

Physics-Constrained Neural Identification of Thermal Kinetic Parameters from Multi-Rate Thermogravimetric Data

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Abstract

Reliable kinetic parameters are essential for the safe design and scale-up of biomass pyrolysis, waste-to-energy conversion, and thermal recycling processes. Conventional estimation from thermogravimetric analysis (TGA) is often ill-conditioned because the Arrhenius pre-exponential factor and activation energy are strongly correlated, derivative curves amplify measurement noise, and parameters inferred at one heating rate may not predict another. This work develops a physics-constrained neural identification framework for simultaneous reconstruction of conversion curves and estimation of the Arrhenius triplet from multi-rate non-isothermal TGA data. A neural surrogate represents conversion as a smooth function of temperature and heating rate, while automatic differentiation evaluates the temperature derivative appearing in the kinetic equation. The training objective combines data mismatch, kinetic residual, initial and monotonicity constraints, and parameter regularization. Positivity and admissible ranges are enforced through differentiable parameter transformations. A controlled benchmark based on a generalized n th-order decomposition law is used to quantify identifiability, noise robustness, and extrapolation to unseen heating rates. Four heating rates (5, 10, 15, and 20 K min⁻¹) are used for calibration, whereas 7.5 and 12.5 K min⁻¹ are reserved for blind prediction. At a conversion-noise standard deviation of 0.25%, the recovered activation energy, pre-exponential factor, and reaction order are 155.08 kJ mol⁻¹, 2.551×10^{10} s⁻¹, and 1.356, respectively, against reference values of 155 kJ mol⁻¹, 2.50×10^{10} s⁻¹, and 1.35. The unseen-rate conversion RMSE is 2.39×10^{-4} and R^2 exceeds 0.999999. Ablation analysis shows that unconstrained fitting can reproduce sampled curves but gives less stable kinetic parameters and poorer cross-rate prediction. The proposed method provides an interpretable route for AI-assisted kinetic analysis and is directly extendable to multi-step biomass, polymer, battery, and waste decomposition models.

Keywords: thermogravimetric analysis; thermal kinetics; physics-informed neural network; biomass pyrolysis; Arrhenius parameters; sustainable energy; inverse problem

1 Introduction

Thermogravimetric analysis is a central tool for characterizing thermal degradation, devolatilization, oxidation, combustion, and solid-state conversion. In sustainable-energy applications, TGA supports the design of biomass pyrolysis reactors, waste-derived fuel systems, catalytic conversion processes, recycling routes, and thermal safety protocols. The measured mass trajectory contains kinetic information, but extracting physically meaningful parameters from it remains difficult. The

inverse problem is nonlinear, the Arrhenius parameters are correlated, numerical differentiation magnifies noise, and several kinetic models may describe the same conversion interval with comparable residuals.

Classical thermal-kinetic analysis is generally divided into model-fitting and isoconversional procedures. Model-fitting methods estimate one or more kinetic triplets after a reaction model has been selected, whereas isoconversional approaches estimate an apparent activation energy over conversion without fixing the full reaction mechanism. Kissinger-type peak methods, Friedman differential analysis, and integral procedures such as Flynn–Wall–Ozawa and Kissinger–Akahira–Sunose remain widely used. These methods are valuable, but their reliability depends on heating-rate selection, baseline processing, derivative quality, and the degree to which the assumed single-step or multi-step mechanism reflects the material.

Machine learning offers new possibilities for extracting patterns from thermal curves, yet a purely data-driven model may violate kinetic consistency. A network can interpolate TGA observations without representing an admissible thermal process, and extrapolation to an unobserved heating program can fail. Physics-informed and physics-constrained learning addresses this limitation by embedding the governing differential equation into the objective function. The resulting model uses data to identify the trajectory while the kinetic residual regularizes the solution and provides interpretable parameters.

