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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 #1

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This paper covers the process for creating a mass-conserving ML framework for a photochemistry code embedded in a larger model. This process is described in detail and appears to be reproducible, and the process is both useful and robust. Given the content of the paper, it seems the title should be altered to specifically mention photochemistry.

Unless I have misread, the crux of this paper's approach to conserving mass or energy seems to be predicting terms that naturally give rise to conservation in the underlying discretization being modeled (e.g., fluxes for radiation or the time-integrated reaction vector, which is re-distributed in a conserving way by the stoichiometry matrix). Seem-

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Discussion paper

ingly one could also create a conservative ML surrogate for, say, a Finite-Volume or Discontinuous Galerkin discretization by predicting the fluxes rather than only the tendencies. This idea is useful but not necessarily novel in itself.

What is very novel is how one extracts a learnable quantity from the more readily available variables in the photochemistry application, a process that took quite a bit of careful attention. This is why I think the title might be better suited to the more novel demonstration of the concept in a complicated application. As I was reading, I was waiting to read about an example using radiation as well (mainly because of the title's generality), even though on a second pass, it was not stated that a radiation example would be given.

While the focus of this paper is machine precision conservation in a ML framework, since a ML surrogate model was indeed produced, it would be helpful to get a sense of the accuracy that was obtained compared to the original codebase for a set of representative examples one might encounter in a realistic model.

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