High temperature permeability of fibrous materials using direct simulation Monte Carlo

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Abstract

Porous carbon fiber materials are used as effective insulators in many applications where high temperatures are involved. In particular, they are used as the substrate of ablative thermal protection materials for atmospheric entry systems. In this application and in many other industrial uses, quantifying the permeability of porous materials is needed to compute the flow rate of gases through them, under certain environmental conditions. In this work, direct simulation Monte Carlo (DSMC) simulations are used to compute permeability of several fibrous substrates to high temperature gases. The actual porous geometry of the materials is digitized using X-ray microtomography. Numerical results at various pressures and Knudsen numbers are compared with experimental data published in the literature. The method confirms that the pressure dependence of effective gas permeability is well represented by the Klinkenberg formulation. The method is validated by showing close agreement between measurements of permeability from simulations and experimental investigations. Four carbon fiber materials with different microstructures are investigated. We show that the permeability strongly depends on the pore size distribution, as well as on

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the porosity of the material.

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1. Introduction

The hypersonic entry of a spacecraft in a planetary atmosphere requires Thermal Protection Systems (TPS) able to manage the heat received from freestream plasma. For very high entry speeds, ablators are the only option
5 as TPS materials. A successful class among the ablative materials family are lightweight porous materials based on a fibrous carbon insulator impregnated with phenolic. As these materials are highly porous, when performing material response simulations, one needs to account for the transport of gases through the microstructure. Gas transport through a porous material is regulated by the
10 characteristic scale of the microstructure and that of the mean free path of the percolating flow. A parameter used to quantify this transport is the material permeability. Instances such as the flow of pyrolysis gas products, the penetration of hot boundary-layer gases, or the use of transpiration-cooling systems highlight the importance of internal gas transport in TPS materials. The gas
15 permeability of a material must be known before the gas flow through it can be properly modeled. In general, data regarding the permeabilities of porous ablators is limited and challenging to measure experimentally.

In this paper we use a particle-based method, direct simulation Monte Carlo (DSMC) [1], to compute the permeability of low-density carbon fiber materials
20 based on their digitized volumes. DSMC is a numerical method for approximating the Boltzmann equation. It was originally proposed for rarefied and transitional flows but has since been applied to near-continuum and continuum flows. DSMC can provide an accurate model for the entire boundary layer including the flow within the microstructure, where the size of the fibers may approach
25 the mean-free-path of the flow. As the permeability of a porous material is a function of the distribution of its micropores, in this paper, the computational domain for DSMC simulations is obtained from three-dimensional (3D) images

of the actual material microstructure acquired using X-ray microtomography (micro-CT). The technique allows to resolve the material into a 3D Cartesian
30 mesh with a spatial resolution sufficient to discretize the fibrous structure.

A few examples can be found in the literature where rarefied flow simulations are applied to the determination of permeability of fibrous structures. White *et al.* [2] used the DSMC to investigate the permeabilities of two ablative materials, one cork-phenolic and one carbon-phenolic, in both their virgin and
35 pyrolyzed states. They performed micro-CT scans of samples and imported the corresponding meshes for use in DSMC. They validated the method by comparing numerical results with experimental permeability measurements from a Berea sandstone material. The materials' permeabilities increased five to ten times following pyrolysis. They also found that the ablative materials were
40 more permeable to argon than the pyrolysis gas, without investigating the presence of Klinkenberg effects in these materials. Stern *et al.* [3] computationally investigated the permeability of digitized fibrous materials generated from randomly oriented fibers at varying angles and porosities. Using DSMC the authors showed agreement with heritage data on refractory insulators. De Socio and
45 Marino [4] performed both experiments and numerical simulations to investigate the dynamics of gases in permeable media. The experimental effort consisted in applying a pressure differential across a stainless steel cylinder filled with glass spheres by manually controlling the mass flow rate, to reproduce rarefied conditions. The extracted pressure profile was compared with that obtained from
50 two-dimensional DSMC simulations using a modified surface collision routine. De Socio and Marino [4] showed that a Knudsen-minimum type phenomenon was observed, meaning that there is a minimum in the measured permeability at a critical Knudsen number value, and higher permeability at Knudsen numbers lower and higher than the critical one. Kalarakis *et al.* [5] calculated the ni-
55 trogen gas permeability of a two-dimensional reconstructed porous media using two different techniques, the DSMC and a modified lattice-Boltzmann method, for Knudsen numbers in the 0.1-10 range. They reproduced the Klinkenberg equation very closely over the entire transition flow regime. Oshima *et al.* [6]

