Micro-kinetic Modeling of Temporal Analysis of Products Data Using Kinetics-informed Neural Networks

Supplementary Information

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S1 Multi-pulse ideal scenario

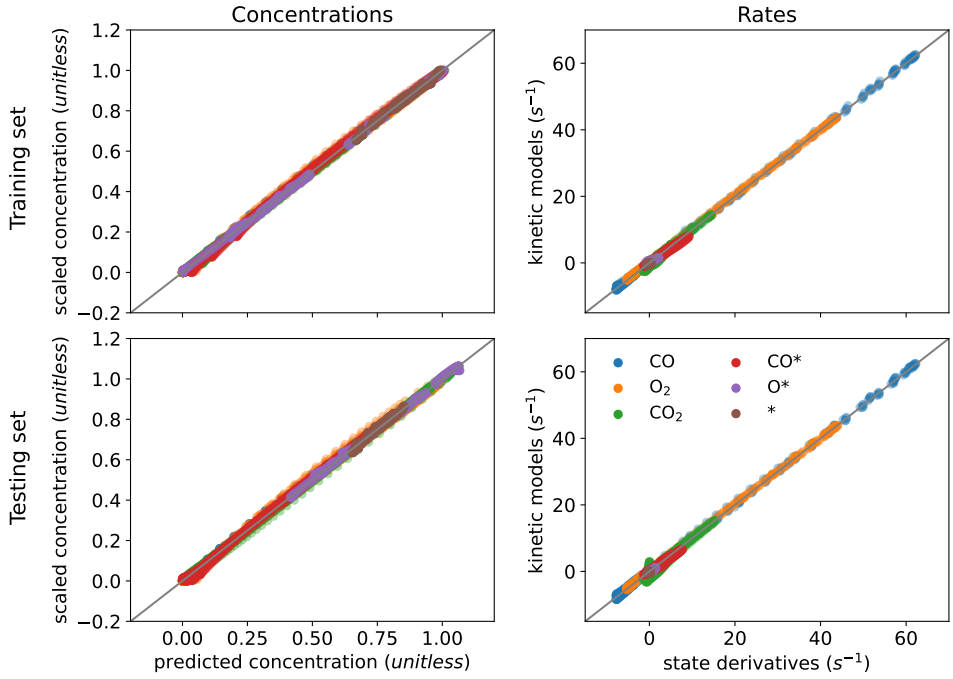

Figure S1: Training (top) and testing (bottom) performance on the concentration prediction and kinetic model fitting for multi-pulse ideal scenario.

