MACHINE LEARNING-BASED PROCESS SIMULATION APPROACH FOR REAL-TIME OPTIMIZATION AND ACTIVE CONTROL OF COMPOSITES AUTOCLAVE PROCESSING

Keith D. Humfeld[1], Navid Zobeiry[2]
[1] Boeing Research and Technology, Seattle, WA, USA
[2] Materials Science & Engineering, University of Washington, Seattle, WA, USA

ABSTRACT

For manufacturing of composites, several parts may be processed simultaneously in an autoclave or oven. Depending on the equipment design, tool/part geometries, and tool nesting, convective heat transfer Boundary Conditions (BCs) may vary around parts in each load. As a result, temperature histories in some of the parts may not conform to specifications such as limits on maximum part temperature, or part temperature rate. To mitigate risk, in addition to conducting finite element simulations prior to fabrication based on assumed BCs, leading and lagging thermocouples, embedded in parts or placed in proxy locations, are used to monitor temperature history during processing. In this study, a recently developed machine learning framework, CompML (Composites Machine Learning) is used for active control of the autoclave. CompML uses TC data at the start of the autoclave processing for real-time inverse modeling of the thermo-chemical problem, and to identify BCs for all parts in each load. The results are then used for real-time optimization of autoclave cure recipe to the shortest cycle that satisfies specifications in all parts. A successful virtual demonstration of the approach for HEXCEL AS4/8552 parts processed on Invar tools is discussed in the paper.

Keywords: machine learning, process simulation, active control, inverse modeling, process optimization, autoclave processing
Corresponding author: Navid Zobeiry

1. INTRODUCTION AND BACKGROUND

For processing of aerospace composites, parts are commonly heated via convection in ovens or autoclaves. To ensure end-part quality, part temperature history must conform to specifications (i.e. specs) which may be defined based on part temperature or part temperature rates during heat-up and dwell steps [1, 2]. Out-of-spec parts may suffer from a variety of process-induced defects such as under-curing, porosity, fiber waviness/wrinkling, and high degree of residual stresses leading to dimensional changes and micro-cracks [3-7]. A combination of experimental thermal profiling and numerical process simulation approaches [8-11] are used in advance of manufacturing, to design robust cure cycles conforming to all specs. Based on experiments and/or simulations, lagging and leading locations (i.e. hottest and coldest zones) of parts are identified. Typically, thermocouples are placed near these locations at the backside of the tool as proxies to monitor part temperature history. For large aerospace parts where a dedicated autoclave is used, the distribution of convective BCs around the part can be measured with a relatively high degree of confidence [9]. However, for cases where multiple parts are cured together in an autoclave/oven, convective BCs are typically not known. This is due to many contributing factors that change the airflow pattern inside the autoclave or oven including the number of parts cured together, tool nesting and orientation, part geometry and overall thermal mass [12].

Away from the part edges and tooling sub-structures, the most dominant mode of heat transfer for thin composite parts is through thickness. Consequently, 1D numerical simulations of thermo-chemical processes are frequently conducted to speed-up analysis [1, 2, 10]. Consider a 1D representation of a composite part with a thickness of L_1, placed on a tool with a thickness of L_2 as shown in Figure 1. Also assume that the heat transfer BCs, h_1 and h_2, are unknown. To monitor part temperature history, a proxy tool thermocouple (TC) is placed under the tool. As shown in Figure 1, during heat-up, part temperature initially lags behind the air temperature. This is due to the tool and part thermal masses and combined convective and conductive thermal resistances. Once the exothermic curing reaction starts in the part, temperature at the center of the part may increase beyond the air temperature as shown in Figure 1. Based on heat transfer analysis of a range of assumed BCs, a robust cure cycle may be designed to satisfy specs. However, this may introduce unnecessary constraints on the solution, to increase processing time. In another approach, data from tool proxy TC may be used to back-calculate BCs using trial-and-error simulations. Given that this is a time-consuming process, it cannot be implemented for real-time optimization of the cure cycle during processing in an active control environment.

