

Clustering-enhanced deep learning method for computation of full detailed thermochemical states via solver-based adaptive sampling

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Supporting Information Available

Empirical threshold choosing experiment: an example for C_2H_4 case

Table S1 presents the loss function values obtained after training for the C_2H_4 case, with four different clusters (the optimal cluster number as highlighted in the paper). As mentioned in Section 4.1, the thresholds for clustering are chosen empirically. The table displays the training/validation/test loss functions, represented as Mean Squared Error (MSE) errors, for each cluster. For Cluster 0, which represents the gas burn-up region with low chemical reactions, the training errors are significantly larger when using a smaller threshold. This is because of the numerical instabilities which are not physically meaningful. On the other hand, when selecting a threshold above the highest value where numerical instabilities occur, the impact of the threshold for training performance becomes insignificant. In this study, when comparing the thresholds $\epsilon = 10^{-10}$ and $\epsilon = 10^{-12}$, the latter seems to yield better training results. The mean squared error in Cluster 2 is notably lower for the threshold $\epsilon = 10^{-12}$ compared to the threshold $\epsilon = 10^{-10}$.

Table S1: Loss values obtained for cases of C_2H_4 training with different threshold in datasets.

	cluster 0	cluster 1	cluster 2	cluster 3
threshold 10^{-10}				
training loss	2.18×10^{-6}	3.05×10^{-7}	3.04×10^{-6}	2.48×10^{-6}
validation loss	2.46×10^{-6}	2.98×10^{-7}	3.46×10^{-6}	2.57×10^{-6}
test loss	2.46×10^{-6}	3.44×10^{-7}	3.36×10^{-6}	2.65×10^{-6}
threshold 10^{-12}				
training loss	1.87×10^{-6}	3.43×10^{-7}	3.44×10^{-7}	3.43×10^{-6}
validation loss	1.91×10^{-6}	3.67×10^{-7}	3.31×10^{-7}	3.55×10^{-6}
test loss	2.01×10^{-6}	3.70×10^{-7}	3.88×10^{-7}	3.55×10^{-6}
threshold 10^{-15}				
training loss	9.64×10^{-1}	7.20×10^{-7}	6.03×10^{-8}	1.13×10^{-6}
validation loss	5.00×10^{-3}	8.63×10^{-7}	6.35×10^{-8}	1.46×10^{-6}
test loss	6.50×10^{-2}	7.30×10^{-7}	6.85×10^{-8}	4.87×10^{-6}
threshold 10^{-20}				
training loss	3.30×10^{-2}	1.76×10^{-5}	5.16×10^{-8}	8.62×10^{-6}
validation loss	4.90×10^{-2}	7.71×10^{-6}	5.37×10^{-8}	1.49×10^{-6}
test loss	1.35×10^{-1}	9.97×10^{-6}	5.80×10^{-8}	2.81×10^{-5}

0D simulation using DNN models for chemical species

Figures S1, S2, and S3 present the inference simulations for several chemical species in the reaction system, serving as additional examples for Section 5.4. The simulations are conducted with initial conditions $T_{01} = 1620.0K$, $\phi_1 = 0.75$, and $T_{02} = 1790.0K$, $\phi_2 = 1.45$, and the resulting trajectories correspond to the CVODE simulation results. On the other hand, Figures S4, S5, and S6 display the trajectories in logarithmic scales, where the total dynamic systems are separated by the clustering algorithm.

