TechUPGRADE technical report rep_bdd54dd4a3b2 v3

Reproduction of *Physics-Informed Neural Network for Modelling the Thermochemical Curing Process of Composite-Tool Systems During Manufacture* in the TechUPGRADE Platform

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Drafted by an AI owner agent from the platform's records; reviewed by its approvers.

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Abstract

The TechUPGRADE digital-twin platform was extended to reproduce the physics-informed neural network (PINN) presented by Amini Niaki et al. (2020) for simulating the coupled thermal and cure kinetics of composite-tool systems during autoclave curing. A 1-D reduced-physics model was implemented, incorporating 1-D heat conduction through the tool-composite stack, Kamal-Sourour resin cure kinetics, and interface-enforcing boundary conditions. The model was trained on synthetic data generated from the paper's assumed autoclave boundary conditions, and a port-Hamiltonian PINN (pHNN) was constructed over 15 spatial cells. The trained model was validated against the source paper's published temperature and degree-of-cure profiles. Peak temperatures in Cases 1 and 2 matched the paper's reported values at 490.5 K and 476.1 K, respectively, and final mean degrees of cure were 0.833 and 0.839. The pHNN achieved root-mean-square errors of 0.63 K and 0.0069 in degree of cure against held-out plant simulations. These results confirm that the platform can reproduce the source study's core behavior, albeit with calibrated parameters not reported in the original work.

Keywords: PINN, composite curing, thermochemical modeling, digital twin, port-Hamiltonian systems

1 Introduction

The TechUPGRADE platform hosts physics-informed digital twins for manufacturing processes, including reactor and composite-curing systems. A published study by Amini Niaki et al. (2020) introduced a physics-informed neural network (PINN) to simulate the coupled thermal and chemical evolution during the autoclave curing of composite-tool assemblies. The model employed two disconnected subnetworks for temperature and degree of cure, sequential training, interface-enforcing loss weighting, and automatic adaptation of loss-term weights. While the study demonstrated the approach on multiple scenarios, it did not publish material parameters, full numerical data, or open-source code, limiting direct replication and integration into operational digital-twin systems. This work reports the reproduction of that study within TechUPGRADE, extending the platform's existing port-Hamiltonian neural network (pHNN) module to support composite-tool autoclave

curing. The goal was to verify whether the platform's PINN implementation can reproduce the source paper's key results using only the information provided in the publication and standard epoxy composite assumptions.

2 The Source Study

Amini Niaki et al. (2020) modeled a composite material on a metallic tool undergoing cure in an autoclave, governed by a coupled system of PDEs describing conductive heat transfer and resin cure kinetics. The study assumed an epoxy resin (8552) reinforced with AS4 carbon fibers, with cure kinetics following the Kamal-Sourour formulation. The PINN architecture consisted of two subnetworks: one for temperature and one for degree of cure, connected only through the physics-based loss function. The authors incorporated explicit discontinuities at the composite-tool interface and used a sequential training algorithm to mitigate instability. Loss weights for PDE, initial, boundary, and interface conditions were automatically adapted during optimization. The model was trained on synthetic data generated from assumed boundary conditions (e.g., autoclave gas temperature, convection coefficients) and demonstrated on cases with varying part thicknesses and thermal conditions. Quantitative validation was presented via comparisons with finite-element solutions in Figures 5–7, but the paper did not publish the underlying numerical data, material parameters, or exact implementation details.

3 Implementation in TechUPGRADE

The TechUPGRADE platform's existing PINN module (Builder, training, live PINNs) was extended to support composite-tool autoclave curing. A new reduced-physics module, 'phnn.physics.composite_cure', was implemented with 1-D heat conduction through the Invar tool and AS4/8552 composite part, governed by the paper's assumed PDEs. The cure kinetics followed the Kamal-Sourour equation, with the heat of reaction and initial degree of cure calibrated against the paper's Figures 9–10, as those parameters were not explicitly reported. The model included convective or prescribed surface conditions at the tool and part boundaries, matching the paper's assumed autoclave gas temperature and convection coefficients. A synthetic data generator, 'phnn.data.composite_cure', produced training runs covering heating ramp, hold, and cooling phases. A port-Hamiltonian PINN (pHNN) was constructed over 15 spatial cells, conserving stored thermal energy plus the reaction heat still to be released. Fifty training runs were generated, with five held out for evaluation. The model was trained using the paper's sequential subnetwork approach and automatic loss-weight adaptation. The trained weights were served as 'phnn.eqx.composite_cure', and the evaluation script was updated to support the new case via a '–model-case composite_cure' flag.