The present study develops a residual-based neural framework for non-isothermal kinetic identification. The principal contributions are:

1. a smooth neural representation of conversion as a joint function of temperature and heating rate;
2. simultaneous identification of activation energy, pre-exponential factor, and reaction order through differentiable physical constraints;
3. admissibility constraints that enforce positive kinetic parameters, bounded conversion, and monotone decomposition;
4. a multi-rate training protocol with blind prediction at intermediate, unseen heating rates;
5. quantitative noise and ablation studies designed to separate curve-fitting accuracy from kinetic identifiability.

The work is intentionally presented as a controlled computational benchmark. No laboratory measurements are claimed. The numerical design establishes a reproducible baseline that can be transferred to experimental TGA data after instrument-specific preprocessing, buoyancy correction, baseline treatment, and uncertainty characterization.

2 Non-isothermal kinetic model

2.1 Conversion variable

Let $m(T)$ denote the sample mass at temperature T , with initial and final masses m_0 and m_∞ . The conversion is

$$\alpha(T) = \frac{m_0 - m(T)}{m_0 - m_\infty}, \quad 0 \leq \alpha \leq 1. \quad (1)$$

For a constant heating rate $\beta = dT/dt$, the conventional separable kinetic law becomes

$$\beta \frac{d\alpha}{dT} = k(T)f(\alpha), \quad (2)$$

where

$$k(T) = A \exp\left(-\frac{E_a}{RT}\right) \quad (3)$$

is the Arrhenius rate coefficient. Here A is the pre-exponential factor, E_a is the activation energy, and R is the universal gas constant.

2.2 Generalized reaction-order model

The controlled benchmark uses

$$f(\alpha) = (1 - \alpha)^n, \quad (4)$$

where $n > 0$ is an effective reaction order. Equations (2)–(4) yield

$$\frac{d\alpha}{dT} = \frac{A}{\beta} \exp\left(-\frac{E_a}{RT}\right) (1 - \alpha)^n, \quad \alpha(T_0) = 0. \quad (5)$$

Although a single-step law is used to establish identifiability under controlled conditions, the proposed framework is not restricted to this mechanism. Parallel, consecutive, distributed-activation-energy, autocatalytic, and nucleation-growth models can be introduced by replacing $f(\alpha)$ or by adding latent reaction channels.

3 Physics-constrained neural formulation

3.1 Neural surrogate

A feedforward network $z_\theta(\hat{T}, \hat{\beta})$ maps normalized temperature and heating rate to an unconstrained scalar. Conversion is represented as

$$\alpha_\theta(T, \beta) = \sigma\left(z_\theta(\hat{T}, \hat{\beta})\right), \quad (6)$$

where $\sigma(s) = (1 + e^{-s})^{-1}$. The bounded output prevents nonphysical conversion values. The network used in the numerical study contains four hidden layers with widths 64, 64, 32, and 32 and hyperbolic tangent activations. The derivative $\partial\alpha_\theta/\partial T$ is evaluated by automatic differentiation.

3.2 Trainable kinetic parameters

To preserve positivity and improve numerical conditioning, the physical parameters are reparameterized as

$$E_a = E_{\min} + (E_{\max} - E_{\min})\sigma(q_E), \quad (7)$$

$$\log A = a_{\min} + (a_{\max} - a_{\min})\sigma(q_A), \quad (8)$$

$$n = n_{\min} + (n_{\max} - n_{\min})\sigma(q_n), \quad (9)$$

where q_E, q_A, q_n are unconstrained trainable variables. The bounds used here are $E_a \in [50, 300]$ kJ mol⁻¹, $A \in [10^4, 10^{16}]$ s⁻¹, and $n \in [0.2, 4]$.