In a forward finite element simulation approach, a known thermal stack (h_1, L_1, L_2 and h_2) and air temperature profile (T_{air}) are needed to simulate the 1D curing process and obtain part temperature history (T_{part}). Aligned with recent advances in applications of Machine Learning (ML) for composites [13-16], a ML framework may be developed to solve the inverse heat-transfer problem. Based on tool proxy TC data (T_{tool}) and known geometries (L_1 and L_2), a ML model may be trained to calculate unknown BCs (h_1 and h_2). This information can be used to calculate the part temperature history (T_{part}) in a forward simulation, hence checking the conformity to specs. Given the speed of simulation in trained ML models, in cases where the part temperature does not satisfy the specs, ML can be used to quickly identify the shortest cure cycle that satisfies all the specs. However, it should be noted that the inverse heat transfer is mathematically an ill-posed problem. This means that multiple solutions may be obtained for the inverse heat transfer problem based on TC data. A robust ML framework should be able to identify all plausible solutions and design a cure cycle that satisfies specs in all of them.

In this paper, a recently developed ML framework is presented, where data from multiple tool TCs are used to solve the inverse thermo-chemical problem and identify all potential thermal stacks. ML framework can then optimize the cure cycle in real-time to identify the fastest cycle to satisfy specs. A demonstration is presented where the temperature profile for curing three HEXCEL AS4/8552 parts on three Invar tools is optimized. Such a framework can be implemented in industrial settings for active control of processing based on TC data.

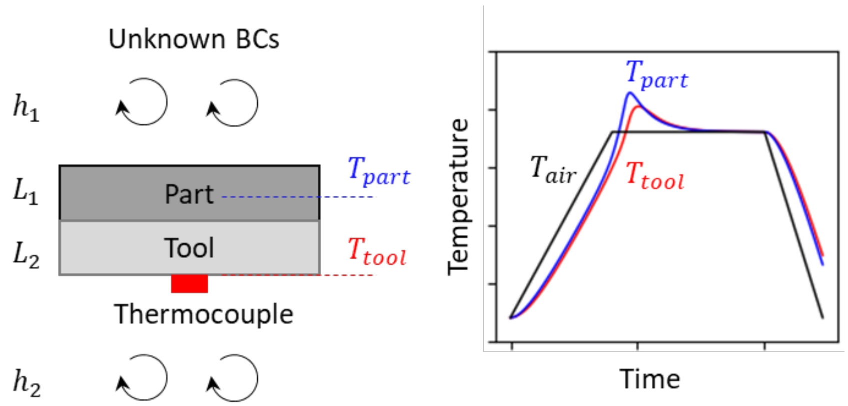

Figure 1. 1D representation of curing of a composite part on a tool in a convective environment. Air temperature profile and temperature histories at the tool back-side and center of the part are shown.

2. DEVELOPING A MACHINE LEARNING FRAMEWORK

Considering the ill-posedness of governing equations for the thermo-chemical process in composites, a forward ML model was developed for fast evaluation of a wide range of BCs. Such a model can quickly identify all plausible solutions based on tool TC data only. The ML framework consists of three Neural Networks (NN) as shown in Figure 2 and Figure 3 and described below:

- Similar to FE, two NNs with LSTM (Long short-term memory) architectures were designed (Figure 2) to predict the entire part and tool temperature histories as a function of known thermal stacks and air temperature. The advantage of the network over FE is the speed. On a typical computer workstation, the trained LSTM network can perform about 50 simulations per second. This is approximately 200 times faster than existing FE models for 1D simulation. This allows the LSTM model to quickly check a wide range of BCs and identify cases with similar temperature histories to measured tool TC data.

- A third NN was designed with a simple feedforward architecture (Figure 3). For given thermal stacks and air temperature profiles, this NN can classify all cases that satisfy the specs. On a typical workstation, this NN can classify about 30,000 cases every second. The identified thermal stacks from the LSTM model can be used as inputs in this NN, to search a wide range of potential cure cycles.

Using this framework and based on the initial data gathered from proxy TCs, all BC solutions for all parts can be identified. Based on these solutions, the cure cycle can be optimized in real-time to the shortest cycle that satisfies specs in all parts. The networks were trained based on data generated from an in-house developed FE model to solve 1D thermo-chemical reactions in composites. HEXCEL AS4/8552 material model [17] along with Invar thermal properties were used [9] to generate 100,000 1D simulations with random thermal stacks and air temperature profiles. Training was done using Tensorflow library in Python 3.6.8.

