DESIGNING PHYSICS-CONSTRAINED NEURAL NETWORKS TO DEVELOP THERMOCHEMICAL MODELS FOR MATERIAL RESPONSE CODES

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Introduction

A neural network is a collection of algorithms that work together in a manner similar to the human brain to recognize trends. Much like the human brain they are capable of recognizing patterns that help to categorically identify objects; however, they can also identify more complex mathematical and physical trends among large samples of data. This research seeks to make use of these capabilities to develop models that predict material response of materials. The property of interest is the effective permeability of carbon composites used in thermal protection systems. Currently, a verified means of generating the extensive database of effective permeability measurements that will train the neural network has been established and a discussion of such composes the majority of this presentation.

Effective permeability is an important property for carbon composites as it impacts the mitigation of heat transfer during the entry process of space capsules. Carbon composites used as TPS materials are low-density materials that consist of a network of carbon fibers infused with a resin (also referred to as the matrix). The composites used on space capsules are highly porous with the fiber and resin occupying no more than 20% of the total volume. The high porosity allows gases to flow through the material. For example, the resin decomposes (process called pyrolysis) and travels through the charred (completely pyrolyzed) network of fibers. Similarly, boundary layer gases can penetrate the material causing in-depth gas-phase and gas-surface reactions [1].

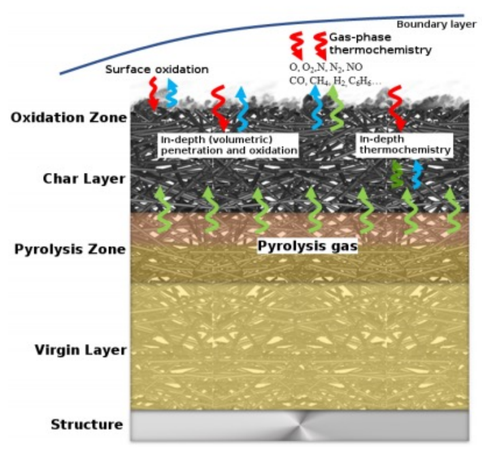

Figure 1. Physical processes occurring on carbon-phenolic TPS

Current material response codes formulate the momentum transport from these penetrating gases through the use of volume-averaged models. Such approaches require model closure: effective permeability of the composite. The goal of this research was to demonstrate the ability of the SPARTA direct simulation Monte Carlo (DSMC) solver to accurately and efficiently model the effective permeability of porous media. The synthetic microstructures used for these purposes were generated using Fibergen, which was shown to reproduce the effective permeability measurements for the Fiberform heatshield material of Marschall and Milos [2]. Results were also compared against the experimental dataset of Panerai et al. [1]

Methodology

All microstructures were generated with the use of Fibergen, and permeability calculations were performed using the DSMC method. Fibergen uses dimensions of the domain to be simulated, target bulk porosity, nominal fiber orientation, nominal fiber radius, and specified variances to generate cylindrical fibers. To replicate the FiberForm microstructure, the radius of a cylindrical fiber is sampled from a Gaussian distribution with a mean of 5 μm and standard deviation of 0.1 μm [3]. The DSMC technique is a stochastic approach that simulates the Boltzmann equation. A detailed description of the DSMC technique and models can be found in Refs. [4]. The DSMC simulations are performed using the open-source DSMC solver Stochastic Parallel Rarefied gas Time-accurate Analyzer (SPARTA) [5, 6, 7], which uses a multi-level Cartesian mesh to track and collide particles.

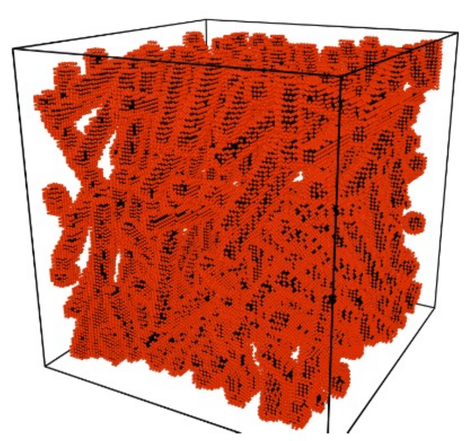

Figure 2. A sample microstructural image generated synthetically using Fibergen

Results

It was observed that the microstructures of FiberForm generated using Fibergen reproduced the effective permeability from two independent experimental measurements [1, 2] with errors within 10 % at low temperatures and high pressures. A systematic increase in the error was observed at high temperatures and low pressures for some samples, which could arise from the limitation of the Klinkenberg formulation that was used to interpret the experimental and simulation results. The initial validation with FiberForm was extended to the full composite through a novel infusion approach for the digital microstructures. Comparison of the effective permeability with the experimental data indicated good agreement. A new relation for the effective permeability was obtained through additional DSMC simulations, and it was demonstrated that the relation could be used for gaseous species that were not explicitly simulated to derive the relation. Avenues for new targeted experiments have been identified and additional validation will be performed in the future.

