Accelerating Composite Cure Cycle Optimization with Combined Probabilistic Machine Learning and Finite Element Process Simulation

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ABSTRACT

Advanced composites are widely used in industries such as aerospace. To certify aerospace structures, the manufacturing process of composites is tightly controlled to ensure compliance with process specifications (i.e., process specs). For example, in autoclave curing of thermoset composites, process specs often limit the maximum temperature in the composite part due to exothermic reaction, maximum thermal lag between the part and autoclave temperature cycle, as well as maximum part porosity and minimum degree of cure. Given all the requirements in process specs, optimizing the temperature cycle in autoclave curing to reduce cycle time and hence increase production throughput is often challenging. While Finite Element (FE) process simulation is used for coupled analysis of heat transfer and thermo-chemical curing reaction of composites during the curing process, due to the long simulation time of high-fidelity simulation models, optimization in the entire design spectrum is not feasible, and most often relies on trial-and-error and engineering insights. In this study, we present a novel framework based on combined probabilistic Machine Learning (ML) and FE to accelerate the process optimization of composites. The probabilistic ML is developed based on the underlying theory of curing and a mathematical foundation of Gaussian Process Regression (GPR). Instead of trial-and-error or time-consuming grid search, this approach relies on targeted FE evaluation of selected cure cycles by the ML model, such that in a step-by-step simulation approach, an optimized solution is obtained. While this approach minimizes the effort to optimize cure processing conditions, it also enables the evaluation of non-traditional cycles such as multi-ramps and holds to minimize the autoclave cycle time. For validation, the framework is applied to optimize the cure cycle of a thick HEXECL AS4/8552 composite laminate cured on a typical Invar tool. A validated FE model is used for process simulation along with the ML model for targeted evaluation. Results show that with only a few analysis steps, an optimized solution can be obtained to satisfy process specs while minimizing cycle time.

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INTRODUCTION

Aerospace-grade fiber-reinforced thermoset composite parts are typically processed using an autoclave. The autoclave parameters during the curing process have a tremendous impact on the quality of end-products, such as the wing panel or fuselage in Boeing 787. However, the autoclave curing process is typically time-consuming with high operational costs. As such, it is common to perform comprehensive experimental thermal profiling combined with process simulations beforehand, to optimize autoclave processing parameters, including the temperature cycle.

Traditionally, Finite Element (FE) is heavily used in the process simulation and analysis[1-3]. However, given the complexity of the large aerospace parts, coupled with uncertainties associated with heat transfer in the autoclave, conducting a parametric study and process optimization using high-fidelity 3D FE process simulation proves to be quite expensive and time-consuming.

To accelerate this optimization process, Machine Learning (ML) based methods have been employed in recent years, including applications for process simulation and analysis using Deep Learning (DL) and Neural Networks (NN)[4-7]. Given that the success of these approaches heavily depends on the quantity and quality of training data, most of these approaches use either high-fidelity FE models or reduced-order, low-fidelity FE models to generate large amounts of data. For instance, an ML framework integrating two Recurrent Neural Networks (RNN) and one classification NN was developed for the active manufacturing control of autoclave curing process, utilizing data from reduced-order FE models[8]. In a separate study, a combination of data from reduced order 1D FE models and higher-fidelity 2D FE models was used to train surrogate NN models, aiming to optimize the curing process and stringer geometry for a stiffened wing panel[9].

However, generating data from experiments or simulation is both costly and limited, which in turn reduces the effectiveness of neural networks in engineering applications. Therefore, other machine learning methods that perform well with small datasets, such as Gaussian Process Regression (GPR)[10], are more advantageous when dealing with this scarcity of data. For composites applications, GPR-based optimization methods have been explored for various purposes, including accelerated kinetics characterization[11], failure characterization[12], and process monitoring[13] and others.

In this work, we present a novel GPR-based approach to optimize the cure cycle in an autoclave using a limited number of simulation iterations, as opposed to the time-consuming trial-and-error and method or grid-search. This automated GPR algorithm significantly accelerates the multi-objective optimization process of cure cycles for advanced aerospace composite. The effectiveness of the methos is demonstrated in the curing of a thick composite part, where with just a few simulation iterations, the cycle is minimized while meeting process specification requirements related to exotherm.

