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Imposing Atom Conservation on Physics-Informed Neural Networks for Chemical Reactor Surrogates

Felix Döppel[1]*, Mauro Bracconi[1], Matteo Maestri[1]
*Lead presenter: felix.doeppel@polimi.it
[1] Laboratory of Catalysis and Catalytic Processes, Politecnico di Milano, Italy

Introduction Machine learning has emerged as an important tool in chemistry reduction, and simulation acceleration. Beyond the purely data-driven approach, physics-informed neural networks (PINNs) leverage a priori physical knowledge to provide highly performant, yet physically plausible model predictions. They facilitate process design and optimization, allow real-time evaluations for model-based control and accelerate reactive CFD. However, PINNs consider the strict law of atom conservation only through soft constraints. Recently, we developed a neural network layer which guarantees atom conservation as a hard constraint [1]. Here, we generalize this atom conservation layer by using a weight matrix to accurately predict the behavior of species with low concentrations, which is critical for reactive CFD applications. We showcase the potential of the method by applying atom conserving PINNs (AC-PINNs) to generate surrogates of the chemical sub step at catalytic surfaces in reactive CFD simulations.

Results and Discussion We apply the newly proposed AC-PINN to predict the gas composition over Rh catalysts for H_2 oxidation based on a detailed microkinetic surface mechanism [2], using only inlet-outlet composition data. While standard PINNs (Fig. 1, dashed) provide only qualitative agreement and violate the atom balance significantly, the new AC-PINN provides excellent agreement and a perfectly closed atom balance (Fig. 1, dotted), even outside the original training range. The AC-PINN accelerates the chemistry sub step by a factor of $\sim 10^4$ and allows for the adoption of any variable simulation time step Δt required by the CFD without retraining. We will implement the AC-PINN also for the detailed description of ammonia and methane catalytic combustion.

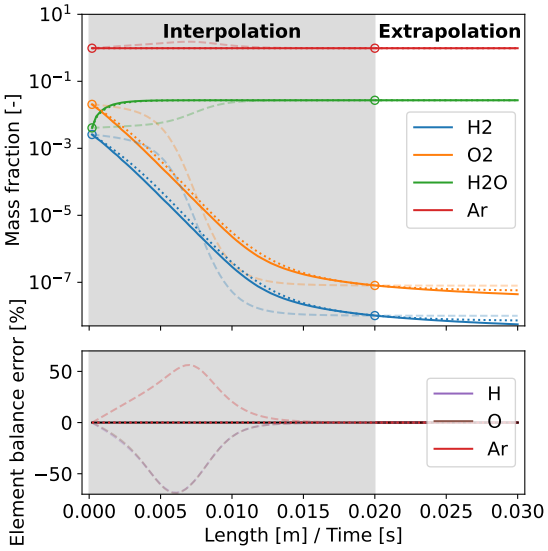

Figure 1: AC-PINN (dotted) prediction compared to the exact composition profile (full lines) and standard PINN (semi-transparent, dashed) along a catalytic H_2 oxidation reactor. The model perfectly closes the atom balance.

References

[1] Döppel F and Votsmeier M. Robust mechanism discovery with atom conserving chemical reaction neural networks. Proceedings of the Combustion Institute. 2024;40(1-4):105507.

[2] Karakaya C and Deutschmann O. Kinetics of hydrogen oxidation on Rh/Al2O3 catalysts studied in a stagnation-flow reactor. Chemical Engineering Science. 2013;89:171-184.