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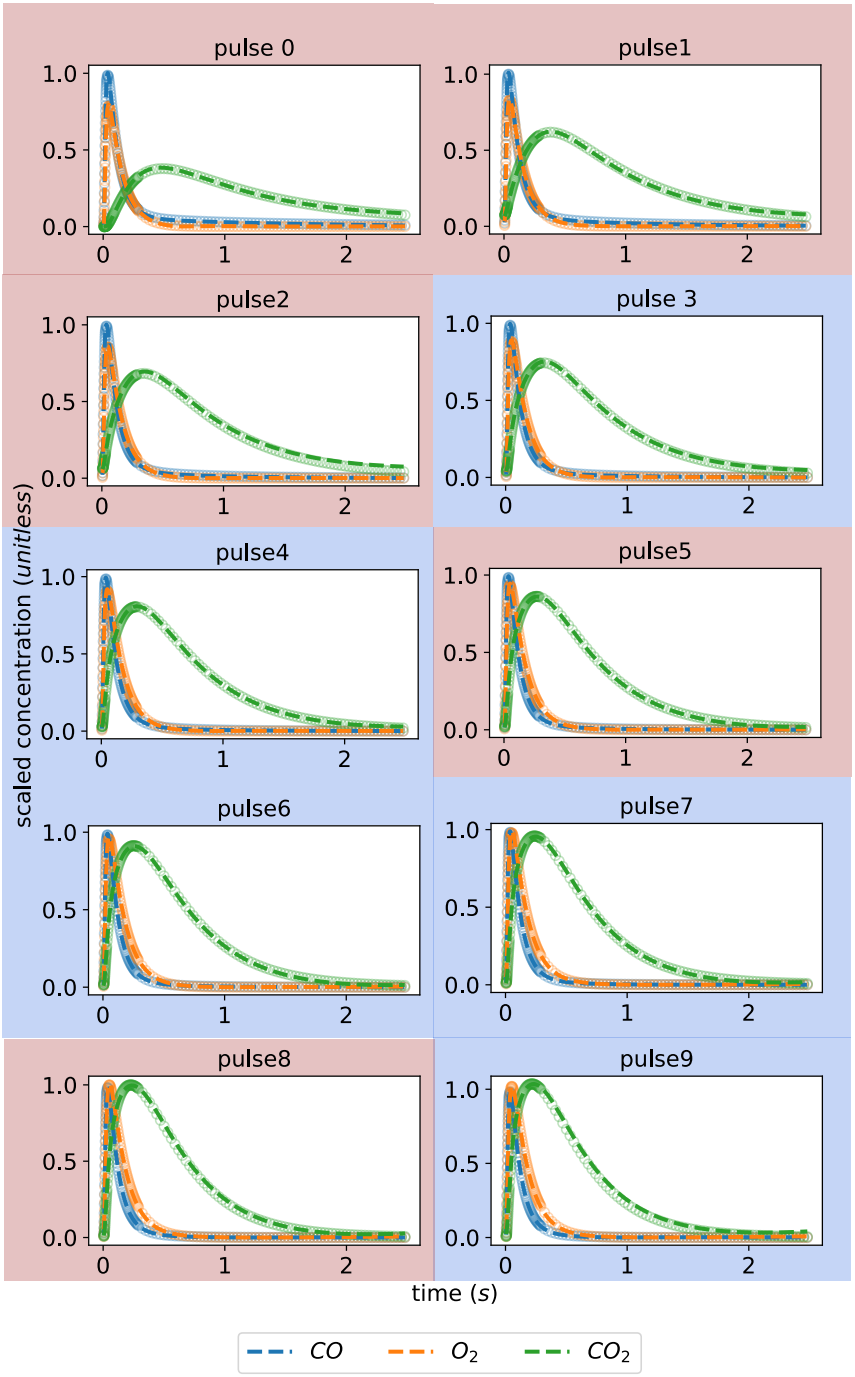


Figure S2: KINN's predicted scaled concentration (dash line) and target ground truth value (dot) for the training set (red background) and interpolating to the testing set (blue background) for gas species.