1. PART AND MATERIAL

From 1989 to 1995, a joint NASA-Boeing program titled Advanced Technology Composite Aircraft Structure (ATCAS) was conducted to investigate the design and manufacturability of composite components, with a focus on reducing cost and weight[14, 15]. One of the projects within the ATCAS program involved exploring the manufacturing capability of a thick composite part made from HEXCEL AS4/8552, a carbon fiber reinforced epoxy prepreg[16]. An illustration of this composite part (cross section) is shown in Figure 1. This part is 152 cm in length, 2.82cm in thickness and 45.7 cm in width. This flat part tested as a potential design for a future keel panel, features a thick solid laminate at the forward end (left end in Figure 1) to redistribute the high compressive keel chord loads. As the sandwich design is introduced from the aft (right end in Figure 1), ply drops and core tapers are arranged in such a way that the overall thickness of the panel remains constant at 2.82 cm from one end to the other. In the original ATCAS research, 30 thermocouples (TCs) were placed at various positions across the cross-section for thermal profiling.

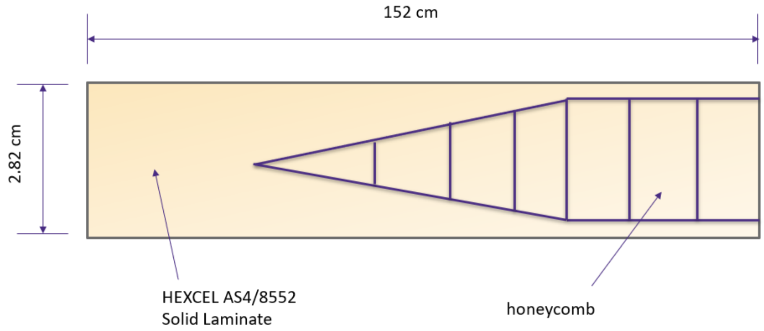

Figure 1. The Illustration of Composite Part (Cross-Section) in ATCAS Program[14]

For such a thick laminate, especially considering the high reactivity of HEXCEL 8552, the manufacturer's recommended cure cycle (MRCC) proves ineffective due to the excess heat buildup in the center of the solid section of the part during exothermic polymerization. Therefore, it becomes imperative to develop a custom cure cycle for such a part to regulate the temperature induced by the exothermic reaction, keeping it within acceptable limits. For the ATCAS program, reducing the total cycle time was not a focus. To lower the maximum part temperature, an additional 90-minute hold at 150°C was designed and validated, alongside MRCC holds at 110°C and 180°C. However, this resulted in a total cure time for this part of approximately 700 minutes in the ATCAS program, a duration which might be considered excessively long by today's standards. In this paper, for the same thick composite part considered in the ATCAS program, our primary interest lies in identifying the shortest cycle that meets process specifications with the least effort.

2. METHODOLOGY

2.1 Finite Element Process Simulation and Optimization

For the curing process simulation, several key material properties need to be characterized. These include the cure kinetics of the material, thermal properties of the part and tool (including specific heat capacity, thermal conductivity, and density), and heat transfer coefficients in the autoclave. In our study, we will employ an in-house python code developed at the University of Washington for 1-Dimensional FE Process Simulation, alongside previously characterized material properties[17, 18]. The simulated thermal stack is schematically shown in Figure 2. Both the part and the tool were discretized into ten elements, and the part's temperature history was recorded at three locations across its thickness.

For process simulations, based on the details of the ATCAS program, following assumptions were made:

- The leading TC is located at the solid section of the part (left end in Figure 1) with a thickness of $L_1 = 28\ mm$.
- The tool is an Invar tool with a thickness of $L_2 = 10\ mm$
- The heat transfer coefficients (HTCs) are set to be constant and $60\,\frac{W}{m^2K}$ above the part and $40\,\frac{W}{m^2K}$ below the Invar tool.