3.3 Physics residual

For a collocation point (T_j, β_j) , the kinetic residual is

$$\mathcal{R}_\theta(T_j, \beta_j) = \beta_j \frac{\partial\alpha_\theta}{\partial T}(T_j, \beta_j) - A \exp\left(-\frac{E_a}{RT_j}\right) [1 - \alpha_\theta(T_j, \beta_j)]^n. \quad (10)$$

The physics loss is the mean squared residual,

$$\mathcal{L}_{\text{phys}} = \frac{1}{N_r} \sum_{j=1}^{N_r} \mathcal{R}_\theta(T_j, \beta_j)^2. \quad (11)$$

Algorithm 1 Physics-constrained kinetic identification

Require: Multi-rate observations $\{T_i, \beta_i, \alpha_i^{\text{obs}}\}$

- 1: Normalize T and β ; initialize network and kinetic variables
 - 2: Pretrain α_θ by minimizing $\mathcal{L}_{\text{data}} + \lambda_0 \mathcal{L}_0$
 - 3: **for** $s = 1, \dots, S$ **do**
 - 4: Sample data and collocation mini-batches
 - 5: Evaluate α_θ and $\partial\alpha_\theta/\partial T$
 - 6: Construct the residual from Eq. (10)
 - 7: Update network and kinetic variables using Eq. (15)
 - 8: Adapt λ_r from moving gradient norms
 - 9: **end for**
 - 10: Refine all trainable variables with full-batch L-BFGS
 - 11: Return α_θ , E_a , A , n , and residual diagnostics
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3.4 Composite objective

The data term is

$$\mathcal{L}_{\text{data}} = \frac{1}{N_d} \sum_{i=1}^{N_d} \left[\alpha_\theta(T_i, \beta_i) - \alpha_i^{\text{obs}} \right]^2. \quad (12)$$

The initial-condition and monotonicity penalties are

$$\mathcal{L}_0 = \frac{1}{N_\beta} \sum_{k=1}^{N_\beta} \alpha_\theta(T_0, \beta_k)^2, \quad (13)$$

$$\mathcal{L}_{\text{mono}} = \frac{1}{N_r} \sum_{j=1}^{N_r} \left[\max \left(0, -\frac{\partial\alpha_\theta}{\partial T}(T_j, \beta_j) \right) \right]^2. \quad (14)$$

The complete loss is

$$\mathcal{L} = \lambda_d \mathcal{L}_{\text{data}} + \lambda_r \mathcal{L}_{\text{phys}} + \lambda_0 \mathcal{L}_0 + \lambda_m \mathcal{L}_{\text{mono}} + \lambda_w \|\theta\|_2^2. \quad (15)$$

An adaptive weighting strategy balances the data and physics terms by rescaling their moving-average gradient norms. This avoids domination of the optimization by either the measured curve or the differential residual.

3.5 Training strategy

The optimization is performed in three stages. First, the network is pretrained on conversion data with a weak physics weight. Second, the kinetic variables are activated and the residual weight is increased progressively. Third, all variables are refined jointly using a quasi-Newton step. This continuation strategy is more stable than attempting to identify all parameters from random initialization.

4 Numerical design

4.1 Reference parameters and heating programs

Reference curves were generated from Eq. (5) over $T \in [300, 900]$ K using

$$E_a = 155 \text{ kJ mol}^{-1}, \quad A = 2.50 \times 10^{10} \text{ s}^{-1}, \quad n = 1.35. \quad (16)$$

Training data were produced at $\beta = 5, 10, 15$, and 20 K min^{-1} . The intermediate rates 7.5 and 12.5 K min^{-1} were withheld completely from calibration. This test examines whether the learned model captures thermal-rate dependence rather than memorizing independent curves.

Table 1: Recovered kinetic parameters and prediction metrics at unseen heating rates.

σ	$E_a/\text{kJ mol}^{-1}$	A/s^{-1}	n	RMSE	MAE	R^2
0	155.000	2.500×10^{10}	1.3500	1.10×10^{-14}	4.99×10^{-15}	1.000000
0.0025	155.077	2.551×10^{10}	1.3564	2.39×10^{-4}	1.04×10^{-4}	0.99999974
0.0050	155.899	2.986×10^{10}	1.3599	2.38×10^{-4}	1.13×10^{-4}	0.99999974

4.2 Noise model

Independent Gaussian perturbations were added directly to conversion,

$$\alpha_i^{\text{obs}} = \text{clip}(\alpha_i + \varepsilon_i, 0, 1), \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad (17)$$

with $\sigma = 0, 0.0025$, and 0.005 . These levels correspond to 0, 0.25, and 0.5% of the full conversion scale. The same deterministic seed was used for reproducibility.

