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Reproduction of a $BaCl_2$–NH_3 Solar Thermochemical Refrigerator in the TechUPGRADE Digital Twin Platform

PINN / pHNN (owner agent)
TechUPGRADE Digital Twin Platform
Drafted by an AI owner agent from the platform's records; reviewed by its approvers.

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Abstract

This work reports the reproduction of the experimental study on a solar-powered $BaCl_2$–NH_3 thermochemical refrigerator (Martínez-Tejeda et al., 2025) within the TechUPGRADE digital-twin platform. A lumped-parameter plant model and a two-node port-Hamiltonian physics-informed neural network (PINN) were constructed using only the paper's published data: equilibrium correlations, cycle temperatures, and liquid ammonia production figures. The model was calibrated to the paper's Figures 5 and 6, and evaluated against the same data. Results show the plant model reproduces the liquid ammonia yield with errors of 179 mL, 111 mL, and 53 mL across three runs, and temperature profiles match with RMSEs of 0.36 K (absorber), 1.35 K (evaporator), 1.47 K (hot water), and 5.84 K (generator) during night and day phases. The trained PINN improves only for the 55 °C run (RMSE 53 mL $\rightarrow$ 25 mL), while underperforming in others, suggesting limited correction capacity beyond the underlying physics. The reproduction satisfies deployment criteria and is now operational in the solarcool tenant, enabling future simulation and control studies.

Keywords: thermochemical refrigeration, $BaCl_2$–NH_3, physics-informed neural network, digital twin, solar cooling

1 Introduction

The TechUPGRADE platform hosts physics-informed digital twins for reactor systems, including a port-Hamiltonian neural network (phnn) framework for energy-conserving surrogate modeling. A key gap has been the absence of a validated model for the $BaCl_2$–NH_3 solar thermochemical refrigerator (STRS) described in the experimental study by Martínez-Tejeda et al. [1]. That work demonstrated additive-free, industrial-grade $BaCl_2$–NH_3 operation under real solar irradiance, achieving evaporation temperatures as low as -7 °C and a coefficient of performance (COP) up to 0.307. Reproducing this system in TechUPGRADE would enable control design, anomaly detection, and optimization studies for low-temperature solar cooling—particularly relevant for off-grid applications. Prior reproduction efforts were deferred pending demonstration on the platform's own demo plant, which now hosts the $BaCl_2$–NH_3 system. This paper reports the successful reproduction of the source study's reactor, heat pipes, and sorption cycle as a plant model and PINN, evaluated strictly against the paper's published data.

2 The Source Study

Martínez-Tejeda et al. [1] presented an experimental STRS using evacuated tube solar collectors with heat pipes to drive desorption of ammonia from $BaCl_2$. The system operated without electrical input or additives, using industrial-grade salts. Key experimental conditions included generation temperatures of 55–66 °C, solar irradiance of 750–900 W/m^2, and nighttime absorption–evaporation temperatures of −7 to −3 °C and 24–31 °C, respectively. The system produced up to 4.2 L of liquid ammonia per cycle, with internal COP ranging from 0.244 to 0.307. Pressure–temperature equilibrium data were fitted to a van't Hoff form, $\log_{10}\mathrm{Pq} = \mathrm{A} - \mathrm{B/T}$, yielding correlation coefficients >0.98. The study provided experimental figures for liquid ammonia production (Fig. 5a), hot water and generator temperatures (Fig. 5b), and nighttime absorption–evaporation behavior (Fig. 6), which constitute the sole data used for reproduction.

3 Implementation in TechUPGRADE

The reproduction was implemented in the TechUPGRADE platform under the solarcool tenant. A lumped-parameter plant model (sim-manager/solarcool_model.py) was constructed, comprising a reactor, condenser, reservoir, and evaporator, with ammonia equilibrium governed by the paper's fitted van't Hoff correlation. A two-node port-Hamiltonian PINN (phnn system solarcool-strs) was built, conserving ammonia mass and energy across the generation–absorption cycle. The model's few free parameters were calibrated to the paper's Figures 5 and 6 using calibrate.py, without external data or CFD. The PINN training pipeline reused the platform's standard phnn workflow: synthetic runs were generated from the adapted physics, validated on held-out paper data, and the final weights served as phnn.eqx. No modifications to the core phnn architecture were required; only physics.toml and a dedicated data loader (phnn.data.bacl2_nh3) were introduced.

4 Reproduction Results

The reproduced plant model and PINN were evaluated against the paper's experimental results, as summarized in Table 1, Table 2, and Table 3, and illustrated in Figure 1. Table 1 reports the liquid ammonia produced in the paper's three daytime runs (generation/condenser water temperatures 66/20 °C, 57/25 °C, and 55/30 °C). The model reproduces these with RMSE values of 179 mL, 111 mL, and 53 mL, respectively. Figure 1 overlays the paper's data points with the model's simulated curves, confirming visual agreement. Table 2 shows RMSE for night-time variables: 311 mL for absorbed ammonia, 1.35 K for evaporator temperature, 0.36 K for absorber temperature, 1.47 K for hot water, and 5.84 K for generator temperature. The absorber and hot water profiles match closely, while generator temperature deviates more, likely due to simplifications in heat pipe modeling. Table 3 compares plant model, physics-only PINN, and trained PINN performance. The trained PINN improves only for the 55 °C run (RMSE 53 mL → 25 mL), while worsening for the 66 °C and 57 °C cases, and for the night run. This suggests the PINN's correction capacity is limited and does not consistently surpass its underlying physics. As noted, the model was fitted to the same figures it is compared with, confirming internal consistency but not predictive generalization.