For the process optimization, the following constrains are applied:

- Temperature cycle must be a two-hold cycle as shown in Figure 2, with the variable parameters: T_1', T_2', t_1, T_1
- The heating rates, T_1' and T_2', must lie between 1 and 7 °C/min:
$$1 < (T_1'\ and\ T_2') < 7\ ℃/min$$
- The second hold must be at 180 °C for 120 minutes.
- The final cool down rate must be -3.5 °C/min.

The objectives of process optimization are as follows:

- The maximum part temperature due to the exothermic reaction < 185 °C
- The total cycle time must be minimized.

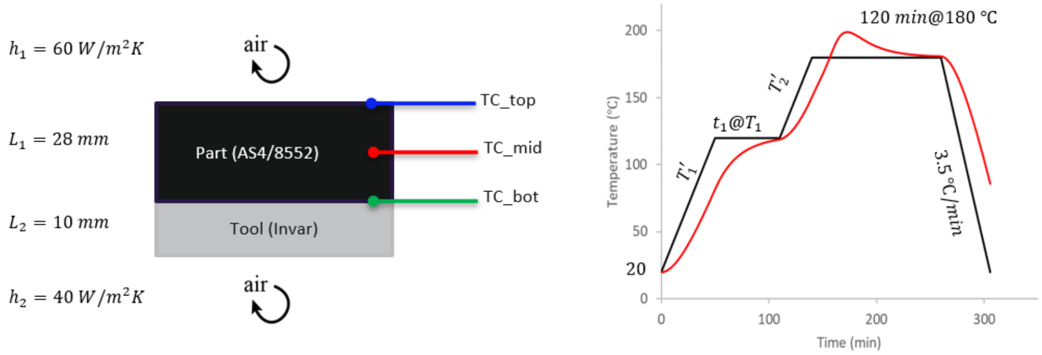

Figure 2. 1D Finite Element Process Simulation

2.2 Automated GPR Search

Gaussian Process Regression (GPR), a popular Probabilistic Machine Learning method, is the approach we have chosen in this study. The 1D FE process simulation detailed in section 2.1 will be incorporated inro the automated GPR algorithm. The flowchart for the automated GPR optimization is illustrated in Figure 3. Before initializing the GPR search, we first need to define a Cost Function for the optimization process which will be discussed in section 2.2.1. Based on this cost function and underlying optimization, we design a specific kernel for the GPR. For GPR initialization, several initial guesses are provided to initialize the search. Typically, in less than 15 iterations, we expect to find an optimal solution based on minimization of the cost function, and targeted evaluations by the GPR algorithm. After every iteration step, a new FE simulation is conducted to generate a targeted data point. This step can be potentially replaced with experiments in the future. If satisfied, the GPR optimization engine will break and stop the search process. Otherwise, the search engine will restart until we get the desired solution.