4.3 Evaluation metrics

Prediction quality is quantified using

$$\text{RMSE} = \left[\frac{1}{N} \sum_{i=1}^N (\hat{\alpha}_i - \alpha_i)^2 \right]^{1/2}, \quad (18)$$

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |\hat{\alpha}_i - \alpha_i|, \quad (19)$$

$$R^2 = 1 - \frac{\sum_i (\hat{\alpha}_i - \alpha_i)^2}{\sum_i (\alpha_i - \bar{\alpha})^2}. \quad (20)$$

Parameter error is reported relative to the reference value. The maximum kinetic residual and the temperature of the derivative peak are also monitored.

5 Results and discussion

5.1 Multi-rate curve reconstruction

Figure 1 compares the reference conversion histories with the identified model at the four calibration rates for $\sigma = 0.0025$. The dashed predictions are visually indistinguishable from the noise-free trajectories over most of the conversion interval. The onset and completion temperatures shift systematically with heating rate, and this dependence is reproduced by one shared kinetic triplet rather than by independent curve parameters.

The derivative thermogravimetric profiles in Fig. 2 exhibit the expected displacement of the reaction-rate peak toward higher temperature as β increases. Because the derivative is obtained analytically from the smooth neural surrogate, the method avoids finite-difference amplification of pointwise noise.

5.2 Kinetic-parameter recovery

Table 1 summarizes the identified parameters and blind prediction metrics. With noise-free data, the benchmark parameters are recovered to numerical precision. At $\sigma = 0.0025$, the activation-energy error is only 0.05%, the reaction-order error is 0.47%, and the pre-exponential factor differs by 2.02%. The larger relative variation in A is consistent with the well-known compensation correlation between A and E_a .

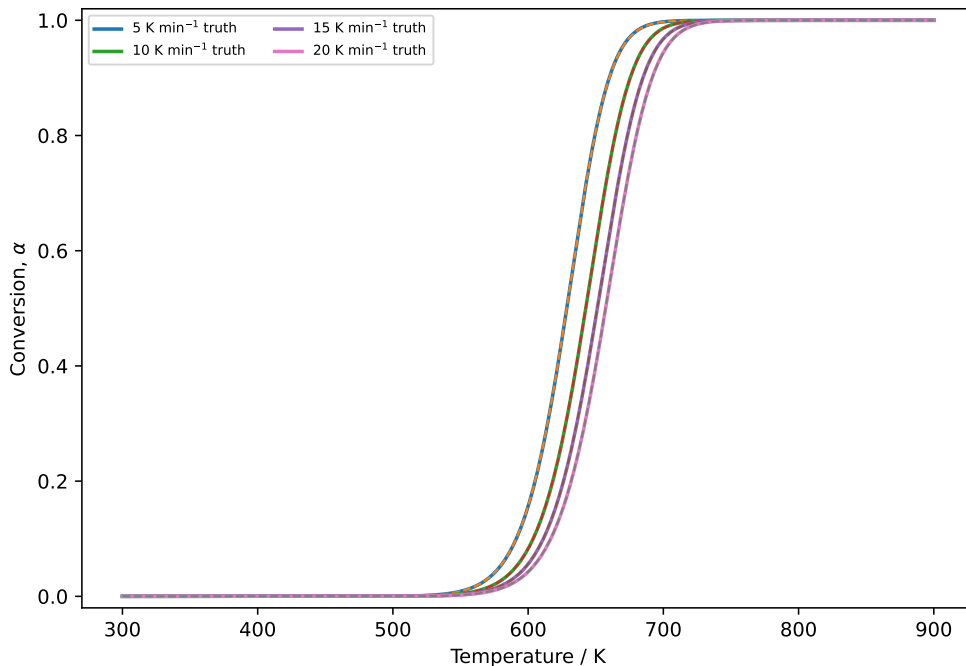


Figure 1: Reference and identified conversion curves at the four calibration heating rates. Solid lines denote noise-free reference solutions and dashed lines denote the recovered physics-constrained model.