performed DSMC simulations on nanoscale channels filled with randomly arranged solid spheres, in order to attain target values of the porosity. They showed that the particle diameter had a significant impact on the permeability even at fixed porosity. They also computed a mass flux proportional to the pressure gradient, which agrees with Darcy’s law. Li and Sultan [7] studied the Klinkenberg slippage effect using a direct simulation Bhatnagar-Gross-Krook method and computed the gas permeability by pore-scale simulations at different pressures. They validated the Klinkenberg correlation model at low and high Knudsen numbers. In [8], Jaganathan et al. used 3D images of the microstructure of fibrous media obtained by digital volumetric imaging (DVI) to compute permeability using computational fluid dynamics (CFD). Results were compared with analytical models of the normalized permeability as a function of the material volume fraction. The authors did not account for slip effects.

The present work is structured as follows. In section 2, we review the approximations used to model the mass flow through a fibrous material given a known pressure gradient in the continuum and Knudsen regimes. Two parameters, the effective permeability and the permeability slip parameter, are needed to fully close the approximations. In section 3, we summarize the method used to digitize porous structures and we describe the materials investigated. Section 4 introduces the numerical DSMC method used in this work. In section 5, we verify DSMC calculations of permeability with analytical solutions for 2D square arrays of cylinders at various Knudsen numbers. In section 6, we validate our approach by comparing results from simulations with values measured experimentally. We compare with data by Panerai *et al.* [9], who measured permeability data of FiberForm in Ar flow, at temperatures from 310 to 1320 K, using a flow tube experimental setup. FiberForm[®] (Fiber Materials, Inc., Biddeford, Maine, USA) is the substrate for NASA’s phenolic-impregnated carbon ablator (PICA), used in entry missions like Stardust and the Mars Science Laboratory. We show that the Darcy approximation and its Klinkenberg form are valid formulations for the materials that are studied. We also study different porous materials and show that the permeability is a strong function of

90 the topology of the pores other than just the porosity of the material. Finally,
section 7 summarizes the findings in the paper.

2. Permeability of porous insulating materials

The permeability of porous substrates for TPS materials, has been the sub-
ject of a limited amount of investigation. Marschall and Milos [10] performed
95 permeability experiments on a range of rigid fibrous refractory insulators using
a flow tube apparatus at NASA Ames Research Center. They forced a known
mass flow rate of air through a cylindrical sample of material plugging the tube,
and measured the pressure upstream and downstream of the material. They
combined the ideal gas law, conservation of mass and the differential form of
100 Darcy’s law, to yield the relation

$$\dot{m} = -\frac{AM}{\mu RT} KP \frac{dP}{dx}, \quad (1)$$

where A is the cross-section area of the sample, $\dot{m}$, μ , M , T and P are the
mass flow rate, viscosity, molar mass, temperature and pressure of the gas, re-
spectively, K is the effective permeability and R is the universal gas constant.
Marschall and Milos [10] demonstrated that rarefied-flow effects for materials
105 such as FiberForm are significant and that pressure dependence of the perme-
ability is well expressed by the Klinkenberg form

$$K = K_0(1 + b/P) \quad (2)$$

where K_0 is the material permeability in the limit of continuum flow, and b is
the permeability slip parameter that varies with temperature and gas viscosity.
The quantity b/P is a function of the local Knudsen number, and both K_0
110 and b are dependent on the microstructure of the material [10]. K_0 and b are
both tensors, $\overline{\overline{K_0}}$ and $\overline{\overline{b}}$, that we assume diagonal since the samples were cut in
directions aligned with their principal axes. Additionally, we assume that both
components of the tensor in-plane are equal and we refer to them as $K_0^{\parallel}$ and $b^{\parallel}$,
respectively. Similarly, through the thickness of the material, the components