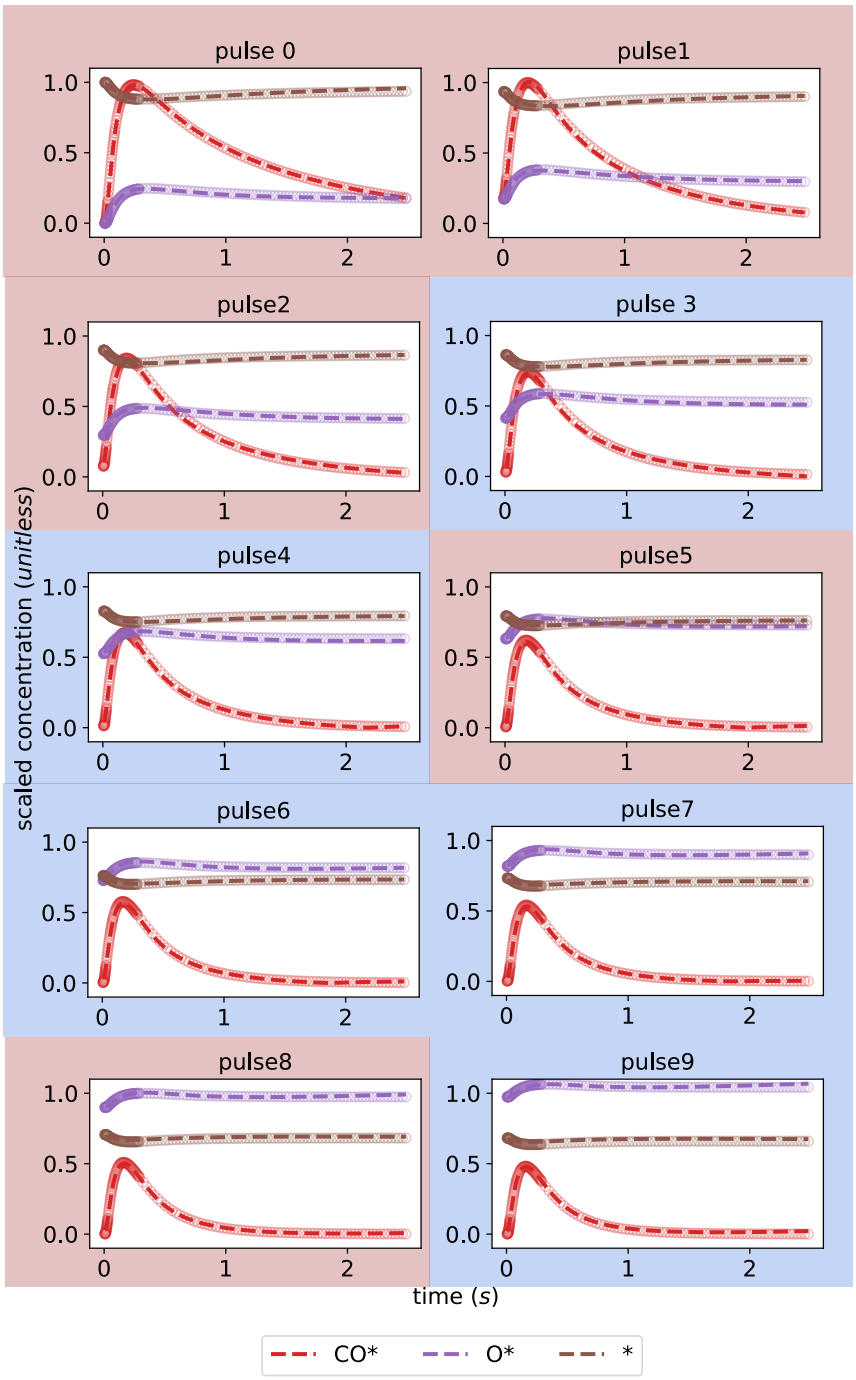


Figure S3: KINN's predicted scaled concentration (dash line) and target ground truth value (dot) for the training set (red background) and interpolating to the testing set (blue background) for adspecies.