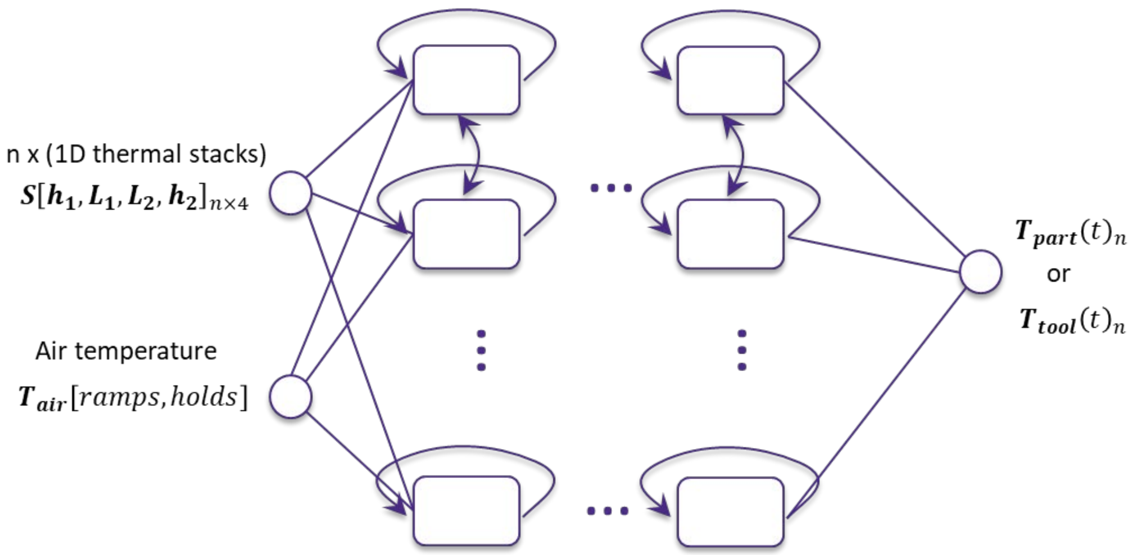

Figure 2. LSTM Neural Networks to predict part and tool temperature histories.

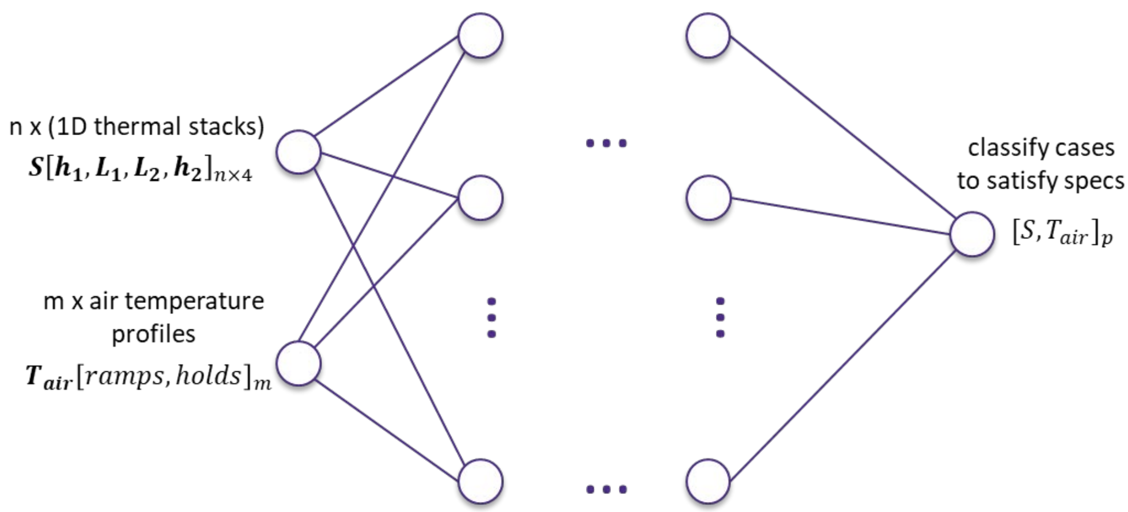

Figure 3. Feed Forward Neural Network to classify thermal stacks and temperature profiles that satisfy specs.

3. APPLICATION AND VALIDATION

The framework described in previous section was recently implemented in a python-based machine learning software developed at the University of Washington, CompML (Composites Machine Learning). For demonstration, CompML is used here for inverse modeling and optimization of cure cycle for simultaneous processing of three parts. To validate the obtained solution, the finite element module in CompML was used to simulate the forward problem to compare with ML predictions.

