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Tomography-based determination of porosity, specific area and permeability of snow and comparison with measurements

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ABSTRACT

Micro-computed tomography (μ-CT) of snow replicas is used to characterize 34 snow samples by determining their specific surface area, porosity, effective permeability, anisotropy, and tortuosity. Their 3D geometrical representation obtained by μ-CT is used in direct pore-level simulations (DPLS) to numerically solve the governing mass and momentum conservation equations for fluid flow through porous media. It is found that inertial effects, given by a second and third order correction in Darcy's law, influence the air flow even at low Reynolds numbers. Correlations are derived for permeability, the Dupuit–Forchheimer coefficient and the third order coefficient of Darcy's law as a function of density and grain size. Comparison with the experimentally measured data yields good agreement and confirms the applicability of DPLS for determining the transport properties of snow.

1. Introduction

Snow consists of sintered ice grains, whose complex porous microstructure changes over time. Its mass transport properties are pertinent to a wide range of environmental processes (Albert et al., 2004). Permeability (K) and Dupuit–Forchheimer coefficient (F) have an influence on the snow metamorphism (Neumann and Waddington, 2004), the snow structure in seasonal and polar snowpacks (Courville et al., 2010; Massman, 2006; Massman and Frank, 2006; Sommerfeld and Rocchio, 1993; Sommerfeld et al., 1996), the heat transfer rate at the earth surface (Morin et al., 2010), the snow–air exchange processes relevant to the composition of the lower atmosphere (Clifton et al., 2007; Grannas et al., 2007), and the composition of the air trapped in snow, with implications to climatology and paleoclimatology (Wolff et al., 2007).

Snow permeability was first measured in 1939 (Bader et al., 1939) and recently measured in Antarctica and Greenland (Albert and Shultz, 2002; Albert et al., 2000; Courville et al., 2007). Several relevant studies include parameterization in relation to density and grain size (Albert and Shultz, 2002; Albert et al., 2000; Hörhold et al., 2009; Shimizu, 1970; Sommerfeld and Rocchio, 1993; Sommerfeld et al., 1996) due to the ease of measuring those parameters experimentally. However, parameterization in relation to pore size and/or porosity — and not grain size — improve the parameterization (Courville et al., 2010; Rick and Albert, 2004). A permeameter for field measurements was developed (Albert et al., 2000; Conway and Abrahamson, 1984) and a model to predict the transport properties of polar firn at the pore scale was formulated (Freitag et al., 2002). More recently, permeability, porosity, and specific surface per unit mass were measured for a large number of different samples (Arakawa et al., 2009). A matching correlation was found between their microstructural parameters, but substantial uncertainty remains. As the samples of this latter study were cast with dimethyl phthalate and conserved, it was possible to scan them later by sublimation tomography (Heggli et al., 2009) in order to conduct the present study.

The experimental study of snow properties is problematic due to fast changes that modify the snow microstructure during the measurements. Tomography allows the microstructure to be kept constant while performing several simulations on the same sample. The transport of snow without changing its microstructure and properties is also problematic. The method of casting snow with diethyl or dimethyl phthalate allows the microstructure to be kept stable and later analysis by micro-computed tomography (μ-CT). The use of a permeameter would not be possible after the snow is cast. In a previous paper (Zermatten et al., 2011), we introduced an alternative method for determining permeability (K) and the Dupuit–Forchheimer coefficient (F) of snow using direct pore-level simulations (DPLS). DPLS allows the simulation of macroscopic physical parameters of complex porous

Abbreviations: CFD, computational fluid dynamics; DMP, dimethyl phthalate; DPLS, direct pore-level simulations; REV, representative elementary volume; NRMSE, normalized root mean square error; SSA, specific surface area (m^{-1}); μ-CT, micro-computed tomography.

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materials (Haussener et al., 2010; Petrasch et al., 2008a, 2008b). Moreover, DPLS allows the determination of pore size, which provides a better parameterization of permeability than grain size (Courville et al., 2010; Rick and Albert, 2004).