S2 Multi-pulse practical scenario

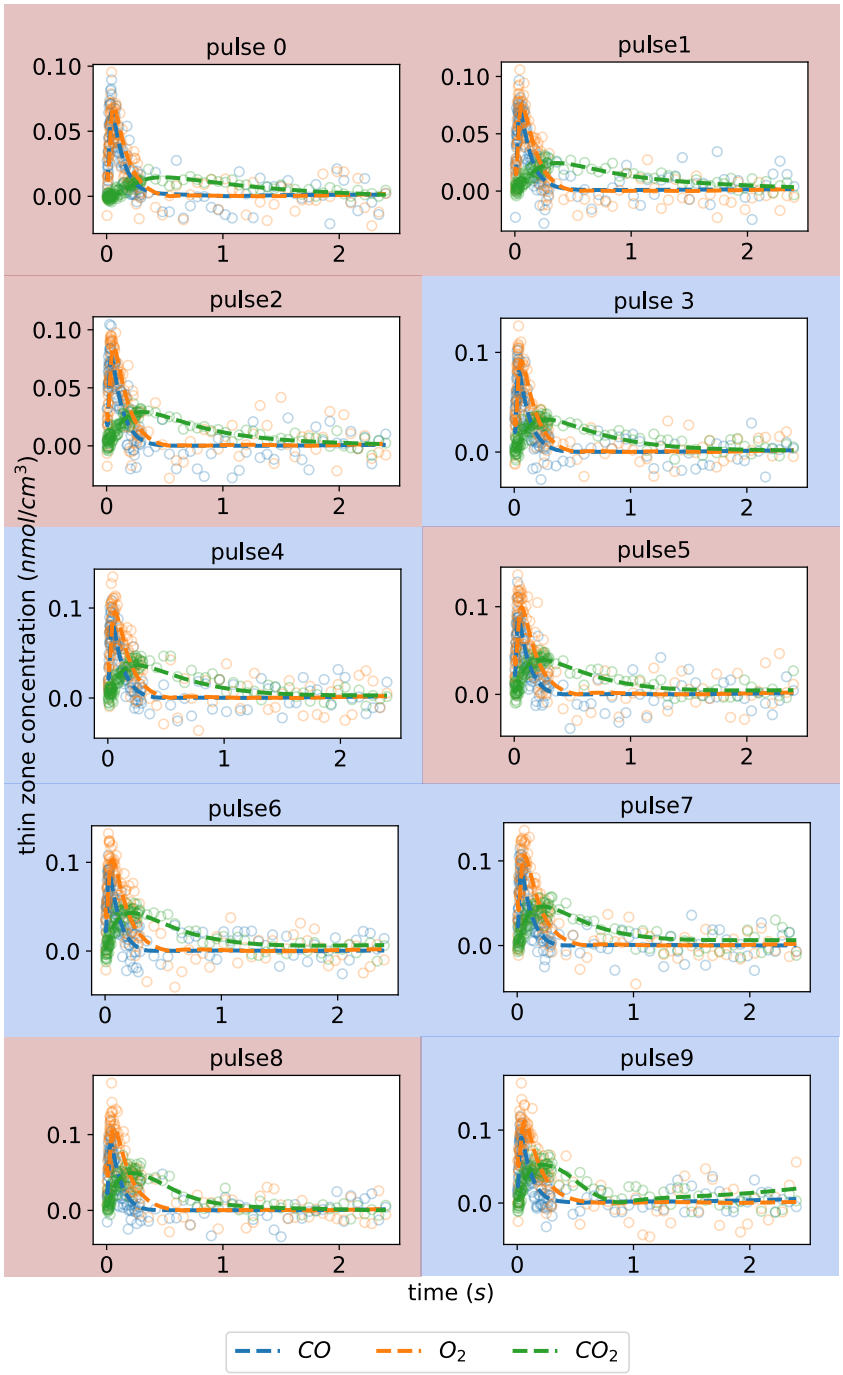


Figure S4: KINN's predicted scaled concentration (dash line) and target ground truth value (dot) for the training set (red background) and interpolating to the testing set (blue background) for gas species. The discontinuity at 0 happens because the absolute value is taken at the output layer as we consider negative concentration is invalid, but the continuous states goes negative because of the noise. A use of softplus/swish layer can solve this discontinuity by test.

