

Interactive comment on “A Mass- and Energy-Conserving Framework for Using Machine Learning to Speed Computations” by Patrick Obin Sturm and Anthony S. Wexler

Anonymous Referee #2

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The current study uses an energy and mass conservation framework in a machine learning module to speed up the atmospheric chemistry computations in large scale simulations. The authors have suggested the use of machine learning tools to memorize the fluxes of change in quantities instead of change in quantities themselves which guarantees adhesion to conservation principles. The paper is well written and is within the scope of the journal, I have some minor suggestions to be included.

1. The authors in line 105 mentions that models usually don't give the flux “S” as output yet while providing the solution for a photochemical module in line 161, the authors in step 3 talk of generating the ΔC and S. How do the authors get the “S” value here?

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2. The authors are suggested to clearly mention and segregate the steps taken to generate the test and train data and then the steps from which machine learning tools are used to learn the relationship of S with other factors in section 3, 4 and 5. In short the authors should clearly mention the steps to be done using Chemical Transport Models (CTM) and the steps where the machine learning algorithm is used to determine the relationship of S with other factors.

3. The authors doesn't mention regrading the errors in approximating equations 11 and 12. Any suggestions to reduce the same?

4. The authors mention 2 problems which may occur a) regarding the stiffness of atmospheric chemistry problems b) regarding high dimensionality of atmospheric chemistry problems. Can the authors add more explanation with suitable examples for the problem as well as the suggested solution for better understanding?

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