This is an interesting paper that addresses a most relevant issue of incorporating background knowledge about processes in question into machine learning (ML) algorithms.

Clearly, in ML we are hoping to program computers by telling them what we want to achieve without having to explicitly instruct them how to achieve such goals. But, what is it that we want from those programs? Do they just need to be accurate or should we also be able to interpret them? In the scientific contexts, the ambition is clear: we are looking for a learning machine capable of finding an accurate approximation of a natural phenomenon, as well as expressing it in the form of a meaningful or an interpretable model. The authors adopt this view, and I fully subscribe to such a working hypothesis.

At the same time, this bias towards meaningfulness and interpretability opens several additional issues. The computer-generated hypotheses should take advantage of the already existing body of knowledge about the domain in question. In the case of two equally good approximations of the same data set: the one which blindly fits the data and the other which, in addition to the fit, also respects the background knowledge, we should be biased toward the latter one.

However, there are few questions that I would appreciate authors could address in the manuscript to a greater depth.

1.) The fashion in which we express knowledge about the processes and make it available to the learning machine remains rather unclear. One can insist on strict adherence to the background knowledge principles - such as 100% mass balance accuracy. We declare this desire and hence this is referred to as declarative bias. Alternatively, one can treat the
bias as an additional objective that should be treated simultaneously with the goodness of fit in the learning process. This is referred to as preferential bias. Declarative bias reduces search space but results in so-called broken ergodicity. Preferential bias results in a Pareto-optimal set of solutions. For further discussion in the context of water management see:

M Keijzer and V Babovic, 2002, Declarative and preferential bias in GP-based scientific discovery, Genetic Programming and Evolvable Machines 3 (1), 41-79

In the present paper, it would appear that authors prefer declarative treatment of background knowledge. However, I would appreciate further analysis, comparison, and, if that is not possible, at least a discussion on preferential vs. declarative bias in the case studies described in theirs work.

2.) Bias Variance Tradeoff. Arguably incorporation of the knowledge bias affects model variance. In this case, bias denotes the difference between the average prediction of a model and the correct value which it is trying to predict. Variance is the variability of model prediction for a given data point or a value that tells us the spread of our data. For in-depth discussion see:

Hastie, T; Tibshirani, R; Friedman, J. H. (2009). The Elements of Statistical Learning, Springer

I would love to see a more in-depth analysis of the bias-variance tradeoff in the present case, and am looking forward to reading more about it in the revised version of the manuscript.

3.) Models vs. Predictions.

LSTM-type of ML models are extremely good at forecasting. The authors have eloquently argued in favour of the approach in this (as well as in previous) published research works. At the same time, one must consider if such a n ML approaches induce models or forecasters. On this topic I would advise the following recent works:


HMVV Herath, J et al, 2021, Genetic programming for hydrological applications: to model or forecast that is the question, Journal of Hydroinformatics
In general, this is an interesting and potentially valuable contribution to the hydrological society. I am looking forward to reading revised version of the manuscript.