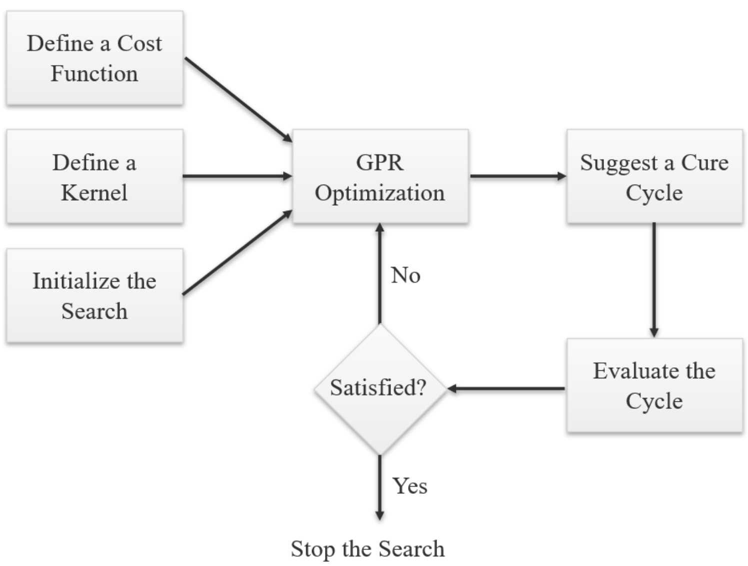

Figure 3. Flowchart for Automated GPR Search

2.2.1 COST FUNCTION

As shown in Figure 4, for GPR optimization, a custom cost function is designed based on maximum part temperature and total cycle time. The function is smooth, with slopes guiding the GPR toward the optimal solution. Notably, the function increases rapidly when approaching 185°C, which is the upper limit for the maximum part temperature. As with other regression problems in machine learning, our aim is to minimize the cost function to find the optimal solution. However, considering the time efficiency of the search algorithm, we have set up a threshold value for the desired cost function. If the function falls below the threshold, the GPR search engine will stop and produce a solution for further validation.

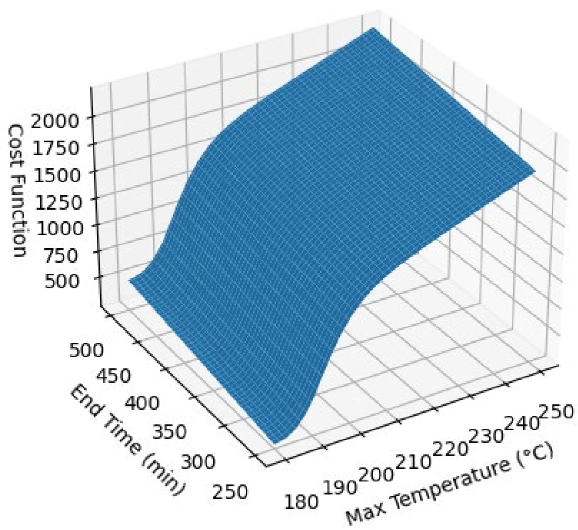

Figure 4. Cost Function to be minimized.

2.2.2 GPR KERNEL

To capture the complexities of the cost function, we have selected a linear combination of the dot product and Matérn kernel[10] with weight c_1 and c_2, respectively, as shown in equation (1). This forms the covariance function for Gaussian Processes.

1) The first part of the kernel is a dot product, which represents the linear covariance structure between the data points. This is designed to capture the linear trend in the cost function.

2) The second part of the kernel is a Matérn kernel with a smoothness parameter ν=2.5. This value is commonly chosen in machine learning problems[19]. The aim of the Matérn kernel is to model the non-linear structure of the response surface. The length scale, l, defines the range of spatial scales that the kernel can capture, spanning from small to large patterns. The combined effect of c_1 and l, and the resultant variety of shapes that the Kernel function can capture, is illustrated in Figure 5.

$$\Sigma(x_i, x_j) = c_1 \cdot (x_i \cdot x_j) + c_2 \cdot \left(1 + \sqrt{5}\frac{\|x_i - x_j\|}{l} + \frac{5}{3}\left(\frac{\|x_i - x_j\|}{l}\right)^2\right) e^{-\sqrt{5}\frac{\|x_i - x_j\|}{l}} \tag{1}$$