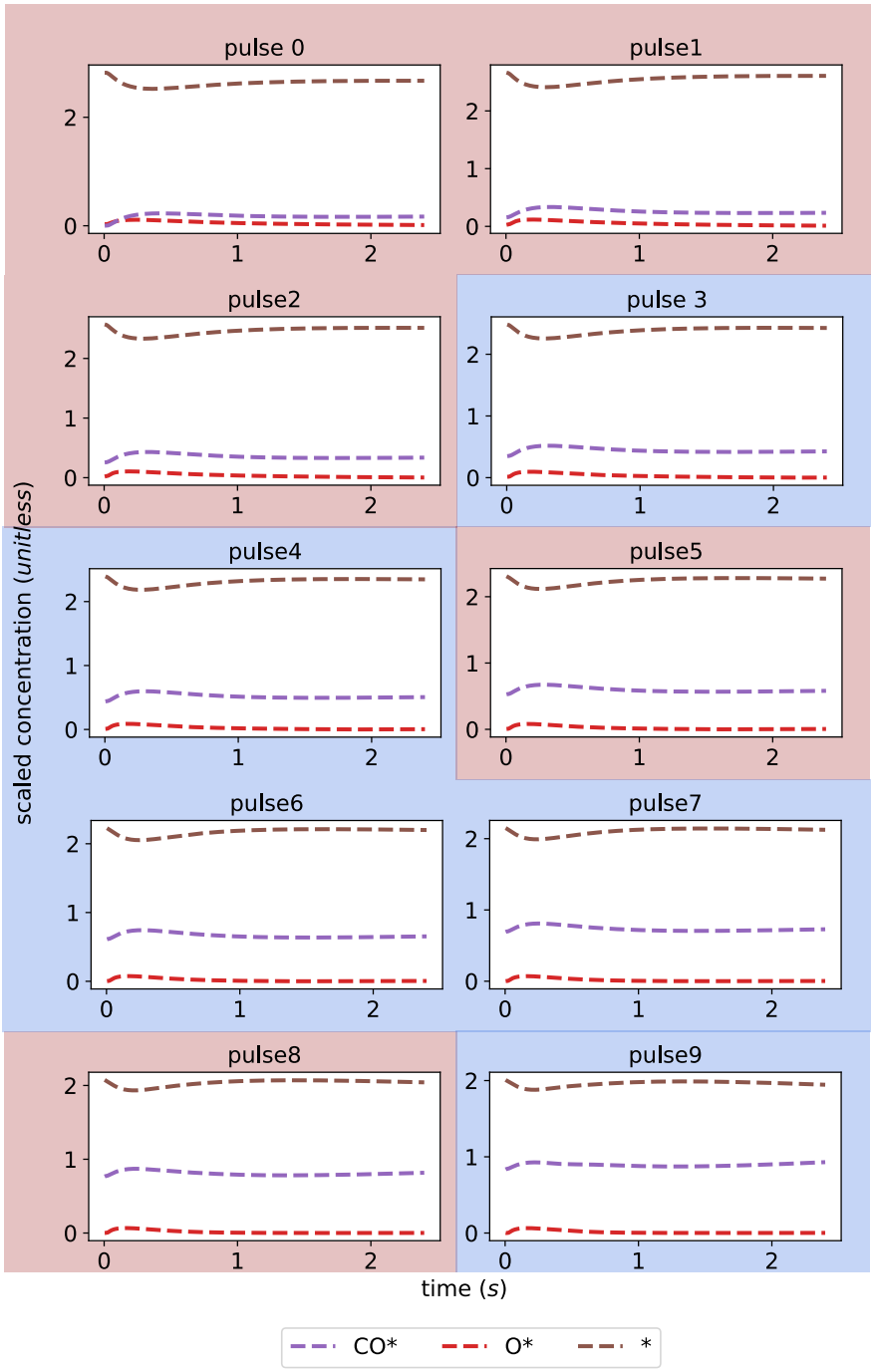


Figure S5: KINN's predicted scaled concentration (dash line) for the training set (red background) and interpolating to the testing set (blue background) for adspecies. The ground truth concentrations are not available in practical scenario, so only the predicted values are shown. Compared to Figure S3, the scaled concentrations are different because they are scaled with different values. In the ideal case, the adspecies concentrations are rescaled with the maximum ground truth values of each species; in the practical case, they are rescaled with the maximum atomic uptake value.

S2.1 Multi-pulse training effect on kinetic model quality

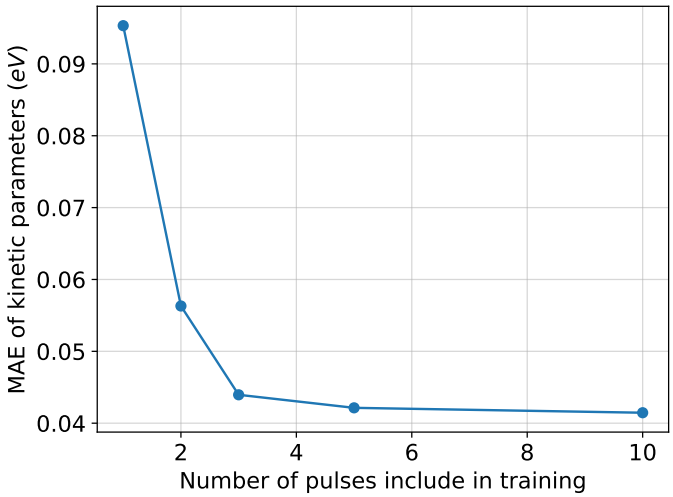


Figure S6: MAE of kinetic parameters as a function of the number of pulses included in training for the practical multi-pulse scenario. Note that the MAE is higher than reported in the main text since fewer epochs were used and the α value was not as carefully optimized.