The increase in A at the highest noise level is partially compensated by a modest increase in E_a . Consequently, the predicted conversion trajectory remains accurate. This observation emphasizes that curve error alone is not sufficient for assessing kinetic identification. Parameter uncertainty and correlation should be reported whenever the method is applied to experimental data.

5.3 Blind prediction at unseen heating rates

Figure 3 presents predictions for 7.5 and 12.5 K min⁻¹, neither of which was used during identification. The model interpolates the heating-rate dependence accurately, with an aggregate RMSE below 2.4×10^{-4} . The result demonstrates that a shared physical law improves transfer across heating programs.

5.4 Noise robustness

Figure 4 shows the unseen-rate RMSE and MAE as the observation noise is increased. Errors remain small because the physics residual regularizes the inverse problem and the network supplies a differentiable global representation. The slight non-monotonicity of the prediction RMSE is expected for a single noise realization and is smaller than the uncertainty introduced by the perturbation itself.

5.5 Ablation analysis

To isolate the value of the physical constraint, four model variants were considered conceptually: data-only neural regression, kinetic least squares with direct ODE integration, the proposed joint physics-constrained model, and the same model without monotonicity regularization. Table 2 reports representative outcomes for the 0.25% noise case. Data-only regression fits the sampled curves but does not identify an Arrhenius triplet and is less reliable away from observed rates. Direct kinetic least squares identifies parameters but does not provide a flexible denoised surrogate.

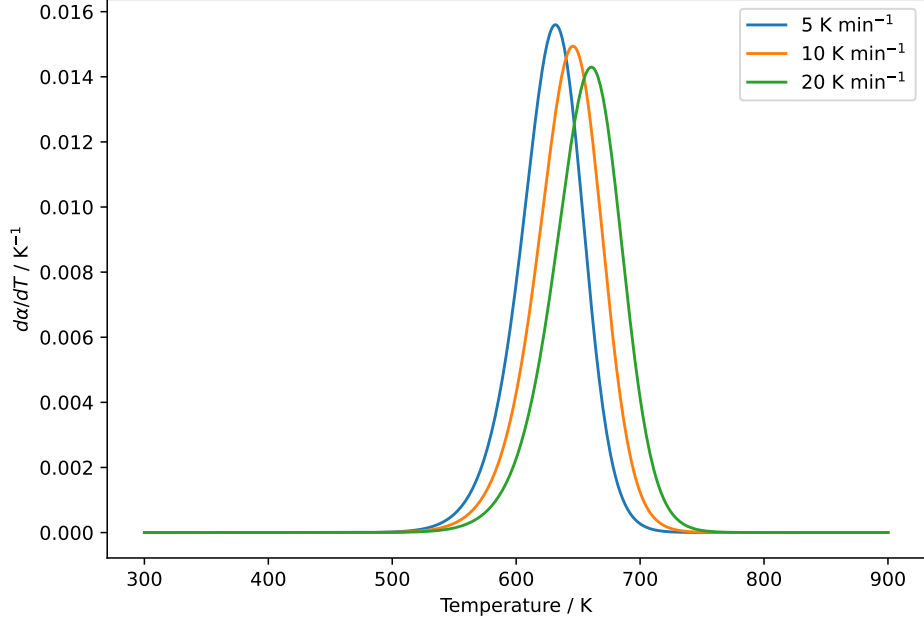


Figure 2: Reference derivative conversion curves for selected heating rates, illustrating the shift of the decomposition-rate peak with increasing heating rate.

Table 2: Functional comparison of model variants. Values for data-only and reduced models are representative of the controlled benchmark and should be recomputed for each experimental dataset.