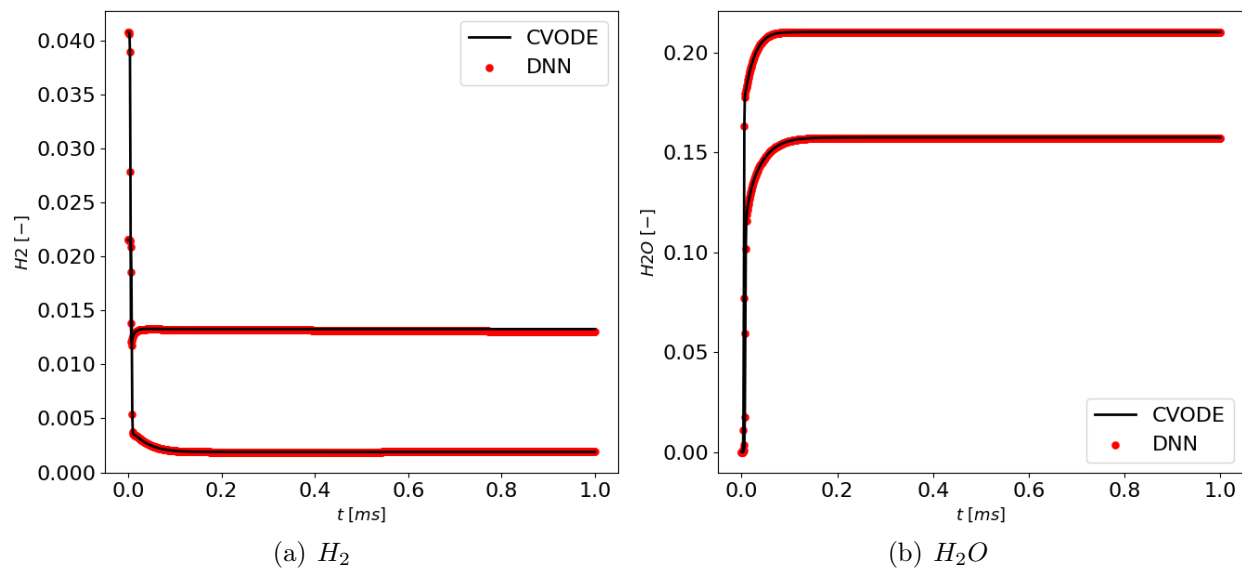


Figure S1: Continuous inference simulation for H_2/air case with 2 trajectories: $T_{01} = 1620.0K, \phi_1 = 0.75$ and $T_{02} = 1790.0K, \phi_2 = 1.45$.

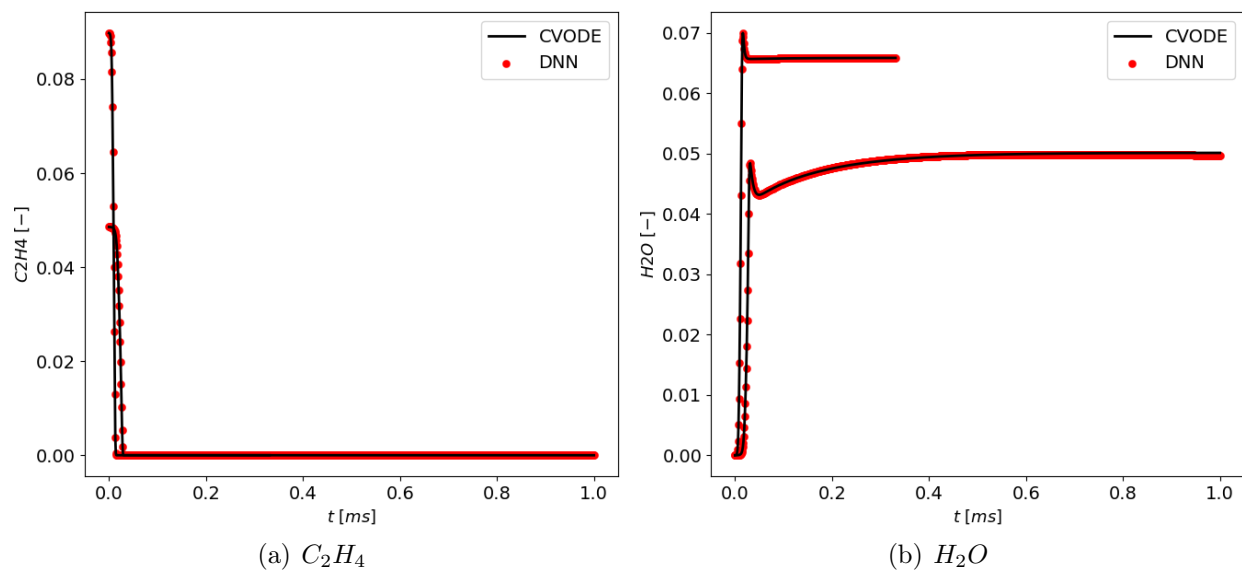


Figure S2: Continuous inference simulation for C_2H_4/air case with 2 trajectories: $T_{01} = 1620.0K, \phi_1 = 0.75$ and $T_{02} = 1790.0K, \phi_2 = 1.45$.