Consider curing of three HEXCEL AS4/8552 parts on three Invar tools as shown in Figure 4. 1D thermal stacks for these parts are listed below:

- $A: h_1 = 60 \frac{W}{m^2K}, L_1 = 10\ mm, L_2 = 10\ mm, h_2 = 40\ W/m^2K$
- $B: h_1 = 80 \frac{W}{m^2K}, L_1 = 20\ mm, L_2 = 10\ mm, h_2 = 40\ W/m^2K$
- $C: h_1 = 40 \frac{W}{m^2K}, L_1 = 15\ mm, L_2 = 10\ mm, h_2 = 40\ W/m^2K$

For this example, two specifications on part maximum temperature, and part temperature rate (at the transition time when air temperature reaches 180 °C) were considered:

- $\max(T_{part}) - 180\ ℃ < 5\ ℃$
- $1\ ℃/min < T'_{part}(T_{air} = 180\ ℃) < 3\ ℃/min$

The three parts are subjected to a one-hold cycle from room temperature to 180 °C with a heating rate of 2 °C/min, followed by two hours hold and then cool-down to room temperature with a rate of 3.5 °C/min. For the forward problem, part and tool temperature histories were predicted using FE as shown in Figure 4. Based on this analysis, none of the parts satisfy the specifications:

- $A: exotherm = 12.0\ ℃, T' = 2.9\ ℃/min$
- $B: exotherm = 33.8\ ℃, T' = 3.3\ ℃/min$
- $C: exotherm = 26.7\ ℃, T' = 2.9\ ℃/min$

For comparison, CompML was used assuming unknown BCs, but with known thicknesses and tool proxy TCs. For unknown BCs, values between 20-100 W/m^2K were considered for evaluation with ML model with a step size of 5 W/m^2K (i.e. 16 values). Consequently, for 3 parts and 2 unknown BCs around each part, a total of 768 cases were considered ($16 \times 16 \times 3$). Initially, CompML predicted the tool temperatures for all combinations of thermal stacks for the first 15 minutes of the cure, and compared them with tool TC data from the first 15 minutes. The entire calculation took 21 seconds to complete. From 768 cases, CompML selected 128 cases based on similarity to tool TC data with a maximum error of 1 °C. For the second calculation, data from the first 30 minutes of the cycle was used with the existing 128 thermal stacks. CompML reduced these to 58 potential thermal stacks in 4.4 seconds. CompML then predicted the temperature at the middle of parts for all 58 potential cases. The potential thermal histories obtained from envelopes of possible responses for the three parts are highlighted in Figure 5, and are compared with FE results with known BCs. This validates the capability of CompML to correctly identify the zone of potential solutions only based on 30 minutes of TC data.

After this step, 2000 potential cure cycles were constructed by varying hold temperature, time, and heating ramps using 1-hold and 2-hold cycles. These cycles were evaluated with all 58 potential thermal stacks to find the shortest cycle to satisfy specs in all 58 cases. This calculation took 1.6 seconds, and the result are shown in Figure 6, and are compared with FE predictions in a forward problem with known BCs. Based on the following measurements, the optimized cycle satisfies specs in all parts:

- $A: exotherm = 0.8$ °C , T'=2.3

- $B: exotherm = 1.2$ °C , T'=2.0

- $C: exotherm = 1.0$ °C, T'=1.8

The results are summarized under Table 1. While the original cycle was 245 minutes, the new optimized cycle is 327 minutes, but it satisfies all the specs for all potential thermal stacks. CompML was able to find 15 additional cycles to satisfy the specs but all were longer than 327 minutes.