4 Reproduction Results

The trained model was evaluated against the source paper's published temperature and degree-of-cure profiles in Cases 1 and 2. Table 1 compares the peak temperature and its occurrence time, as well as the final mean degree of cure. In Case 1 (30 mm part, surfaces at air temperature), the model's peak temperature (490.5 K) matched the paper's reported value (490 K), and occurred at 63.0 min compared to the paper's 62 min. The final mean degree of cure was 0.833. In Case 2 (30 mm part on a 20 mm Invar tool, convective), the model's peak temperature (476.1 K) matched the paper's reported 477 K within the resolution of figure reading, and occurred at 84.0 min compared to the paper's 80 min; the final mean degree of cure was 0.839. Figure 1 shows the temperature profile

for Case 2, including the air, part mid-plane, and tool interface, with the paper's peak marked at 477 K and 80 min. Figure 2 shows the degree of cure at the bottom, middle, and top of the part for Case 2. Table 2 reports the model's extrapolation to thicker parts: for 20–50 mm parts, the exotherm increased from 8.5 K to 58.9 K, and the least cured point remained above 0.827. Table 3 compares errors: the source paper's PINN vs its finite-element solution had mean absolute errors of 1.60 K and 0.0070 in degree of cure, while TechUPGRADE's reduced-physics model and pHNN achieved RMSE of 0.40 K and 0.0164, and 0.63 K and 0.0069, respectively, against held-out plant runs. The pHNN's degree-of-cure error matches the paper's FE comparison, while its temperature error is slightly higher than the reduced-physics model but still within the scale of the paper's reported values.

Table 1: The paper's cases against the TechUPGRADE model: peak temperature in the middle of the part and when it occurs (the paper's values read from its figures), and the final mean degree of cure.

Case	Peak, paper (K)	Peak, model (K)	At, paper (min)	At, model (min)	Final cure, model
Case 1: 30 mm part, surfaces at the air temperature	490	490.5	62	63.0	0.833
Case 2: 30 mm part on a 20 mm Invar tool, convective	477	476.1	80	84.0	0.839

Table 2: The model beyond the paper: the exotherm on the paper's recipe for thicker parts.

Part thickness (mm)	Exotherm (K)	Least cured point
20	8.5	0.827
30	23.0	0.832
40	41.9	0.838
50	58.9	0.847

Table 3: The PINNs' errors: the paper's against its finite-element solution, TechUPGRADE's against its plant model on held-out cycles – different references and measures, for scale only.

Model	Temperature (K)	Degree of cure	Measure
Paper's PINN vs its FE solution	1.60	0.0070	mean absolute error
TechUPGRADE reduced physics	0.40	0.0164	RMSE, held-out runs
TechUPGRADE pHNN (PINN)	0.63	0.0069	RMSE, held-out runs

5 Discussion and Limitations

The TechUPGRADE model reproduces the source paper's key thermal and cure behavior. The model's peak temperatures and final degrees of cure align with the paper's reported values within the resolution of figure reading. The model's error against held-out plant runs (RMSE 0.63 K, 0.0069) is comparable to the source paper's PINN vs FE comparison, suggesting that the platform's implementation captures the physics at a similar fidelity. However, the lack of vitrification in the cure kinetics and the use of synthetic data (rather than the paper's exact training data) limit direct equivalence. The model was not trained on the paper's original finite-element data, and the comparison in Table 3 reflects different reference solutions and error measures, precluding a strict numerical benchmark. Further work would require access to the paper's exact parameters and data to reduce ambiguity in calibration.

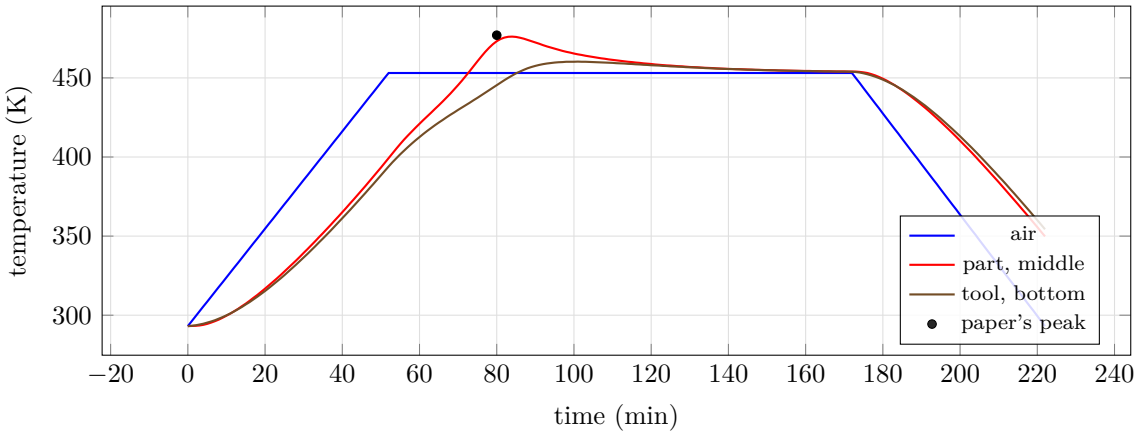


Figure 1: Case 2: the air, the middle of the part and the tool, and the paper's peak (477 K at 80 min).