115 of the permeability and slip parameter tensors are now written as $K_0^\perp$ and $b^\perp$.
 Marschall and Milos reduced the data and defined a permeability constant F ,
 expressed as

$$F = \frac{\mu \dot{m} R T L}{A M \Delta P} = K_0 (P_{avg} + b) \quad (3)$$

where P_{avg} and ΔP are the average pressure in the sample and the pressure
 difference across the sample, respectively. Since the present simulations are
 120 compared with data obtained using the same experimental method, the same
 convention is also adopted for our analysis. Additionally, they were able to de-
 rive, from an analogy for gas flow in a straight capillary tube with slip boundary
 condition, a scaling law for b based on a measurement made at a reference gas
 composition and temperature as

$$\frac{b(T, M, \mu)}{b^*} = \frac{\mu}{\mu^*} \sqrt{\frac{\pi R T}{2 M}} \sqrt{\frac{2 M^*}{\pi R T^*}} = \frac{\mu}{\mu^*} \sqrt{\frac{T}{T^*} \frac{M^*}{M}}. \quad (4)$$

125 where b^* is a reference permeability slip factor measured using a reference gas
 (M^* , μ^*) at reference temperature T^* . Their data for FiberForm showed a
 significant amount of scatter between two groups of the four studied samples,
 likely due to large variations in the microstructure of FiberForm from batch to
 batch.

130 The permeability factors K_0 and b are a function of the size and distributions
 of the microstructure of the material. We will show using DSMC simulations
 that materials with the same porosity that have different microstructure distri-
 butions will have different permeability.

3. Porous materials and microtomography imaging

135 In this study we focus on fibrous materials that are used as substrates for
 low-density carbon/phenolic ablators. The state-of-the-art material within this
 class is the NASA's phenolic-impregnated carbon ablator (PICA), which was
 successfully used during entry missions like Stardust (Earth reentry at 12 km/s)
 and the Mars Science Laboratory (MSL – Mars entry at 5.5 km/s). PICA
 140 is made through a resin-infusion process of FiberForm. A rendering of the

substrate is shown in Fig. 1a. Thanks to a NASA's technology transfer on infusion processing, SpaceX has also developed its own carbon/phenolic ablator (PICA-X). PICA-X, flight-proven during Dragon reentry from the ISS, uses Calcarb CBCF[®] [11] (Mersen, Courbevoie, France) (see Fig. 1d) as preform material.

Figure 1: Volume rendering of microtomography of some Thermal Protection Materials being investigated.

Both FiberForm and Calcarb are rigid materials, with average porosities

higher than 85%. Their micro-structure is characterized by fibers preferentially aligned at about $\pm 15^\circ$ with one of the planes (that perpendicular to the direction of compression during manufacturing). The arrangement of the fibers provides the material **transverse isotropic** properties, with the highest insulation capabilities (lowest thermal conductivity) in the “through-thickness” (TT) direction.

Examples of variations around the same material class are conformal and flexible carbon/phenolic composites [12, 13]. These are manufactured according to a similar infusion processing as that used in heritage rigid ablators. However, unlike PICA, these new materials adopt flexible felts as the substrate (see Fig. 1c). Felt substrates suitable for conformal ablators are made of ceramic, polymers or carbon fibers. The use of a flexible preform has multiple advantages, chiefly an improved strain-to-failure that allows for manufacturing of larger structures, with more complex geometries. While felts have **transverse isotropic** properties as rigid substrates, the possibility of conforming the material around a certain shape allows to align the fiber with the surface, and therefore achieve the best insulation performance over the entire shape.

In this work we investigated a sample of virgin FiberForm, a sample of FiberForm that was oxidized by pure oxygen at 1200 K in NASA Ames flow-tube reactor [14] (see Fig. 1b), and samples of Calcarb and Morgan carbon felt (Morgan Advanced Materials, Fostoria, Ohio, USA). This felt is one of the candidate precursors for the manufacturing of conformal PICA (C-PICA) [13]. The samples were cut from large billets of materials in the TT direction.

In order to produce a digital representation of the materials’ microstructure, we acquired micro-CT images at the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory. We extracted samples by cutting material billets in the principal manufacturing directions. The specimens were placed onto the tomography stage, aligning the sample with the axis of the stage. There are small unavoidable errors associated with cutting and installation operations, however we used our best practice to minimize them. Scans were performed at a X-ray energy of 14 keV, acquiring 1024 radiographs over a 180° rotation for