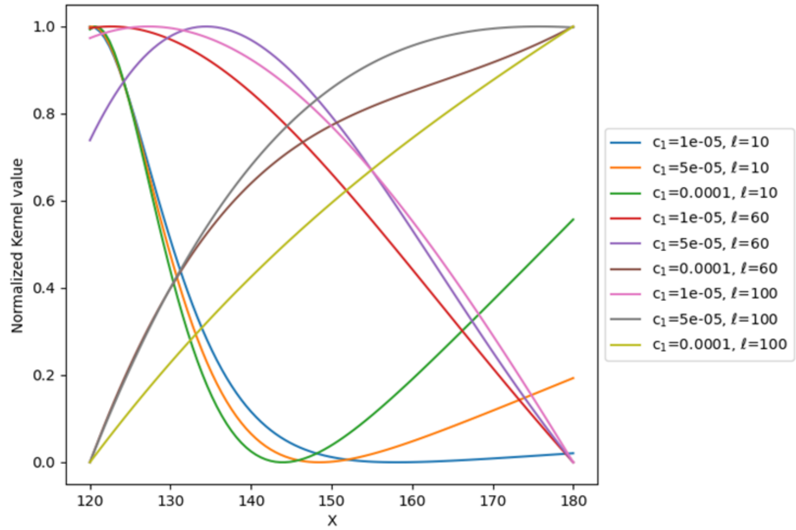

Figure 5. The Combined Effect of c_1 and l

2.2.3 INITIALIZATION

We initialized the GPR search with four initial guesses as shown in Figure 6. These initial guesses are based on our understanding of the impact of a hold temperature on exotherm. When the temperature is held at a specific level for an extended duration, partial exotherm heat is released and dissipated, and the degree of cure plateaus. This phenomenon significantly affects the maximum part temperature at the final hold, when the remaining heat is released. To aid the GPR in capturing this effect and expedite the optimization process, we begin the search with four cycles as shown in Figure 6. Without these initial guesses, the initialization would be random, possibly leading slower convergence of the search.

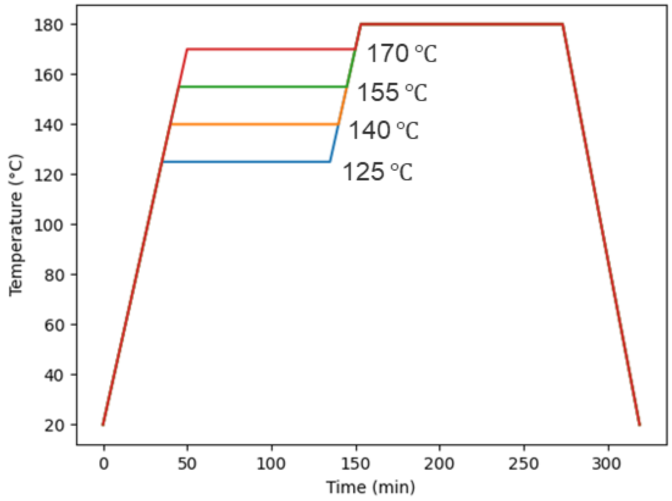

Figure 6. Several Cure Cycles as Initializer for GPR search

3. RESULTS AND DISCUSSION

3.1 GPR Optimization

As shown in Figure 7 and Figure 8, on average, after about 10 iterations, the automated GPR finds a satisfactory cycle based on the minimization of the cost function. After about 15 iterations, it discovers a zone of acceptable cycles that satisfy the exotherm condition (<185℃), with the total cure time less than 300 minutes.