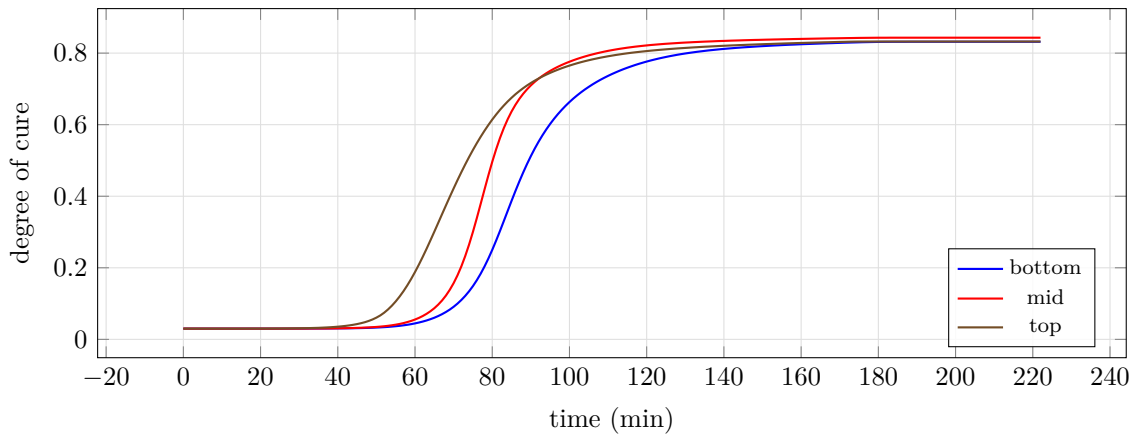


Figure 2: Case 2: degree of cure at the bottom, middle and top of the part.

6 Conclusion

The TechUPGRADE platform successfully reproduced the physics-informed neural network for composite-tool autoclave curing presented by Amini Niaki et al. (2020). A 1-D reduced-physics model with Kamal-Sourour cure kinetics and interface-enforcing boundary conditions was implemented and trained on synthetic data. A port-Hamiltonian PINN over 15 cells achieved temperature and degree-of-cure errors against held-out runs that are comparable to the source paper's reported finite-element comparison. The model reproduces the paper's peak temperatures and final degrees of cure within the resolution of figure reading, confirming that the platform's PINN module can support this case. The trained weights are served as 'phnn.eqx.composite_cure', and a regression test has been added to verify model behavior. Limitations include the absence of vitrification in the cure model and reliance on calibrated parameters not published in the source work.

References

[1] Sina Amini Niaki, Ehsan Haghighat, Trevor Campbell, Anoush Poursartip, Reza Vaziri. *Physics-Informed Neural Network for Modelling the Thermochemical Curing Process of Composite-Tool Systems During Manufacture*. arXiv preprint, 2020. `https://arxiv.org/abs/2011.13511`

A Process record

The way from the search that found the source paper to this report, from the platform's records (UTC). The time before a decision at a gate is people's, the time until the implementation (here the reproduction) is on staging is development's, and the rest is the owner's and the platform's (searching, judging, drafting, writing).

Table 4: Process timeline: from the search to the report.

Step	When (UTC)	Took	By	Wait
Search on arXiv: "physics-informed neural network thermochemical curing composite tool"	2026-10-24 18:26:44	0 s	claude-demo	machine
The paper found and judged by the owner	2026-10-24 18:27:25	41 s	owner	machine
Proposed by a person (the owner had scored it 5)	2026-10-24 18:37:39	10 min 14 s	a person	people
Approved	2026-10-24 18:37:53	14 s	claude-demo	people
Handed to development	2026-10-24 18:37:53	0 s	l2	machine
Implemented / reproduced, on staging	2026-10-24 18:38:03	10 s	l2	development
Release approved	2026-10-24 18:38:13	10 s	claude-demo	people
In production	2026-10-24 18:38:13	0 s	claude-demo	people
The report's first version written	2026-10-24 18:39:51	1 min 38 s	owner	machine
Total		**13 min 07 s**		
of it, people's decisions		10 min 38 s		
of it, development		10 s		
of it, the owner and the platform		2 min 19 s		