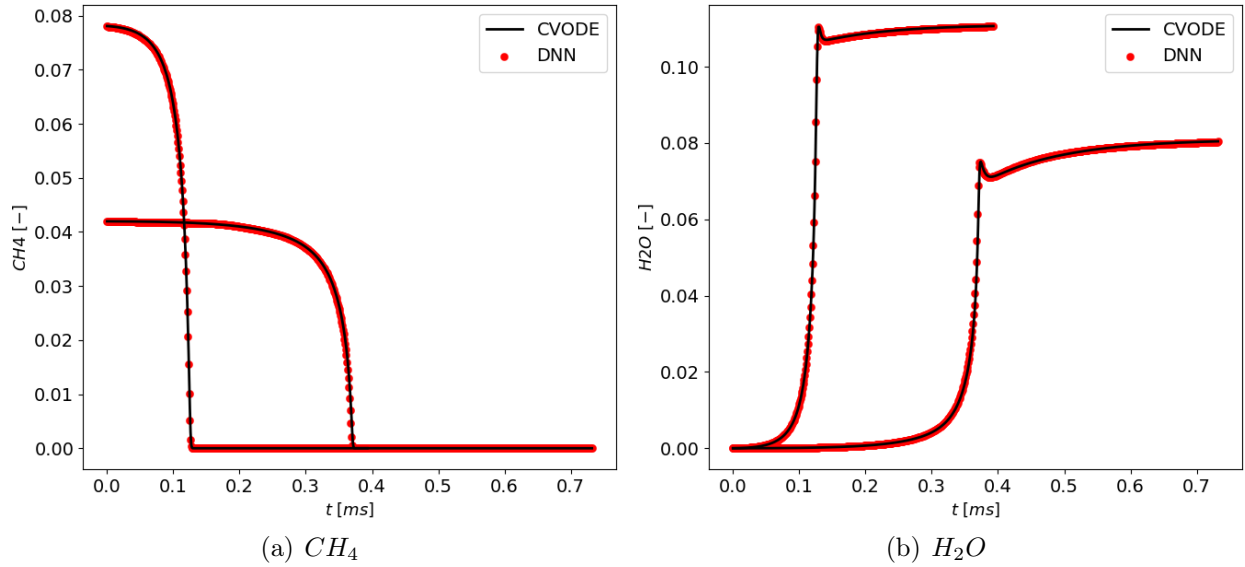


Figure S3: Continuous inference simulation for CH_4/air case with 2 trajectories: $T_{01} = 1620.0K, \phi_1 = 0.75$ and $T_{02} = 1790.0K, \phi_2 = 1.45$.

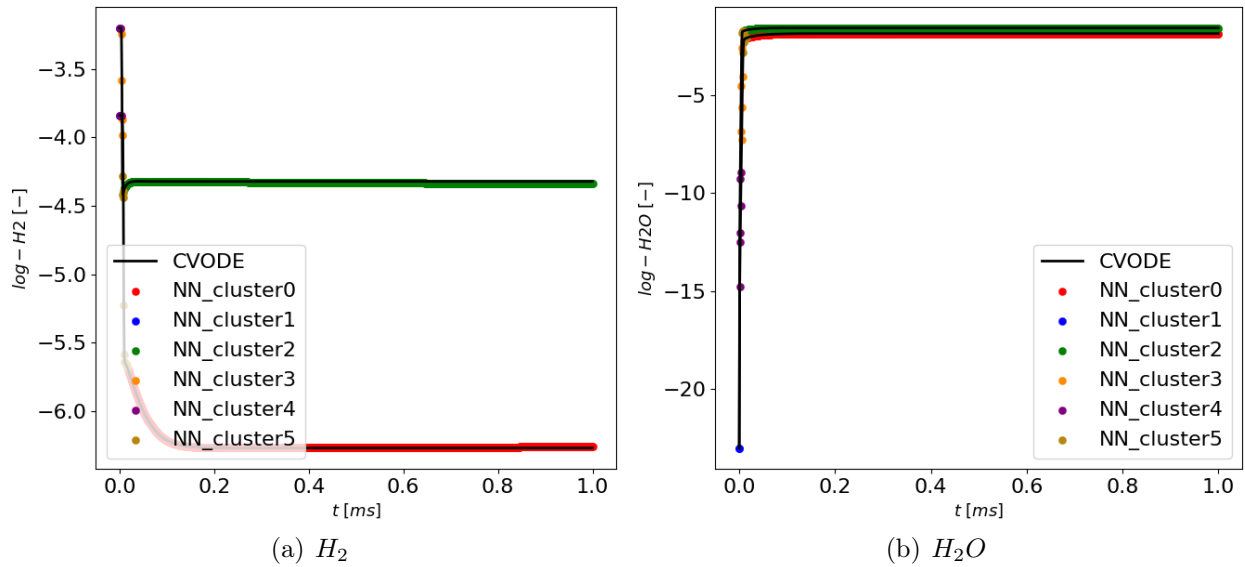


Figure S4: Continuous inference simulation in logarithmic scale for H_2/air case with 2 trajectories: $T_{01} = 1620.0K, \phi_1 = 0.75$ and $T_{02} = 1790.0K, \phi_2 = 1.45$.