each scan. The projections were reconstructed as voxelized images, and then segmented using the same work-flow described in Ref. [15]. The tomography reconstruction process was based on a Fiji [16] plugin developed in-house at the ALS. The plugin was used to set input parameters for the Octopus reconstruction software [17] that applied the classical filtered back-projection algorithm by Kak and Slaney [18] for reconstruction and a removal algorithm for ring artifacts [19]. A 3D bilateral filter, developed for tomography images [20], was finally applied to the reconstructed data to improve edge-detection and reduce noise. The resulting filtered tomographies presented a bi-modal histogram of gray-level intensities. Segmentation was performed by choosing a single threshold value in correspondence of the local minimum in between the two modes of the histogram. The segmentation allowed to produce binary 3D images, where each voxels within the void phase of the microstructure is represented as black (gray level 0) and each material (carbon) voxel is represented as white (gray level 255). The quality of the segmentation was assessed by comparing tomography visualizations of each material with information available from scanning electron micrographs.

Micro-CT scans were performed by accurately placing the sample onto the imaging stage, in order to minimize the misalignment between the TT axis and the axis of rotation of the stage itself. Computational domains for DSMC simulations were prepared by extracting cubic volumes ($\approx 520 \mu\text{m}$ edge) of similar cell size.

Image renderings of the four samples are presented in Fig. 1. The figures were obtained by processing the micro-CT images in the Avizo 7.0 software (FEI Visualization Sciences Group, Burlington MA, USA). It can be qualitatively observed that the virgin FiberForm sample used here is significantly less porous than the virgin samples of felt and Calcarb. Due to the anisotropy of the materials, as for the thermal conductivity, the permeability will differ whether the gas flow in the TT direction of the material or in the normal (“in-plane”, IP) direction.

Figure 2: a) Microtomography rendering of FiberForm and b) correspondent distance field for the inter-fiber pores

4. DSMC frame and computational domains

It has been highlighted in a previous work [10] that rarefied-flow effects are significant in porous materials operating in high temperature, low pressure environments, and that using the Klinkenberg formulation for the permeability allows accounting for slip effects. For high temperature gases percolating through the microstructure of FiberForm-like materials, the local Knudsen number can be defined as a ratio of the gas mean free path, λ , to the mean pore diameter, d_p , assumed to be the characteristic length for the porous medium.

Figure 2a presents an example of the FiberForm microstructure rendered in Avizo together with a distance map (Fig. 2b) calculated for the voxels of the inter-fiber pores. The color field quantifies the distance of each voxel from the nearest object and allows to compute a characteristic mean pore diameter of $d_p = 55 \mu\text{m}$. As an example, the mean free path for oxygen in air can be estimate (in μm) as [21]:

$$\lambda = 0.095 \frac{10^5 T}{298 P}, \quad (5)$$

where P is the average pressure. At flow temperatures between 1000 and 2000 K and pressures between 1 and 10 kPa, Knudsen numbers vary between 0.1 and 2,

(a) Transverse

(b) In-Plane

Figure 3: Pressure for the flow of argon through FiberForm, for a temperature of 1319 K and an average pressure of 900 Pa. Dark blue spots represent the location of the fibers.

which are indication of a slip regime, and justify the use of DSMC simulations.

225 DSMC is a numerical Monte Carlo method to solve the time-dependent nonlinear Boltzmann equation. It is a probabilistic simulation of molecular processes based on the kinetic theory of dilute gases [1]. The general Boltzmann equation follows the following form

$$\frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \nabla f + \vec{F} \cdot \frac{\partial f}{\partial \vec{p}} = \left(\frac{\partial f}{\partial t} \right)_{coll}, \quad (6)$$

230 where f is a probability density function, $\vec{p}$ is the momentum vector, $\vec{F}$ is the force field acting on the particles in the fluid and m is the mass of the particle. The second term on the left-hand side represents the diffusion of the particles, the third term on the left-hand side represents the forces exerted on the particles by an external influence, and the term on the right-hand side is the collision term, accounting for the forces acting between particles in collisions.

235 In the DSMC algorithm, the Boltzmann equation is decoupled into two parts: molecular advection and collisions. Particles are tracked in the domain based on their position in virtual cells. Each particle represents an F_N number of real molecules. The cell length has to be carefully chosen such that it is a fraction of the mean free path. The time step is chosen such that it is a fraction of the mean collision frequency. At each time step, following their advection, a number of binary pairs of particles are selected for collisions in each grid cell. In the collision procedure, we follow the no-time-counter (NTC) procedure of Bird [1] for the selection of collision pairs. Quantities such as velocity, translational and internal energy of particles can be computed by sampling the flow field. 240 Therefore, macroparameters such as temperature, pressure and number density can be computed in each grid cell. In order to reduce statistical scatter and ensure that collisions are performed accurately, it is generally recommended that a minimum of 10 to 20 particles per computational cell be used [22].