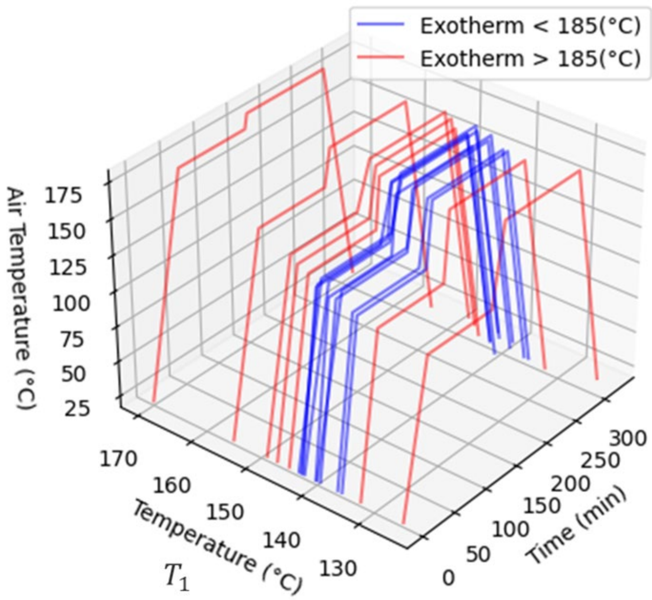

Figure 7. Cure Cycles by Automated GPR Search

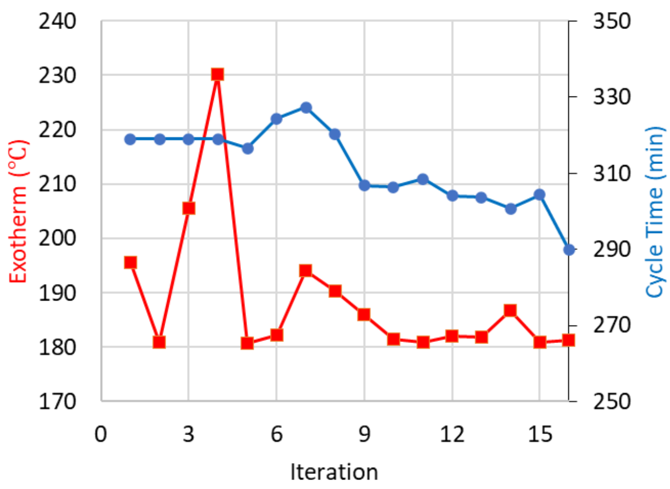

Figure 8. Training History of Automated GPR Search

3.2 Optimized Solution

After 15 iterations, we obtain an optimized parameter set:

- $\mathrm{T}_1' = 5.5\ ^\circ\mathrm{C/min},\ \mathrm{T}_2' = 6.5\ ^\circ\mathrm{C/min},\ \mathrm{T}_1 = 140\ ^\circ\mathrm{C},\ \mathrm{t}_1 = 95\ \mathrm{min}$
- Maximum temperature: 181.5 ℃
- Total time: 288 min

These values were used as input into the 1D FE process simulation (see section 2.1) and the resulting part temperature histories (at top, middle and bottom), degree of cure (at middle), and cure rate (at middle) are shown in Figure 9 and Figure 10.

