3rd International Conference on Tomography of Materials and Structures
Lund, Sweden, 26-30 June 2017, ICTMS2017-137

The Porous Materials Analysis open-source software for material properties and response based on micro-tomography

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Keywords: material properties, oxidation, conductivity, tortuosity

Summary: A framework for determining material properties and response based on its micro-structure is presented. The framework called Porous Materials Analysis (PuMA) allows for the quick import and visualization of tomographic datasets, and for computing properties such as porosity, specific surface area, effective thermal conductivity, tortuosity, and representative elementary volume.

1. INTRODUCTION

Micro-tomography has become a powerful tool in material science applications, allowing for non-destructive characterization of a material micro-structure at a sub-micron resolution. The resulting 3D representations provide an excellent computational grid upon which to calculate effective material properties.

With the goal of supporting the development of material response models for ablative thermal protection systems, the Porous Materials Analysis (PuMA) software has been designed as a computational framework to extract material properties and response from microtomography or artificially generated micro-structures. PuMA allows for the calculation of porosity, specific surface area, effective thermal conductivity, tortuosity, representative elementary volume, and implements a micro-scale decomposition model [1]. PuMA is written in C++, with a graphical user interface built on QT and a visualization toolkit based on OpenGL. A schematic of the software architecture is shown in Fig. 1a.

2. DETERMINATION OF EFFECTIVE MATERIAL PROPERTIES

Using the PuMA computational framework, basic material properties can be calculated. The porosity and volume fractions are calculated as a ratio of void voxels to domain size. The specific surface area of a material is calculated using the marching cubes algorithm as a sum of individual areas of each triangle in the micro-tomography iso-surface.

A finite-difference method [2] is implemented to determine the effective thermal conductivity of a composite material based on its constituent properties. A random walk method is also implemented to solve the conduction through a composite porous media.

The tortuosity of a material as a function of Knudsen number is found through a random walk technique [3] using a Maxwell-Boltzmann velocity distribution for the particles. The continuum tortuosity is computed by solving the diffusion equation in the voids of the material using a second order finite-difference method [2].

Finally, representative elementary volume analysis can be conducted by determining the variance in effective material properties as a function of domain size.

The calculation of each effective material property has been verified against analytical solutions and applied to complex fibrous structures [4].

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3. MICRO-SCALE DECOMPOSITION

At high temperature, carbon fiber ablators undergo mass loss due to oxidation, sublimation, and spallation (mechanical mass loss due to shear). PuMA implements a particle-based method [5] [1] to simulate the micro-scale oxidation of carbon fiber materials. A Brownian motion technique is used to simulate diffusion, and a linear interpolation method [1] is used for collision detection based on the voxel data. A sticking probability method is used to simulate surface recession. The implementation of the method was verified against analytical solutions [6] and was applied to tomographic representations of ablative materials in various regimes [1] [4], as shown in Fig. 1b.

An important feature of the oxidation model is the ability to determine the effective material properties of a material during its decomposition. This becomes critical in macro-scale modeling, but is not typically available through physical experiments.

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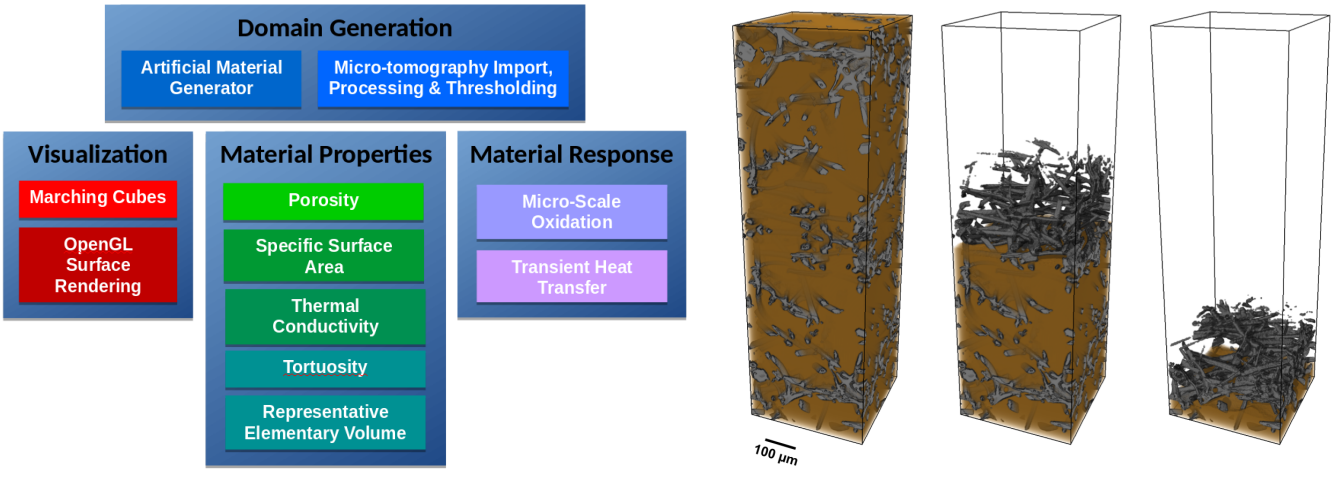

Figure 1: (a) Organizational schematic of the PuMA software. (b) 2000K oxidation simulation on a carbon fiber preform, FiberForm®, filled with a low density phenolic matrix.