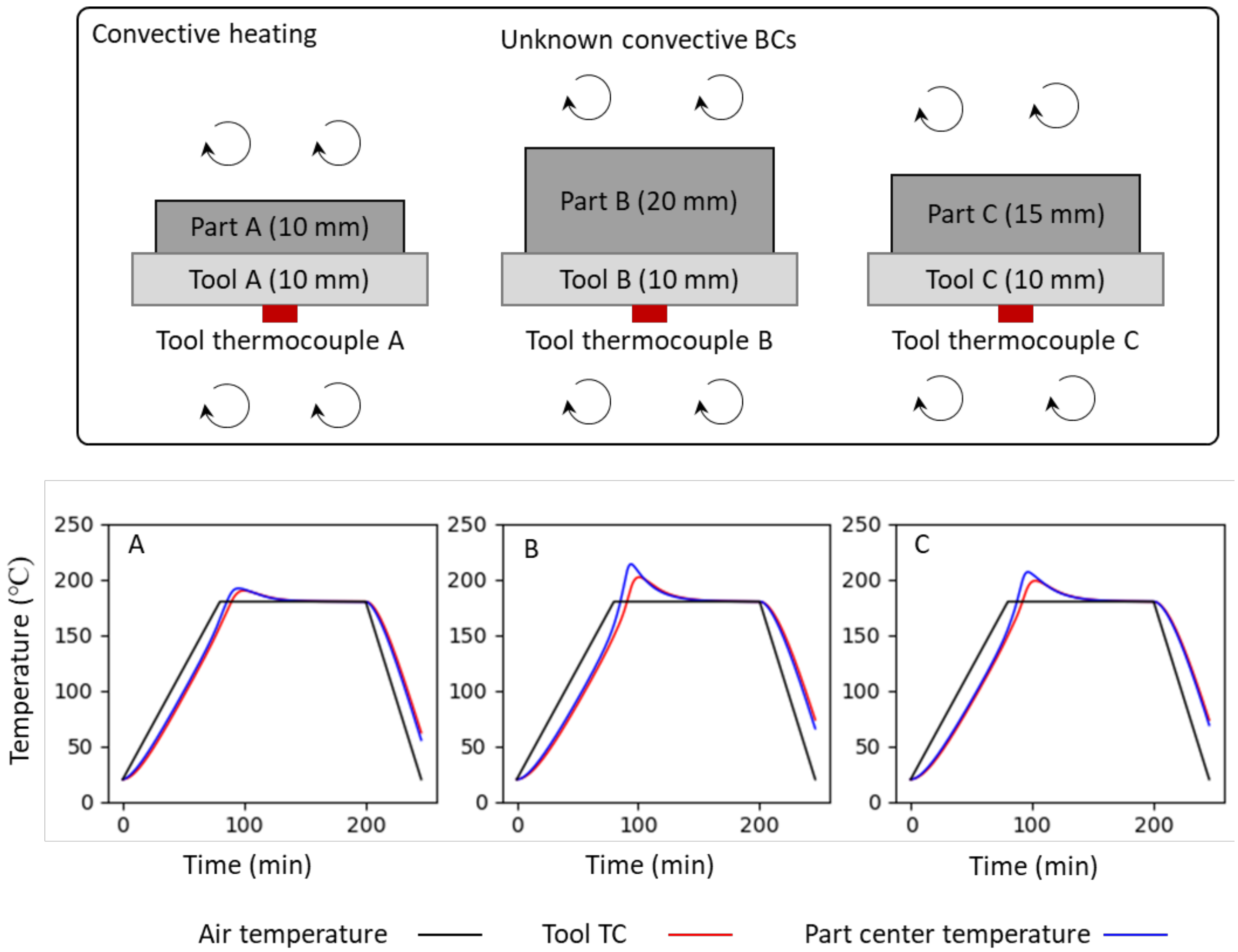

Figure 4. Convective heating and processing of three parts on three tools (A, B and C) with unknown convective BCs, and subjected to a one-hold cure cycle. Air temperature, tool back-side, and part center temperatures are compared.

