Data-driven Kinetics Modeling of Chemical Vapor Infiltration for Ceramic Matrix Composites Manufacturing

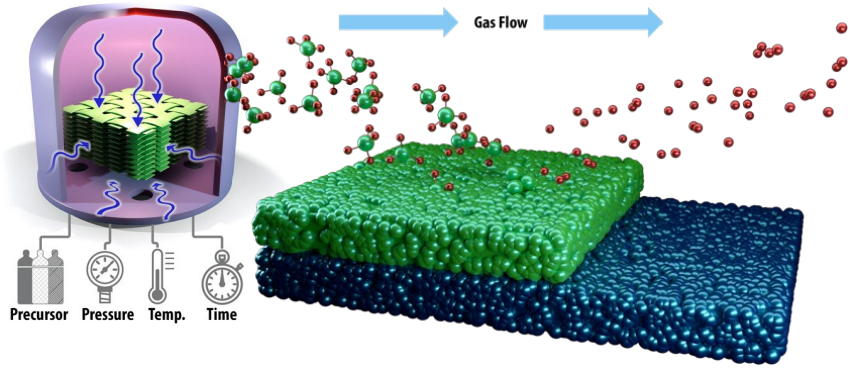
Chemical vapor infiltration (CVI) is a process that can be used to manufacture a phase-pure stoichiometric SiC matrix without the residual Si associated with the more commonly used Melt Infiltration (MI) process of SiC ceramic matrix fabrication. CVI-ceramic matrix composites (CMCs) offer an increase of up to 165°C (300°F) in temperature capability as compared to a melt infiltration (MI)-CMC. This higher temperature capability is anticipated to lead to fuel efficiency benefits in gas turbines while retaining CMC's weight and temperature capability advantage over typical metal alloy components.

However, the CVI process has some drawbacks, including longer process times required to densify the preform and a higher residual porosity in the final CMC component than typically found in MI-CMCs. Overcoming these challenges would allow an expansion of the range of SiC based CMC products and product capability.

This project aims to address the limitations of the CVI process by demonstrating a workflow that integrates chemical kinetics, bulk reactor fluid dynamics, and deposition connecting local physical conditions (i.e., chemical species partial pressures and temperatures) to ceramic deposition rates. The development of an updatable integrated model would provide a step change in assessing risk, optimizing, and making superior CVI-CMC product development decisions.

To address the challenges associated with the CVI process, the GE-ORNL team will build on the foundation of ORNL's recently demonstrated CVISim workflow that integrates high-throughput CFD simulation of chemical reactor fluid flow and temperature via Open Source Field Operation and Manipulation (OpenFOAM) and artificial intelligence.

In this project, researchers used a neural network to create a surrogate model that can efficiently represent computationally intensive CFD calculations obtained from high-performance computing, allowing them to explore the vast parameter space of the CVI process and understand chemical kinetics. They used a ResNet-based neural network to predict the output for a set of chemical kinetic parameters that had not been simulated before. They then used simulated annealing to identify a set of kinetic parameters that can replicate the experimental results. The results show that they find better kinetic parameter sets close to the experiment results as they progress with simulated annealing.



The present study has demonstrated that high-throughput CFD and modern data analytics on the HPC platform can be used to develop a high-fidelity surrogate model that captures the CVI process for rapidly optimizing kinetics parameters. The outcome of this project will enable accurate prediction of advanced processing costs and description of the operational performance of the CVI process before capital investment, as well as reducing scale-up risk and accelerating commercialization.