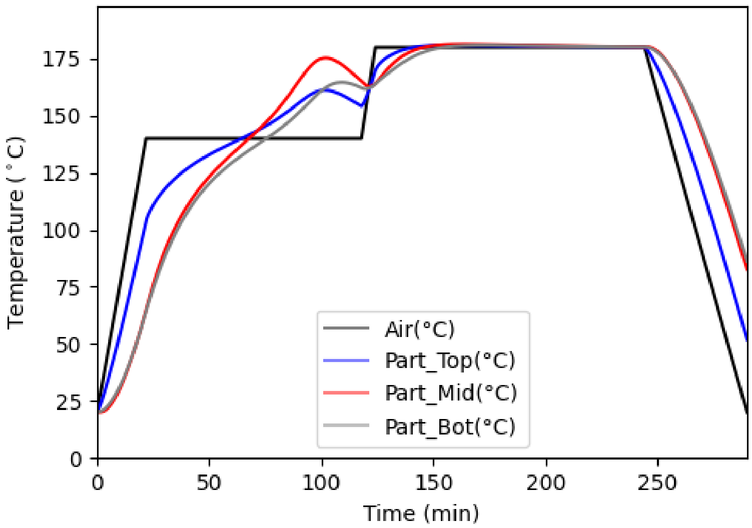

Figure 9. Part Temperature History at Different Position

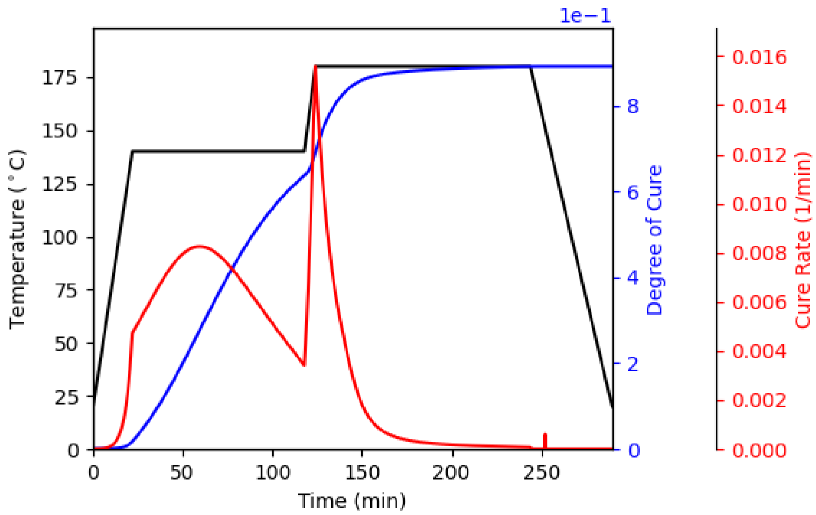

Figure 10. History of Degree of Cure and Cure Rate

3.3 Validation

Having obtained the optimized solution from the automated GPR search, we now compare it with the optimized solution for the same thick composite part from the original ATCAS program. As discussed earlier, in the ATCAS program, reducing total time was not considered. To reduce maximum part temperature, a cure cycle with an extra 90-minute hold at 150 ℃ was designed and validated. This resulted in the total cure time of around 700 min.

For comparison, our automated GPR algorithm predicts a cycle with a 95-minute hold at 140°C, ensuring that the maximum part temperature stays below 185℃. This result is similar to the additional hold (90 minutes at 150°C) introduced in the ATCAS program. The comparison between ATCAS optimized cycle and our selected GPR-derived cycle is shown in Figure 11. The original cycle time in the ATCAS program was about 700 minutes, while our solution, optimized via GPR, has a cycle time less than 300 minutes. Furthermore, the same GPR search engine, after just 15 iterations, has found several solutions with hold temperatures ranging from 135 to 145°C, and cycle times varying from 290 to 325 minutes, as shown in Figure 7 and 8.

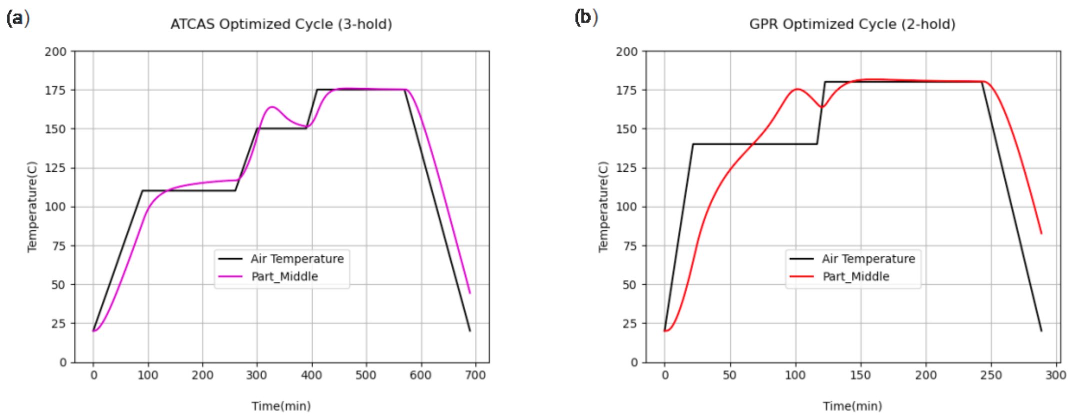

Figure 11. Comparison between ATCAS and GPR Optimized Cycle

4. CONCLUSION

In this paper, we have presented a novel framework combining probabilistic machine learning techniques, specifically Gaussian Process Regression (GPR), and the finite element method to efficiently optimize the cure cycles for advanced composites with limited number of iterations. To validate our approach, we conducted a case study for curing of a thick composite part, which was originally studied under the ATCAS program. Results demonstrated that the implementation of this GPR-based approach can drastically accelerate the optimization of curing cycles with just a few iterations. The results from the GPR-based method were compared with the outcomes from the ATCAS program, demonstrating a similar solution in reducing exotherm, while significantly reducing the total cycle time. This can potentially lead to lower production costs and higher production rates.