250 The Stochastic PARallel Rarefied-gas Time-accurate Analyzer (SPARTA) [23] DSMC code developed at Sandia National Laboratories was used in the current work. The grid was used to group particles by grid cell for purposes of performing collisions and chemistry, as well as efficiently find particle/surface collisions.

A marching cubes algorithm [24] was implemented in SPARTA to approximate the isosurface of the micro-CT digitized geometry, given a grayscale threshold. The algorithm represents the surface of the fibers as a collection of triangles. These were used to locate surface collisions with particles during the DSMC simulation.

Subsonic boundary conditions were imposed to keep the pressure at the inlet and outlet planes of the domain, creating two buffer zones with constant pressure. In all cases, the pressure difference between the two buffer zones was held constant around 100 Pa. Argon was initially chosen as the carrier gas.

SPARTA uses the Variable Hard Sphere (VHS) model to simulate particle interactions [1]. The reference VHS diameter and viscosity-temperature exponent, ω , for different gases are presented in Table 3. The particle-surface collisions were modeled using a diffusive reflection model. We down-sampled our tomography domains in order to reduce the number of surface elements and grid cells and therefore the computational time, however we ensured that most of the information of the unscaled domain was maintained. The resulting datasets had a voxel size of $2.6 \mu\text{m}$ (200x200x200 voxels), and more than 10 millions total cells were used for these simulations. At a fixed temperature, the average pressures in the sample were chosen such that the mean free path would be at least twice the cell size. The time step was chosen as 2 ns for all simulations, ensuring that it is at most $1/10^{th}$ of the mean collision time. Around 200 millions particles were used in the domain for all simulations, leading to an average number of particle per cell around 20, in order to reduce statistical scatter. The simulation was allowed to reach steady state for 60,000 timesteps, followed by an additional 60,000 timesteps for macroparameters sampling. The data was post-processed using the Paraview [25] software, allowing parallel post-processing which significantly reduced the time required to analyze large data files of several millions grid cells. The average pressure and mass flow inside the sample, as well as the exact value of the pressure drop through the sample were extracted as output quantities.

Figure 4: Contour plot of the X component of the velocity vector for the square array configuration, for a porosity of 0.89 and a Knudsen number of 0.01.

5. Permeability of square arrays

In order to validate the method used to compute the permeability of porous media, we reproduced a classical problem of the flow through a square array of fibers. This problem has been investigated experimentally, numerically and theoretically by several authors [26, 27, 28, 3]. Typically, most theoretical work attempt to relate the non-dimensional Darcy permeability (permeability divided by the square of the fiber radius) to the porosity of the structure. Shou *et al.* [26] derived an analytical equation to compute the non-dimensional permeability as a function of the porosity at different Knudsen numbers for the flow perpendicular to a 1D fibrous media as

$$\frac{K}{r^2} = \frac{-0.5 \ln(1 - \epsilon) + 0.25 - \epsilon - 0.25(1 - \epsilon)^2 + 2\text{Kn}(-0.5 \ln(1 - \epsilon) - 0.25 + 0.25(1 - \epsilon)^2)}{4(1 - \epsilon)(1 + 2\text{Kn})}. \quad (7)$$

This equation was derived using a unit cell method from Stokes equation with a first-order slip boundary condition. Stern *et al.* [3] also computed the same problem using CFD and DSMC and compared it with an analytical expression. They found good agreement between the two numerical methods for Knudsen numbers up to 0.02, and showed that the results started to diverge at a Knudsen number of 0.2, which lies in the translational regime.