S3 Multi-pulse analysis compared to differential algebraic programming

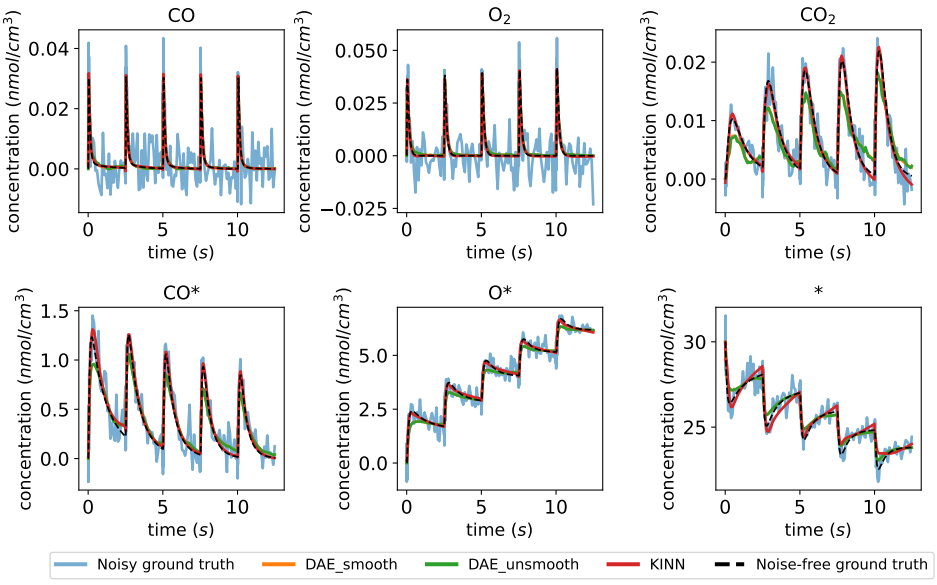


Figure S7: Concentration fitting of DAE and the KINN at 0.5σ noise level.

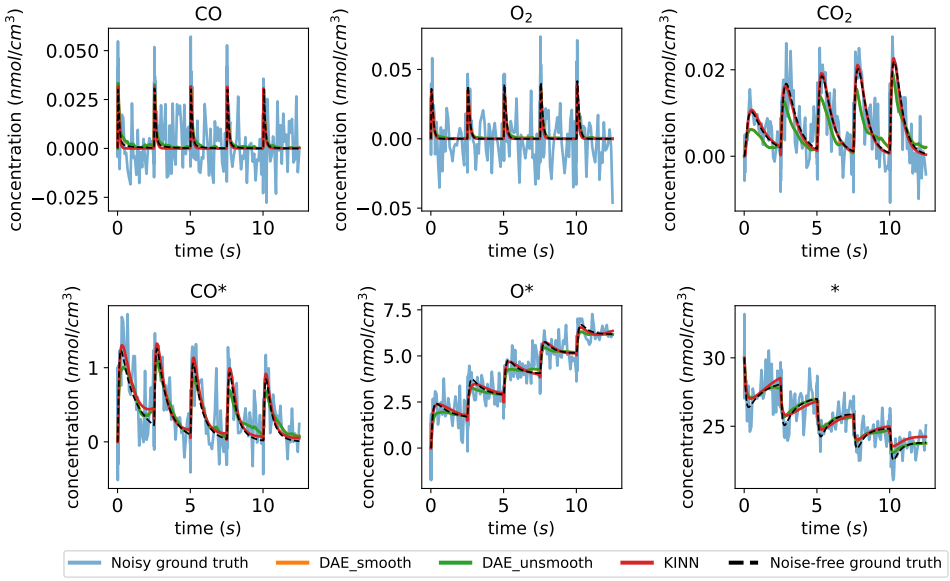


Figure S8: Concentration fitting of DAE and the KINN at 1.0σ noise level.

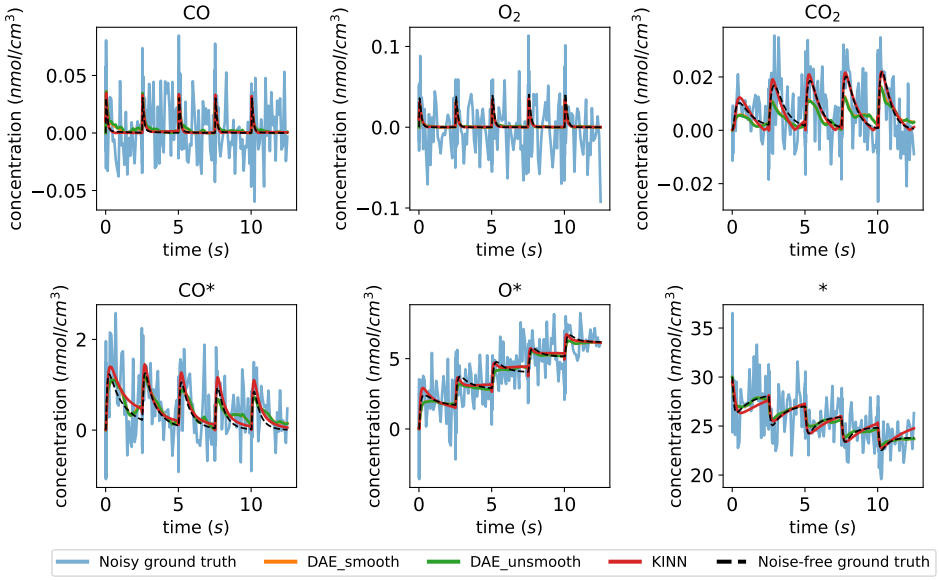


Figure S9: Concentration fitting of DAE and the KINN at 2.0σ noise level.