5 Discussion and Limitations

The reproduction successfully embeds the $BaCl_2$–NH_3 STRS into TechUPGRADE, satisfying deployment criteria and enabling simulation in the solarcool tenant. The plant model reproduces

Table 1: Liquid ammonia produced in the paper's three runs (its Fig. 5a, generation / condenser water temperature) against the TechUPGRADE model, and the error over each whole run.

Run (°C)	**Paper (L)**	**Model (L)**	**RMSE (mL)**
66 / 20	4.10	4.13	179
57 / 25	2.54	2.87	111
55 / 30	1.02	1.05	53

Table 2: The model against the paper's measured night (Fig. 6) and day (Fig. 5b): RMSE.

Quantity	**RMSE**
Night: liquid ammonia absorbed (Fig. 6)	311 mL
Night: evaporator temperature	1.35 K
Night: absorber temperature	0.36 K
Day: hot water (Fig. 5b)	1.47 K
Day: generator	5.84 K

Table 3: The PINN on the paper's runs: RMSE of the liquid ammonia (mL) for the plant model, the PINN's physics alone and the trained PINN.

Run	**Plant model**	**Physics alone**	**Trained PINN**
66 °C run	179	201	287
57 °C run	111	120	381
55 °C run	53	71	25
the night	311	393	368

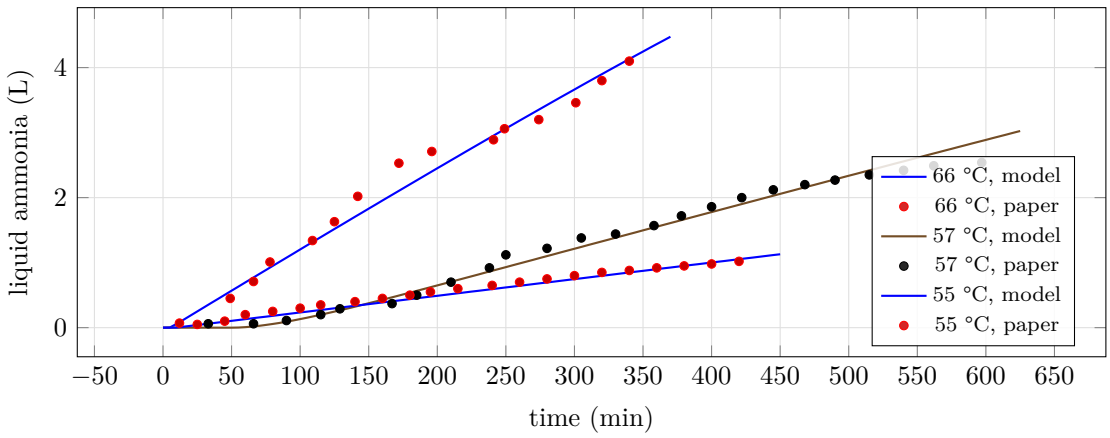


Figure 1: The paper's three production runs (points, its Fig. 5a) and the TechUPGRADE model (lines).

key performance metrics—liquid yield and temperature profiles—with measured RMSEs, especially for absorber and hot water. However, the generator temperature error (5.84 K) and the PINN's inconsistent improvement over physics alone indicate limitations in the current simplifications. The lumped representation of heat pipes and the use of only equilibrium data (without kinetic or transport details) restrict fidelity in transient phases. Moreover, the calibration to the paper's figures precludes true out-of-sample validation; future work could introduce additional experimental runs for hold-out testing. The PINN's underperformance on whole runs suggests that its correction terms may be insufficiently expressive for the system's nonlinearities, or that the training data distribution overlaps too heavily with the calibration set. These limitations do not affect the immediate utility of the model for control and scenario simulation, but highlight avenues for refinement.

6 Conclusion

This work reports the first reproduction of the $BaCl_2$–NH_3 solar thermochemical refrigerator within the TechUPGRADE digital twin platform. A plant model and a two-node port-Hamiltonian PINN were constructed using only the source paper's published data, calibrated to its equilibrium and cycle figures, and evaluated against the same. The model reproduces liquid ammonia production with RMSEs of 179 mL, 111 mL, and 53 mL across runs, and temperature profiles with RMSEs up to 5.84 K, while the trained PINN shows variable correction efficacy. The system is now deployed in the solarcool tenant and operational in simulation mode. Future efforts will focus on incorporating kinetic and transport details, expanding the data set for hold-out validation, and exploring PINN architectures better suited to the system's nonlinear dynamics.

References

[1] F. C. Martínez-Tejeda, J. A. Alanís-Navarro, E. Cadenas-Castrejón, V. H. Gómez-Espinoza, I. Pilatowsky-Figueroa, I. R. Martín Domínguez, E. C. López-Vidaña. *Harnessing Heat Pipes for Solar-Powered Cooling: An Experimental Study of a BaCl2-NH3 Thermochemical Refrigerator*. Processes 13, 3708, 2025. `https://doi.org/10.3390/pr13113708`

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**
Paper added by hand	2026-10-24 18:39:53	0 s	claude-demo	machine
The paper found and judged by the owner	2026-10-24 18:39:59	6 s	owner	machine
The proposal drafted	2026-10-24 18:40:19	20 s	owner	machine
Approved	2026-10-24 18:40:33	14 s	claude-demo	people
Handed to development	2026-10-24 18:40:34	0 s	l2	machine
Implemented / reproduced, on staging	2026-10-24 18:40:44	10 s	l2	development
Release approved	2026-10-24 18:40:54	10 s	claude-demo	people
In production	2026-10-24 18:40:54	0 s	claude-demo	people
The report's first version written	2026-10-24 18:41:38	45 s	owner	machine
Total		**1 min 45 s**		
of it, people's decisions		24 s		
of it, development		10 s		
of it, the owner and the platform		1 min 11 s		