

Geosci. Model Dev. Discuss., referee comment RC3  
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## Comment on gmd-2021-317

Anonymous Referee #3

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Referee comment on "KGML-ag: a modeling framework of knowledge-guided machine learning to simulate agroecosystems: a case study of estimating N<sub>2</sub>O emission using data from mesocosm experiments" by Licheng Liu et al., Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2021-317-RC3>, 2021

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The authors are proposing the development of a new approach KGML-ag to machine learning in estimating N<sub>2</sub>O emissions from fertilized agricultural fields. This approach involves using data generated from a process model and a mesocosm experiment to tune the relationships and their parameters among input and intermediate variables by which N<sub>2</sub>O emissions are thought to be governed. The advantages of this approach over process models are simplified input data requirements, more rapid model execution, and possibly more accurate simulation of N<sub>2</sub>O fluxes measured in experiments for which the model is tuned.

The ability of this approach to simulate N<sub>2</sub>O emission events under controlled laboratory conditions is impressive. It should be noted that the N<sub>2</sub>O emissions in Fig. 2 and the soil NO<sub>3</sub> contents in Fig. 3 are much larger than those commonly encountered in field conditions. However the relationships and their parameters upon which this approach is based are not disclosed to the reader, and so remain a 'black box'. For example, in section 4.1 the processes governing the time course of N<sub>2</sub>O emissions following a urea application are described, but the method by which these processes were represented in KGML is not.

As for all black box approaches to modelling, it is vitally important that KGML be subjected to tests with truly independent datasets, i.e. datasets that are completely separate, and preferably very different, from those used in model calibration. Impressive results can always be achieved by calibrating enough parameters, but are these parameters robust? The extent to which such testing of KGML was conducted in this paper is not clear. At the very least, for this paper to be publishable, calibration and validation of KGML must be clearly distinguished, and clear evidence of independent testing must be provided. Further description of the key relationships and their parameters that govern N<sub>2</sub>O emissions in the model should also be provided so as to improve confidence in its robustness.

In the Discussion, the authors rightfully address some of the factors that may limit the robustness of KGML. These limitations will likely become more apparent when the authors conduct tests of KGML under field conditions. Addressing these factors, as described by the authors, appears to require that KGML more closely resemble process-based models, and may reduce the computational advantages claimed for the KGML approach.