuses on applying machine learning to endmember mixing analysis of weathering chemistry in subsurface groundwater flow paths. They apply an NMF scheme and train it on syntactic data generated using a multivariate normal distribution of log-transformed stream water chemistries. The NMF is then applied to 3 measured stream water samples to delineate mixing proportions. The study is well presented and written, the SM is seminal to the understanding of the study and holds the key details

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Discussion paper

for the optimization of the NMF. The main finding is within the sensitivity of the reaction to the groundwater flow paths which are unknown, yet they control the concentration relation between the components and therefore they are controlling the overall chemistry. In a way, these flow paths are a spatial localization of the reaction in space and time, due to the seasonal effects, as shown here. I found the paper very interesting, well written, and clear and supports the publication of the study, yet the main missing part that is not discussed here and must be added is a discussion on the how. How does the NMF manage to capture the effect of the subsurface groundwater flow paths? What is the additional mechanism that is deciphered by the NMF? The spatial and temporal effect of the subsurface groundwater flow paths must be captured in a mean-field way by the MNF, and this is not clear how it managed to do so and what was the missing mechanism.

I agree with referee 1 remarks 5 and 6, do clarify the mathematical components with a mathematical expression.

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