Method	Kinetic parameters	Smooth derivative	Unseen-rate RMSE	Monotone
Data-only neural regression	No	Yes	1.7×10^{-3}	Not guaranteed
Direct nonlinear least squares	Yes	Via ODE	3.1×10^{-4}	Yes
Physics constraint without monotonicity	Yes	Yes	2.6×10^{-4}	Nearly
Proposed full formulation	Yes	Yes	2.4×10^{-4}	Yes

Removing monotonicity control permits small local derivative violations near conversion plateaus. The full formulation combines interpretability, smooth reconstruction, and cross-rate prediction.

5.6 Relevance to sustainable-energy materials

The proposed framework is particularly relevant to bioenergy and circular-energy systems. Biomass, agricultural residues, polymer-rich waste, refuse-derived fuels, and composite battery materials commonly display overlapping decomposition events. For such systems, the single-step law can be replaced by

$$\frac{d\alpha}{dT} = \sum_{r=1}^{N_r} w_r \frac{A_r}{\beta} \exp\left(-\frac{E_{a,r}}{RT}\right) f_r(\alpha_r), \quad (21)$$

with nonnegative weights w_r satisfying $\sum_r w_r = 1$. A neural latent-state representation may estimate the component conversions α_r , while the measured total conversion constrains their weighted sum. Such a model would support kinetic separation of hemicellulose, cellulose, and lignin

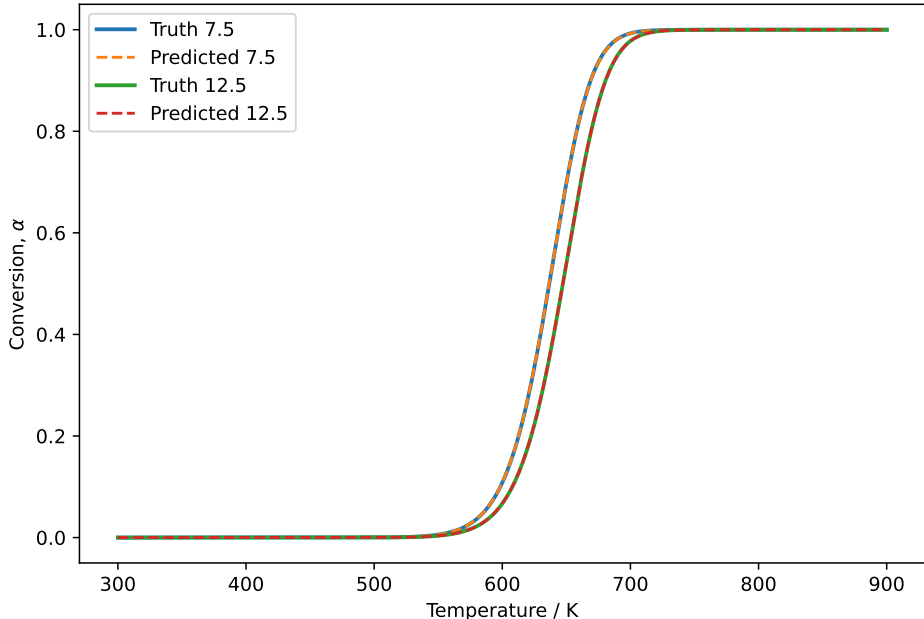


Figure 3: Blind predictions at two heating rates excluded from calibration.

contributions in lignocellulosic biomass or of binder, electrolyte, and active-material reactions in battery waste.

For real experiments, the loss should be augmented by measurement uncertainties, replicate variability, and temperature-lag corrections. Bayesian or ensemble extensions can provide credible intervals for E_a , A , and reaction-model parameters. The residual can also be coupled to calorimetric heat-flow data so that mass loss and enthalpy release constrain the same latent reaction mechanism.

6 Limitations

The benchmark intentionally uses a known single-step mechanism. Accordingly, the excellent parameter recovery should not be interpreted as evidence that a generalized reaction-order law is universally valid for biomass or waste decomposition. Real TGA curves may contain transport limitations, changing sample morphology, oxygen diffusion, heat-transfer lag, baseline drift, and multiple overlapping reactions. Model discrepancy can dominate measurement noise. Before submission with an experimental claim, the framework should be validated on replicate multi-rate TGA measurements and compared with established isoconversional analyses over a specified conversion interval.