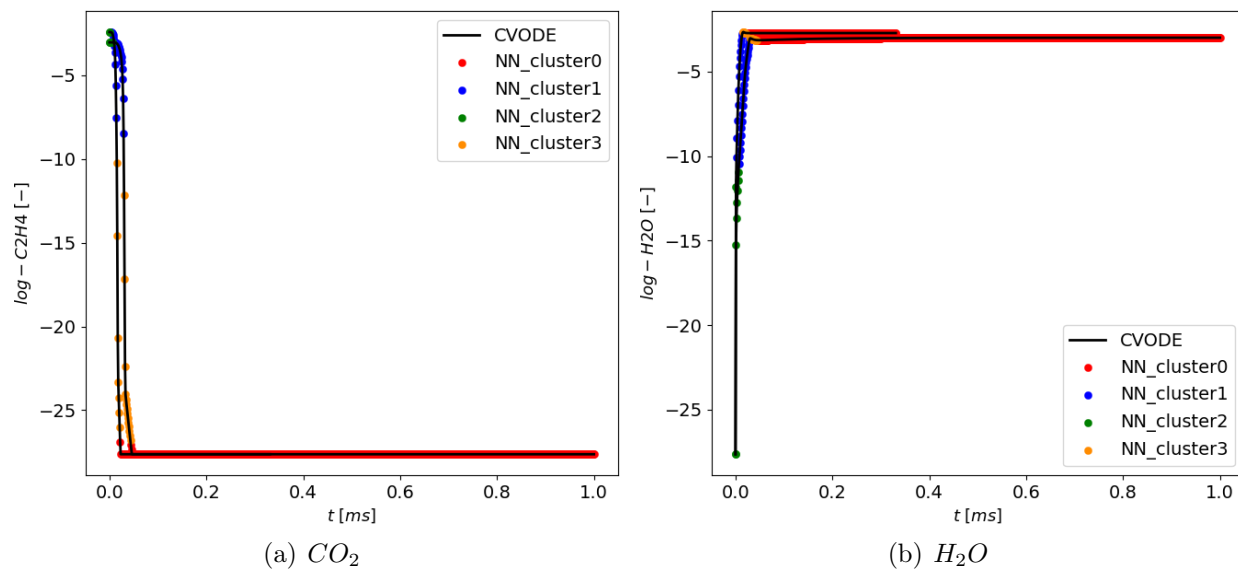


Figure S5: Continuous inference simulation in logarithmic scale for C_2H_4/air case with 2 trajectories: $T_{01} = 1620.0K, \phi_1 = 0.75$ and $T_{02} = 1790.0K, \phi_2 = 1.45$.

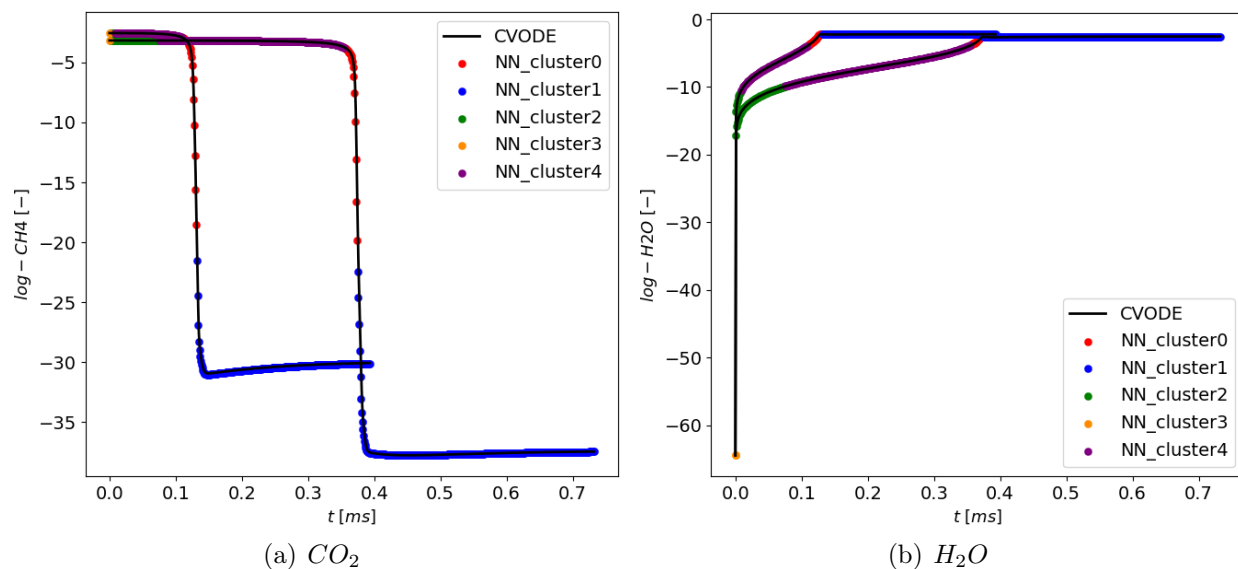


Figure S6: Continuous inference simulation in logarithmic scale for CH_4/air case with 2 trajectories: $T_{01} = 1620.0K, \phi_1 = 0.75$ and $T_{02} = 1790.0K, \phi_2 = 1.45$.