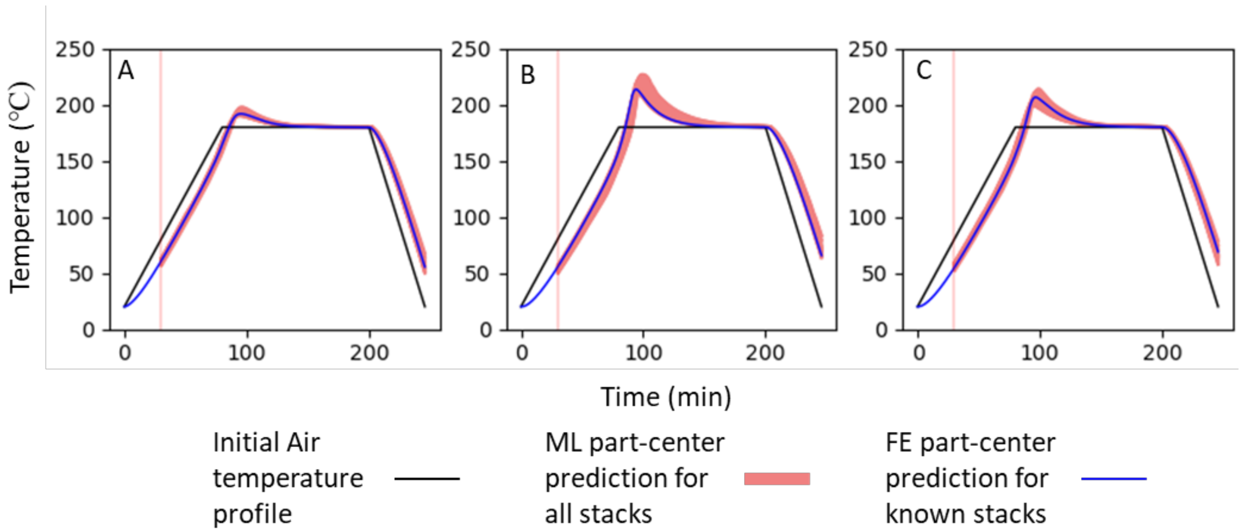

Figure 5. Based on the initial 30 minutes data from tool proxy TCs, CompML predicts all solutions for part temperature histories. The zones of viable solutions are compared with FE results.

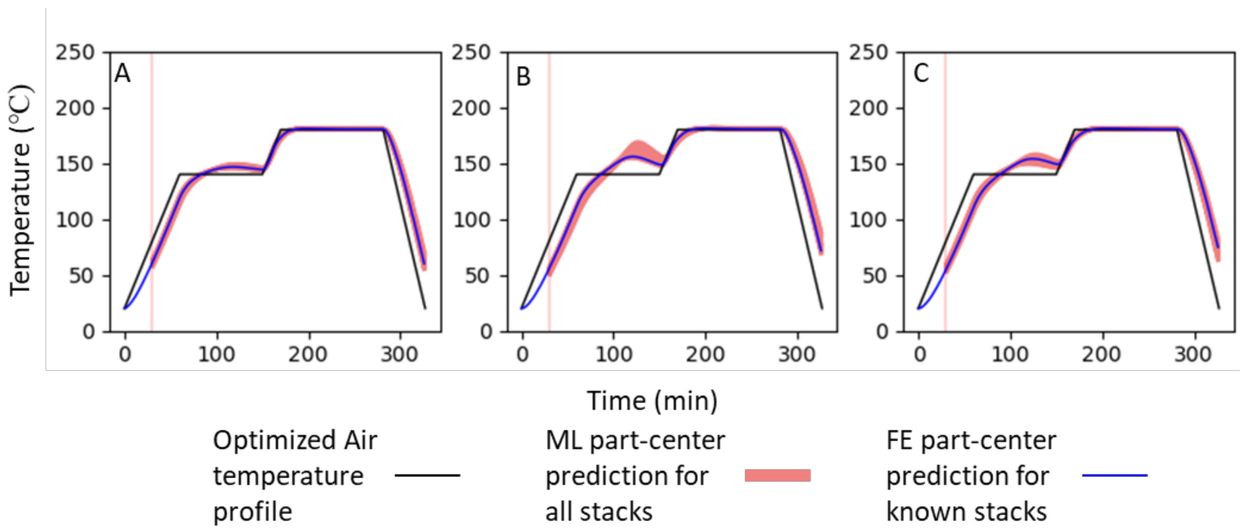

Figure 6. Shortest 2-hold cycle to satisfy specs in all parts.

Table 1. Part max temperatures and heating rates for the initial and optimized cure cycles.

Part	Initial 1-hold Cycle – 245 min		Optimized 2-hold Cycle – 327 min	
	Max temperature	Part heating rate	Max temperature	Part heating rate
A	12.0 °C	2.9 °C/min	0.8 °C	2.3 °C/min
B	33.8 °C	3.3 °C/min	1.2 °C	2.0 °C/min
C	26.7 °C	2.9 °C/min	1.0 °C	1.8 °C/min

4. CONCLUSIONS

In this paper, a novel ML framework was developed and implemented in a python-based ML software, CompML. For multiple parts heated and cured via convection, the capability of the framework was demonstrated to optimize the cure cycle based on tool TC data only, without the knowledge of convective BCs. Based on TC data, trained LSTM models solved the forward problem to identify all plausible solutions based on limited TC data only. The results were then used with a fast classification NN, to identify the shortest cycle to satisfy specs in all parts. The speed of the framework is such that it can be implemented for real-time optimization of curing process with active controlling of ovens/autoclaves. This can mitigate the risk associated with unknown BCs during processing of composite parts and reduce scrap rate in cases where parts go out-of-spec during processing.