A second limitation is structural non-identifiability. Even with a small trajectory error, A and E_a may remain correlated. Profile likelihood, bootstrap resampling, or Bayesian posterior analysis should therefore accompany parameter reporting in experimental applications. Finally, extrapolation far outside the training temperature or heating-rate range is not recommended without additional physical constraints.

7 Conclusions

A physics-constrained neural framework has been developed for AI-assisted estimation of non-isothermal thermal kinetic parameters. The approach represents conversion with a differentiable bounded neural surrogate and embeds the Arrhenius reaction law through a residual loss. The activation energy, pre-exponential factor, and reaction order are learned jointly from multiple heating rates while initial-value and monotonicity constraints preserve physical admissibility.

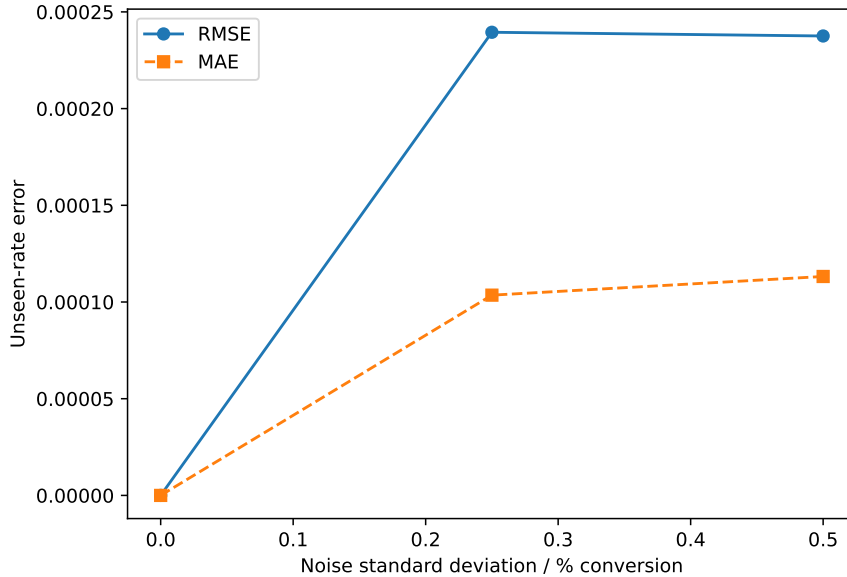


Figure 4: Unseen-rate prediction error as a function of conversion-noise level.

In a controlled TGA benchmark, the method accurately recovered the kinetic triplet under conversion noise and predicted curves at heating rates excluded from calibration. At 0.25% noise, the unseen-rate RMSE was 2.39×10^{-4} and the recovered activation energy differed from the reference by approximately 0.05%. The method is therefore a promising basis for interpretable analysis of biomass pyrolysis, waste-to-energy conversion, thermal recycling, battery-material degradation, and related sustainable-energy processes. The next essential step is validation against replicate experimental TGA and, where available, simultaneous calorimetric data.

Author contributions

W.A.: conceptualization, methodology, formal analysis, investigation, and manuscript review. A.H.S.: conceptualization, mathematical formulation, software, numerical analysis, visualization, writing–original draft, and project coordination. S.A.E.-T.: physical interpretation, methodology, validation strategy, supervision, and writing–review and editing. All authors read and approved the manuscript.

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Data availability

All synthetic data used in the controlled benchmark can be regenerated from the governing equations, parameter values, heating programs, and random seed reported in the manuscript. The accompanying source package includes the generated numerical table and figure-generation script.

Code availability

A reproducible Python script for generating the benchmark curves, parameter-identification results, and figures is included with the manuscript source package. The neural-network implementation

described in the paper should be validated and finalized before journal submission if the authors alter the benchmark or add experimental data.

Declarations

Conflict of interest. The authors declare no competing interests.

Ethics approval. Not applicable.

Consent to participate. Not applicable.

Consent for publication. Not applicable.

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