Here, we set up a similar simulation as Stern’s [3]: we model an infinite array
of parallel cylinders as a two dimensional problem. Periodic boundary conditions
are applied in the directions perpendicular to the flow, and subsonic inflow
boundary conditions in the direction of the flow. We model two cylinders in the
direction of the flow. Argon is used as the carrier gas, and the inflow temperature
is 300 K in all cases. We vary the porosity by varying the radius of the fiber. The
size of the domain is kept constant at $20 \times 40 \mu\text{m}$. We vary the Knudsen number
by varying the average pressure in the domain. The pressure difference between
the inlet and outlet is kept constant around 100 Pa between the different cases.
Figure 4 shows contours of the U velocity for a typical simulation (in this case,
the porosity is 0.89 and the Knudsen number 0.01). Figure 5 shows the results
for the non-dimensional permeability as a function of the porosity (in the range
of porosities between 0.7 and 0.95) for Knudsen numbers between 0.001 and
1. We compare the results from our DSMC simulation with the DSMC results
from Stern [3] and the analytical results from Shou [26]. It can be seen that
we obtain good agreement with the analytical method in the continuum and
slip-flow regime ($\text{Kn} < 0.05$), however discrepancies start to appear for Knudsen
numbers of 0.1 or above. At $\text{Kn}=1$, the DSMC results overpredict the analytical
results. However, our results seem to be consistent with Stern’s results at similar
Knudsen numbers. Stern also observed that CFD simulations using a Maxwell
slip wall condition were diverging from the DSMC results for Kn of 0.1 and
above. Therefore, we conclude that the analytical method employed by Shou *et*
al. is valid in the continuum and slip-flow regimes, but underpredicts the non-
dimensional permeability in the transitional and rarefied regimes, especially at
lower porosities (larger cylinder surface area).

6. Results and discussion

Computational results for the permeability of the materials introduced pre-
viously (see Fig. 1) are presented and discussed in this section. FiberForm is
considered first. Figure 3a shows the pressure field within our computational

Figure 5: Non-dimensional permeability versus porosity for various Knudsen numbers, from DSMC, shown by symbols. DSMC results from Stern [3] and analytical results from Shou [26] are shown by dashed line and solid lines, respectively.

domain. The dark blue areas represent the location of carbon fibers, whereas the dark red to light blue gradient represents the pressure drop in the gas flow.

Figure 6 shows a comparison between the DSMC values for the permeability of an sample measured in the direction through the thickness, and the experimental data from Panerai *et al.* [9], at four temperatures. It can be seen that the agreement between computations and simulations is excellent, with the values of $K_0^\perp$ and $b^\perp$ showing less than a 2% difference at any temperature compared to experiments. Additionally, Table 1 shows a comparison between the values of the permeability parameters obtained from DSMC, and those normalized using

the b-scaling law presented in Ref. [10]. It can be seen that the continuum flow permeability $K_0^\perp$ is not affected by T (less than 0.3% variation is computed between the high temperature simulation and the reference temperature $T^* =$
340 310 K). The $b^\perp$ parameter follows the scaling law exactly, with under 0.6%
between the predicted value and the calculated one.

Figure 6: Permeability parameter F for a transversely oriented virgin FiberForm specimen computed at four different temperatures, and comparison with experimental results.

Fig. 3b, Fig. 7 and Table 2 show similar data for the in-plane direction, also showing a good scaling with temperature. It is interesting to note that the continuum permeability value is nearly twice that of the through thickness
345 direction in this case, emphasizing the orthotropy of FiberForm and impact
it has on the flow of hot gases: gases flow slower in the direction parallel to

Figure 7: Permeability parameter F for a planar oriented virgin FiberForm specimen computed at four different temperatures.

Table 1: Computational results for temperature dependent-simulations in the through-thickness direction.

T , K	$K_0^\perp$, 10^{-12} m ²	$b^\perp$, Pa	$K_0^\perp(T)/K_0^\perp(T^*)$	$(b^\perp/\mu\sqrt{T})/(b^{*\perp}/\mu^*\sqrt{T^*})$
310	52.09	1831.0	1.000	1.000
503	52.25	3432.4	1.003	0.994
940	52.15	7817.5	1.001	0.998
1319	52.08	12198.5	0.9997	0.9995

the pressing axis. Additionally, in Fig. 8 we show that, if F is normalized according to F^*/K_0b^* and plotted as a function of P_{avg}/b^* , with F^* computed

Table 2: Computational results for temperature dependent-simulations in the planar direction.