5. ACKNOWLEDGEMENTS

We would like to acknowledge financial supports by the Boeing company, University of Washington, and State of Washington in USA.

6. REFERENCES

1. J. Fabris, D. Lussier, N. Zobeiry, C. Mobuchon, A. Poursartip. *Development of Standardized Approaches to Thermal Management in Composites Manufacturing*. In SAMPE Technical Conference Proceedings. Society for the Advancement of Material and Process Engineering. Seattle, WA, June, pp. 2-5. 2014.
2. J. Fabris, C. Mobuchon, N. Zobeiry, D. Lussier, G. Fernlund, A. Poursartip. *Introducing thermal history producibility assessment at conceptual design*. In SAMPE conference, society for the advancement of material and process engineering. 2015.
3. M. Mohseni, N. Zobeiry, G. Fernlund, Process-induced matrix defects: post-gelation, Composite Part A, DOI: 10.1016/j.compositesa.2020.106007, 2020.
4. L. Farhang, M. Mohseni, N. Zobeiry, G. Fernlund, Experimental study of void evolution in partially impregnated prepregs, Journal of Composite Materials, 54(11):1511-1523, 2019.
5. N. Zobeiry, A. Poursartip, The origins of residual stress and its evaluation in composite materials, In: Beaumont, P.W.R., Soutis S. and Hodzic A. (eds.), 2015.
6. K. Farnand, N. Zobeiry, A. Poursartip, G. Fernlund, Micro-level mechanisms of fiber waviness and wrinkling during hot drape forming of unidirectional prepreg composites, Composites Part A: Applied Science and Manufacturing, 103:168-177, 2017.
7. N. Zobeiry, A. Lee, C. Mobuchon, Fabrication of Transparent Composites, Composites Science and Technology, 197:108281, 2020.
8. N. Zobeiry, A. Forghani, C. Li, K. Gordnian, R. Thorpe, R. Vaziri, G. Fernlund, G., A. Poursartip, *Multiscale characterization and representation of composite materials during processing*, in: Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences. p. 20150278. https://doi.org/10.1098/rsta.2015.0278, 2016.

9. N. Zobeiry, J. Park, A. Poursartip, *An infrared thermography-based method for the evaluation of the thermal response of tooling for composites manufacturing*. J. Compos. Mater. 53, 1277–1290. https://doi.org/10.1177/0021998318798444, 2019.

10. J. Fabris, C. Mobuchon, N. Zobeiry, A. Poursartip, *Understanding the consequences of tooling design choices on thermal history in composites processing*, in: International SAMPE Technical Conference, 2016.

11. J. Park, N. Zobeiry, A. Poursartip, A, *Tooling materials and their effect on surface thermal gradients*, in: International SAMPE Technical Conference, 2017.

12. G. Fernlund, C. Mobuchon, N. Zobeiry, 2.3 Autoclave Processing, In: Beaumont P.W.R. and Zweben C.H. (eds.), Comprehensive Composite Materials II, 2:42-62, Oxford: Academic Press, 2018.

13. N. Zobeiry, K.D. Humfeld. *A Physics-Informed Machine Learning Approach for Solving Heat Transfer Equation in Advanced Manufacturing and Engineering Applications*. arXiv preprint arXiv:2010.02011, 2020.

14. N. Zobeiry, A. Stewart, A. Poursartip. *Applications of Machine Learning for Process Modeling of Composites*. In SAMPE Virtual Conference. 2020.

15. N. Zobeiry, J. Reiner, R. Vaziri. *Theory-guided machine learning for damage characterization of composites*. Composite Structures, 112407, 2020.

16. N. Zobeiry, K.D. Humfeld, *An iterative machine learning approach for discovery of theories underlying physical phenomena*, arXiv preprint arXiv:1909.13718

17. D. Van Ee, A. Poursartip. *HexPly 8552 Material Properties Database for use with COMPRO CCA and RAVEN*. Version 0.9. NCAMP. Wichita, KS (2009).