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REFERENCES

1. Johnston, A., P. Hubert, G. Fernlund, R. Vaziri, et al., *Process modeling of composite structures employing a virtual autoclave concept.* Science and Engineering of Composite Materials, 1996. **5**(3-4): p. 235-252.
2. Fernlund, G., A. Osooly, A. Poursartip, R. Vaziri, et al., *Finite element based prediction of process-induced deformation of autoclaved composite structures using 2D process analysis and 3D structural analysis.* Composite Structures, 2003. **62**(2): p. 223-234.
3. Zobeiry, N., A. Forghani, C. Li, K. Gordnian, et al., *Multiscale characterization and representation of composite materials during processing.* Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2016. **374**(2071): p. 20150278.
4. Zobeiry, N., A. Stewart, and A. Poursartip. *Applications of machine learning for process modeling of composites*. in *SAMPE Virtual Conference*. 2020.
5. Zobeiry, N., D. van Ee, and A. Poursartip. *Theory-guided machine learning composites processing modelling for manufacturability assessment in preliminary design*. in *Proceedings of the NAFEMS 17th World Congress, Quebec City*. 2019.
6. Humfeld, K.D., D. Gu, G.A. Butler, K. Nelson, et al., *A machine learning framework for real-time inverse modeling and multi-objective process optimization of composites for active manufacturing control.* Composites Part B: Engineering, 2021. **223**: p. 109150.
7. Zobeiry, N. and K.D. Humfeld, *A physics-informed machine learning approach for solving heat transfer equation in advanced manufacturing and engineering applications.* Engineering Applications of Artificial Intelligence, 2021. **101**: p. 104232.
8. Humfeld, K.D., D. Gu, G.A. Butler, K. Nelson, et al., *A machine learning framework for real-time inverse modeling and multi-objective process optimization of composites for active manufacturing control.* Composites Part B-Engineering, 2021. **223**.
9. Fu, H.L. and N. Zobeiry. *A Theory-Guided Machine Learning and Reduced-Order Finite Element Modeling Framework to Accelerate Process Simulation of Aerospace Composite Parts*. in *Aerospace Structures, Structural Dynamics, and Materials Conference*. 2023. San Diego, California.
10. Rasmussen, C.E. and C.K.I. Williams, *Gaussian Processes for Machine Learning*. 2006: MIT Press.
11. Wynn, M. and N. Zobeiry, *Investigating the Effect of Temperature History on Crystal Morphology of Thermoplastic Composites Using In Situ Polarized Light Microscopy and Probabilistic Machine Learning.* Polymers, 2023. **15**(1): p. 18.
12. Freed, Y., N. Zobeiry, and M. Salviato, *Development of aviation industry-oriented methodology for failure predictions of brittle bonded joints using probabilistic machine learning.* Composite Structures, 2022. **297**: p. 115979.
13. Schoenholz, C., S. Li, K. Bainbridge, V. Huynh, et al., *Accelerated In Situ Inspection of Release Coating and Tool Surface Condition in Composites Manufacturing Using Global*

Mapping, Sparse Sensing, and Machine Learning. Journal of Manufacturing and Materials Processing, 2023. **7**(3): p. 81.

14. Ilcewicz, L., P. Smith, C. Hanson, T. Walker, et al., *Advanced technology composite fuselage: Program Overview*. 1997.
15. Poursartip, A., A. Johnston, P. Hubert, and R. Vaziri, *An investigation of autoclave convective heat transfer.* Design and manufacturing of composites, 1998: p. 106-113.
16. HEXCEL, *HexPly 8552 Epoxy matrix (180°C/365°F curing matrix) Product Data 2016.* https://www.hexcel.com/user_area/content_media/raw/HexPly_8552_eu_DataSheet.pdf.
17. van Ee, D. and A. Poursartip *HexPly 8552 MATERIAL PROPERTIES DATABASE for use with COMPRO CCA and Raven.* https://www.wichita.edu/industry_and_defense/NIAR/Research/hexcel-8552/Additional-Documents-2.pdf, 2009.
18. Zobeiry, N., J. Park, and A. Poursartip, *An infrared thermography-based method for the evaluation of the thermal response of tooling for composites manufacturing.* Journal of Composite Materials, 2019. **53**(10): p. 1277-1290.
19. Cornford, D., I.T. Nabney, and C.K. Williams, *Modelling frontal discontinuities in wind fields.* Journal of nonparametric statistics, 2002. **14**(1-2): p. 43-58.