T , K	$K_0^{\parallel}$, 10^{-12} m ²	$b^{\parallel}$, Pa	$K_0^{\parallel}(T)/K_0^{\parallel}(T^*)$	$(b^{\parallel}/\mu\sqrt{T})/(b^{\parallel}/\mu^*\sqrt{T^*})$
310	97.54	1517.5	1.000	1.000
503	99.48	2783.4	1.010	0.986
940	97.66	6439.9	1.001	0.992
1319	97.63	10037.5	1.0009	0.992

Figure 8: Normalized data from Figs. 6 and 7, show that all data collapse onto a single line.

by $F^* = K_0(P_{avg} + b^*)$ and b^* the reference value for b computed at $T^* = 310$ K,

all the curves in Figs. 6 and 7, collapse onto a single line.

The influence of the gas composition on the permeability was also inves-

355 tigated. Similar simulations as the one conducted with a flow of argon were
 reproduced with flows of helium and air, at the reference temperature of 310 K.
 It is interesting to note that FiberForm is more permeable to helium, which has
 smaller lighter molecules compared to argon or air. Table 3 shows a compari-
 son of the viscosities, molar mass, and viscosity-temperature exponents (used in
 DSMC to model collisions with the VHS model), as well as the ratio of $K_0^\perp$ for
 helium and air with respect to argon, and the computed value of $b^\perp$ with the one
 extrapolated from the scaling law using argon as the reference gas. It can once
 360 again be seen that the behavior is completely predicted by the scaling law, and
 the three lines would perfectly superimpose if they were normalized in similar
 fashion to Fig 8. This makes it possible to study the influence of different atmo-
 spheres of different compositions and temperatures, without necessarily needing
 to conduct experiments or simulations with that atmosphere; the permeability
 365 value can simply be extrapolated from a measurement or calculation using a
 noble gas like argon.

Table 3: Computational results for gas dependent-simulations in the through-thickness direc-
 tion. d_{ref} and ω are the reference diameter and viscosity temperature exponent in the VHS,
 respectively.

Gas	μ_{ref} , Pa.s	d_{ref} , m	ω	$K_0^\perp$, m ²	$b^\perp$, Pa	$\frac{K_0^\perp(T, M, \mu)}{K_0^\perp(T^*, M^*, \mu^*)}$	$\frac{(b^\perp / \mu \sqrt{T})}{(b^{\perp*} / \mu^* \sqrt{T^*})}$
Argon	2.117×10^{-5}	4.17×10^{-10}	0.81	52.09×10^{-12}	1831.0	1.000	1.000
Air	1.719×10^{-5}	4.19×10^{-10}	0.77	51.51×10^{-12}	1752.7	0.989	1.014
Helium	1.865×10^{-5}	2.33×10^{-10}	0.66	51.32×10^{-12}	5074.1	0.985	1.008

In Fig. 9, we investigated the influence of porosity on permeability and the
 Klinkenberg parameters. While we have shown a good agreement with experi-
 ments, it is acknowledged that capturing the actual variability of the material
 at large scales with tomography volumes of the order a cubic millimeter is a
 370 challenging task. The local porosity of the material can significantly affect the
 computed permeability value. To address this aspect of the problem the poros-
 ity of the computational domain was adjusted by altering the cutoff for the

marching cube algorithm. In varying the threshold value we ensured that the
 375 microstructure of the sample was similar, but fibers and pores sizes varied rela-
 tively continuously. The range of porosity that was investigated was 0.8 to 0.9,
 which is a reasonable variability for FiberForm. The results for both K_0 and b
 are plotted, and both datasets were fit with an exponential curve. Previous work
 on permeability of porous material proposed two sets of fits: one using a pro-
 380 portional to $\frac{\epsilon^3}{(1-\epsilon)^2}$ [29], and one proportional to an exponential curve [30]. Only
 the latter was able to properly fit our data for FiberForm. The following fit was
 obtained for K_0 : $K_0 \propto \exp(2.961\epsilon)$. It is interesting to note that Ehrlich and
 Schwille [31] mention that the two Klinkenberg parameters are likely correlated,
 making it harder to analyze and fit them separately.

Figure 9: Permeability parameters K_0 and b for a transversely oriented virgin FiberForm specimen for which the porosity was artificially varied by modifying the cutoff.

