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Prediction of Permeability for Porous Materials Using a Surrogate Model

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Abstract: Permeability of porous media is an important material property that dictates the flow of gases through the media. The computation of permeability through complex structures is a computationally intensive and tedious process. Surrogate modeling of physical simulations offer a significantly cheaper alternative to obtain permeability. The main objective of this work is to develop a surrogate model that approximates the physical fluid simulations through a porous material. This work focuses on the development of an objective function which relates the permeability of the porous material with the simulation conditions and porosity of the material. The objective function is realised using support vector regression (SVR), which was found to be a robust technique in order to capture the complex relationship between temperature, average pressure, and porosity of the material. The objective function was validated against a wide range of inputs, even extending beyond the range of trained values, and experimental results to justify the use of the developed surrogate model.

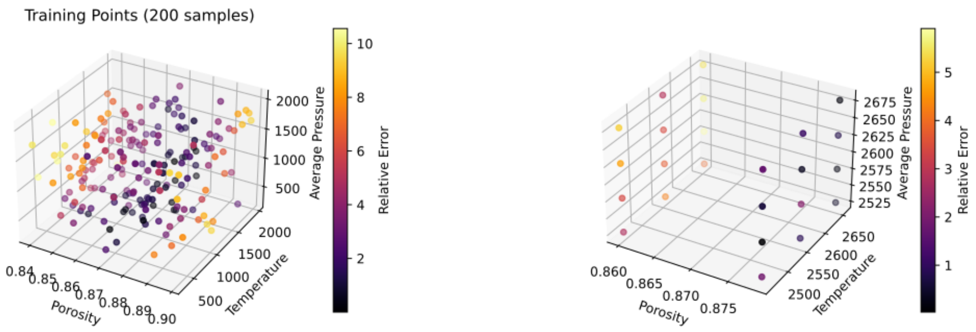
Keywords: Porous media flow, Non-continuum flows, Surrogate models.

1 Introduction

The use of surrogate modeling in the field of computational fluid dynamics (CFD) is gaining traction in recent years mainly because of its ability to effectively eliminate the need for repetitive numerical simulations involved in computing the performance parameter for a wide range of inputs. The current work uses SVR to train a surrogate model that accurately predicts the permeability of porous media, thereby significantly reducing the computational time. To demonstrate the utility of surrogate modeling, permeability of porous carbon composites used as heat shield materials on space capsules [1] is predicted using the trained SVR model. The surrogate model provides the permeability as a function of pressure, temperature, porosity, and the gaseous species flowing through the material. The main advantage of a surrogate model is that an algebraic model that contains relevant physical information can be obtained. These models can then be used in large-scale engineering studies.

2 Problem Statement

Since the entry of space capsules occur at high altitudes, the flow inside porous heat shield materials occur in the non-continuum regime. The analysis of Stardust, a sample return mission indicates that the flow inside the porous heat shield material is either in the transition or slip regime. Therefore, analytical relations that are derived either in the continuum or in the free-molecular limit cannot be used to predict the permeability for flight-relevant conditions. The permeability under these conditions are computed using the direct simulation Monte Carlo (DSMC) technique [2]. The DSMC method can simulate all relevant physics, including convection, multi-component diffusion, gas-phase and gas-surface chemistry, and it is accurate for flow conditions ranging from continuum to free-molecular using the same set of collision model parameters. With the ability to decouple the surface and flow mesh, arbitrarily complex geometries can be imported into



(a) Comparison against training data.

(b) Comparison against test data.

Figure 1: Error between the SVR surrogate model and the *ground truth* obtained from DSMC-Fibergen computations.

DSMC solvers. Therefore, it is an ideal technique to obtain material permeability of complex porous heat shield materials. The porous material is generated using an in-house digital tool called Fibergen. It uses the dimensions of the domain to be simulated (also referred to as "box"), target bulk porosity, nominal fiber orientation, nominal fiber radius, specified variances to generate cylindrical fibers in three-dimensions, and then incorporates the resin into the porous carbon network. The Latin hypercube sampling technique is used to generate over 200 simulation data points, and the SVR network is trained against this data (Fig. 1a). Comparison against test data beyond the range of trained data indicates that the errors are within 5% (Fig. 1b), which is within the statistical uncertainty of the architecture of the porous carbon network.

3 Conclusion and Future Work

In this work, we set out to develop a predictive model to estimate material permeability based on surrogate modeling to minimize the computational costs and to improve the utility of these computations in large-scale engineering studies. The surrogate model predicts the permeability within the statistical uncertainty expected for the material under investigation. Future work includes:

- Validation of the developed surrogate model against the experimental data set of Panerai et al. [3].
- Extending the developed predictive model to multi-species gaseous flow.
- Incorporating the rate of oxidation of chemical species as a mathematical variable in defining the surrogate model.
- Incorporating the effect of pyrolysis on the permeability of the material.

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