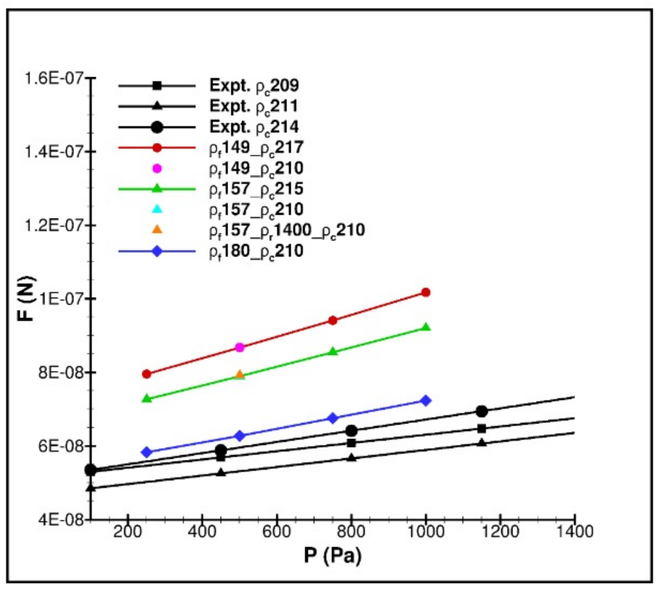

Figure 3. Comparison of DSMC simulations with experimental data of the full composite.

Current/Future Work

The next step in this research is currently underway and involves the development of a robust neural network to autonomously predict effective permeability with high fidelity, efficiency, and accuracy. The objective is to construct a neural network capable of modeling effective permeability for any combination of microstructure and flow properties. It has already been shown that support vector regression (SVR) can replicate permeability calculations of Fiberform with relative accuracy. Figure 2 shows the results of a comparison of the permeability force calculated from the SVR model to that calculated from the experimental results of Panerai et al. [1].

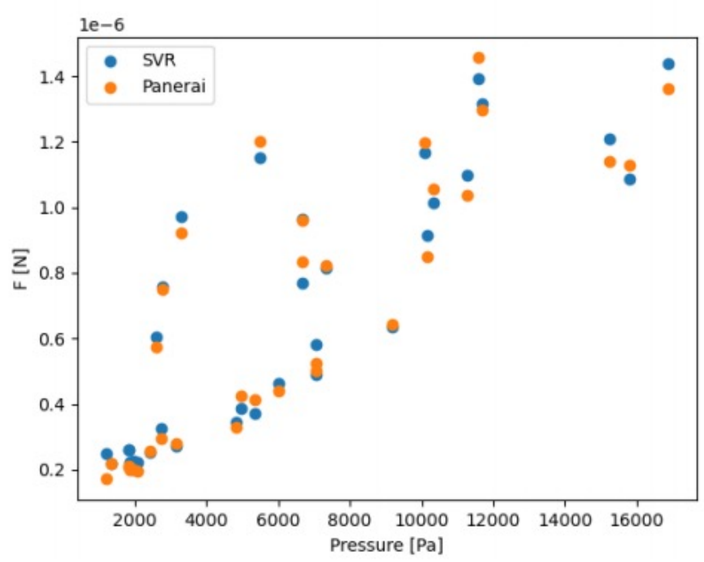

Figure 4. Comparison of SVR and experimental fit of Panerai et al.

With a means to build a permeability database now established and preliminary machine learning results obtained, the next step is to implement ResNet for the sake of summarizing the microstructure voxel image as a more tractable set of values to feed into a convolution neural network along with the other features: temperature and pressure. In this scenario, the microstructure image would be substituted for the porosity/sample density of the material, which has proven to be lacking as a robust representation of the material.

References

[1] F. Panerai et al. International Journal of Heat and Mass Transfer101(2016), pp. 267–273. [2] J. Marschall and F. S. Milos. Journal of Thermo-physics 1 and Heat Transfer12.4 (Oct. 1998), pp. 528–535 [3] F. Panerai et al. Journal of Thermophysics and Heat Transfer28.2 (Apr. 2014), pp. 181–190. [4] . D. Boyd and T. E. Schwartzentruber.Nonequilib-rium Gas Dynamics and Molecular Simulation. Vol. 42.Cambridge University Press, 2017. [5] S. Plimpton et al.Physics of Fluids31.8 (2019), p. 086101. [6] M. A. Gallis et al. PhysicalReview Fluids1.4 (2016), p. 043403. [7] M. Gallis et al. Physical Review Letters118.6(2017), p. 064501.