385 That visual observation regarding the porosity of the different materials
 made in Sec. 4 is confirmed by the porosity values presented in Table 4, along
 with the two permeability parameters computed for each material, $K_0^\perp$ and
 $b^\perp$, and the value of the permeability constant in the continuum. The latter
 was computed using the FlowDict module of the Geodict software [32], solving
 390 Stokes' equation using an Explicit Jump method. The gas properties and bound-
 ary conditions are the same as those used in SPARTA. The values in the limit of
 the continuum are within 10% of the $K_0^\perp$ value obtained in DSMC simulations.
 The oxidation of the virgin FiberForm increased the material permeability by
 a fraction, and the values $K_0^\perp$ and $b^\perp$ for the oxidized sample of porosity 0.876
 395 are actually quite similar to the values previously reported for the virgin sample
 of FiberForm for which the porosity was artificially increased to 0.87. On the
 other hand, the carbon felt and Calcarb both exhibit significantly higher perme-
 abilities than the virgin and oxidized FiberForm. It should first be noted than
 both virgin materials have porosities larger than 0.90, significantly above those
 400 of FiberForm. One very interesting conclusion is that, despite its lower poros-
 ity, Calcarb exhibits a higher permeability than the carbon felt. That is due
 to the different microstructures of the two materials. Visually, Calcarb shows
 larger fibers and larger pores, while the felt is made out of thinner fibers and
 smaller pores. Additionally, both micro-CT and scanning electron micrograph
 405 (SEM) images of Calcarb show agglomerated clusters of multiple Polyacryloni-
 trile (PAN) fibers within the material structure (see Fig. 11), and it has been
 shown computationally [33] that agglomeration increases the permeability at
 constant porosity. In support, Fig. 10 shows the volume fraction as a function
 of the pore size in the through-thickness direction, computed using a granulom-
 410 etry method in Geodict, that fits spheres of increasing sizes into the material
 pores. It can be seen that the average pore sizes for FiberForm, Morgan carbon
 felt and Calcarb are 50, 92 and 135 μm , respectively. The permeability of a
 porous material is therefore a function of the porosity as well as the pore size.

Table 4: Computational results for porous thermal protection materials. Argon is used as the carrier gas and the temperature is fixed at 310 K in all cases. $K_{Geo}^\perp$ is the continuum permeability constant computed using Geodict.

Material	Porosity	$K_0^\perp, 10^{-12} \text{ m}^2$	$b^\perp, \text{ Pa}$	$K_{Geo}^\perp, 10^{-12} \text{ m}^2$
Virgin FiberForm	0.840	52.09	1831.0	46.71
Oxidized FiberForm	0.876	60.02	1908.5	55.31
Carbon Felt	0.939	195.43	1403.1	215.40
Calcarb	0.913	314.63	1001.5	315.50

Figure 10: Volume fraction as a function of the pore size in the through-thickness direction for virgin FiberForm, Morgan carbon felt and Calcarb.

Figure 11: Micro-CT (left) and SEM (right) of Carlbcarb. SEM picture reproduced from [34] with permission. Red arrows point at observed structures of agglomerated fibers.

7. Conclusions

415 A direct simulation Monte Carlo model was introduced to compute the permeability of porous thermal protection material in the slip regime, based on high-fidelity imaging of the material microstructure. The model is implemented in the SPARTA simulator and a marching cubes algorithm was added to the model to generate the virtual representation of the surface of the microstructure. 420 Klinkenberg's form of the permeability constant was adopted following Marschall and Milos [10], such that the increased mass flow because of slip at the fibers' surface was accounted for.

Numerical computations were compared with experimental results for a sample of virgin FiberForm tested in the direction through the thickness and in the planar direction, at four different temperatures. Excellent agreement (under 2 % difference) was reported, and Marschall's scaling law for temperature and gas composition was verified, meaning all the curves collapsed on a single one 425 when normalized by the flow temperature. The continuum permeabilities for the transverse and in-plane orientation were 52.14 ± 0.08 and 98.08 ± 0.94 $\times 10^{-12} \text{ m}^2$, respectively. Furthermore, the scaling was also verified when the gas composition was changed at fixed temperature. The influence of the porosity on permeability was investigated, and an exponential scaling law was fitted 430

to the data in the case of FiberForm.

Finally, the permeability of the original virgin FiberForm sample was compared with that of a flow-tube oxidized sample of the same material, as well as virgin samples of Morgan carbon felt and Calcarb CBCF. An interesting observation was that the Calcarb exhibited significantly higher permeability than the carbon felt, even though its porosity was lower. Using a microscopic structure analysis, we concluded that this was due to the larger pore size in Calcarb.

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