Parameter	KINN	DAE smooth	DAE unsmooth
k_1	10.90	11.60	11.63
k_{-1}	0.129	0.503	0.593
k_2	0.348	0.264	0.263
k_3	0.434	0.625	0.630
k_{-3}	0.020	0.115	0.117
k_4	13.36	10.32	10.19

Table S1: Kinetic parameters extracted from KINNs and DAE on 0.5σ noise level.

Parameter	KINN	DAE smooth	DAE unsmooth
k_1	9.587	10.37	10.40
k_{-1}	0.175	0.793	1.009
k_2	0.322	0.279	0.277
k_3	0.469	19.57	–
k_{-3}	0.029	8.069	–
k_4	10.02	20.92	21.71

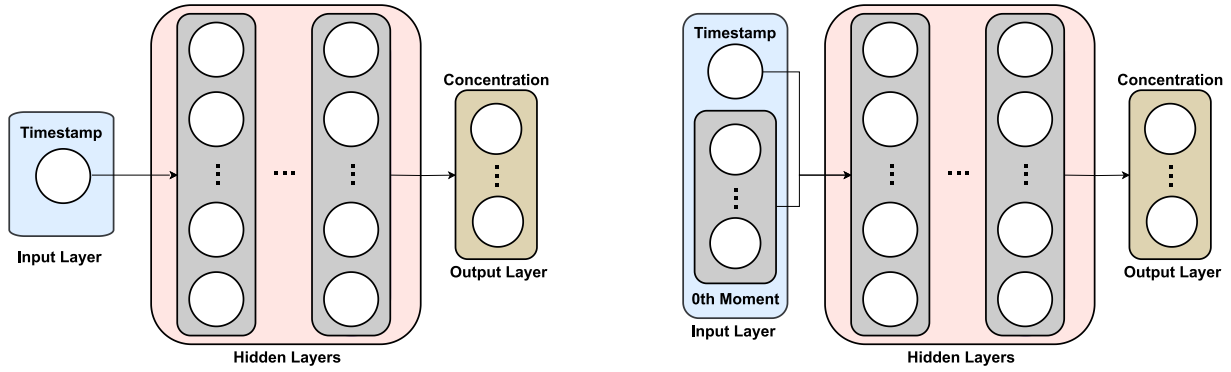
Table S2: Kinetic parameters extracted from KINNs and DAE on 1.0σ noise level.

Parameter	KINN	DAE smooth	DAE unsmooth
k_1	10.07	9.500	9.647
k_{-1}	0.416	1.354	1.780
k_2	0.378	0.312	0.310
k_3	0.290	–	–
k_{-3}	0.021	–	–
k_4	9.761	29.91	32.01

Table S3: Kinetic parameters extracted from KINNs and DAE on 2.0σ noise level.

S4 KINNs Setup

The KINNs stepup and hyperparameters at the ending state are provided in this section. All NN parameters are available on github in .npz format.



(a) Single-pulse

(b) Multi-pulse

Figure S10: Conceptual diagram for the NN structure used for (a) single-pulse and (b) multi-pulse cases.

S4.1 Single-pulse ideal scenario

Activation function	swish
NN structure	[1, 8, 6]
NN parameters initialization scale	1e-2
Model parameters initialization scale	1e-5
Step size	1e-3
Ending α	1

S4.2 Multi-pulse ideal scenario

Activation function	swish
NN structure	[4, 10, 10, 6]
NN parameters initialization scale	1e-2
Model parameters initialization scale	1e-5
Step size	1e-3
Ending α	1e-3

S4.3 Multi-pulse practical scenario

Activation function	swish
NN structure	[4, 10, 10, 6]
NN parameters initialization scale	1e-2
Model parameters initialization scale	1e-5
Step size	1e-3
Ending α	1e-3
Ending β	1

S5 Code

The full code of this work is available at `https://github.com/medford-group/kinn-tap`, Zenodo DOI: 10.5281/zenodo.13754686.