Previous studies on snow permeability applied the linear Darcy's law (Darcy, 1856). However, it has been shown that this law only approximates the pressure drop during laminar flow in porous media (Amaral Souto and Moyne, 1997; Lasseux et al., 2011; Rojas and Koplik, 1998; Skjetne and Auriault, 1999), even at low fluid velocities. In the present study, an extended form of Darcy's law is applied (Rojas and Koplik, 1998).

The objective of the present paper is to show the validity of this methodology and assess its accuracy by comparing DPLS results to the experimental values of permeability obtained from 34 snow samples (Arakawa et al., 2009). Calculations were also performed to determine the threshold air flow velocity for which the second and third order corrections become important in the extended Darcy's law. Recently, increased attention was directed to the anisotropic permeability of snow (Calonne et al., 2012; Hörhold et al., 2009; Riche and Schneebeli, 2010), which is difficult to examine via physical measurements. In this paper, anisotropy of permeability is also examined via DPLS.

DPLS has been successfully applied to complex porous materials such as reticulate porous ceramic foams, porous rocks, and packed beds of opaque and semi-transparent particles (Haussener and Steinfeld, 2012; Haussener et al., 2010, 2012; Petrasch et al., 2008a, 2008b). Their precise digital 3D geometrical representation was obtained by micro-computed tomography (μ-CT) and used in DPLS to calculate their effective transport properties by solving the corresponding mass and momentum conservation equations. Computational fluid dynamics (CFD) has also been applied for the characterization of polar firn (Courville et al., 2010) with a comparison to measurements. A more recent study uses numerical computation to determine snow permeability and anisotropy in permeability of several snow samples (Calonne et al., 2012), but only comparing parameterizations from experimental results. As there exists an infinity of different snow structures that cannot be described by simple morphological properties, our comparison with the same snow samples will give a direct validation of the DPLS methodology and better understanding of its limitations.

2. Methods

More than a hundred different snow samples were collected during the winter 2007–2008 in Hokkaido prefecture, Japan (Arakawa et al., 2009). Each of these samples was cast with dimethyl phthalate (DMP), i.e., the air in the sample is replaced with DMP and frozen at −40 °C to preserve its original structure and to allow its transportation and storage. We scanned a subset of 34 samples using sublimation tomography (Heggli et al., 2009) (Table 1). Firstly, the complete sample was scanned using a Scanco-μCT 40 CT. This way, the air bubbles that could have been trapped in the DMP are also imaged. The ice is then sublimated from the sample by lowering the pressure to about 10^{-2} mbar at −20 °C. The remaining, which is scanned, is therefore a negative of the snow sample. The tomography was done using a voxel edge length of 10 μm. The scanned samples had a dimension around 8 × 8 × 8 mm^3. The image of the pore space and the image of the snow matrix were then superimposed and the air bubbles trapped in the DMP were removed by image processing. A threshold was set to separate the gray values into ice and void phase. Two-point correlation function (Haussener et al., 2010; Petrasch et al., 2008a) was used to determine morphological properties, namely: the porosity (ε) and specific surface area (SSA), here defined as the phase boundary surface divided by the total snow volume. The representative elementary volume (REV) is defined as the minimum volume for which the continuum assumption is valid. We determined the REV based on modeled pressure drop and velocity calculations for subsequently growing volumes until the pressure drop and the velocity asymptotically reached a constant value within a given error band.

Each 3D image was meshed using an in-house mesh generator (Friess et al., 2013), which first covers the domain with tetrahedral elements and then performs systematic refinements on the phase boundaries. Deforming or splitting surface-crossing elements establishes boundary conformity. Furthermore, the algorithm features automatic adaptation of the mesh density to the surface structure, which is characterized by the local roughness obtained from numerical integration over small, suitably selected regions. For each sample, the largest mesh element length was 0.25 mm and the smallest possible mesh element measured 15.625 μm. This refinement was chosen after a grid convergence study using the model with a tolerance of 5% for the calculated pressure drop. Preliminary calculations of the REV were carried out for various sample sizes to elucidate the trade-off between computational time and accuracy of the results. It was observed that the width of the sample parallel to the flow direction can be chosen 2 to 3 times shorter than the perpendicular length without jeopardizing the precision of the results (Zermatten et al., 2011). For the determination of K and F, it has been shown (Haussener et al., 2010; Zermatten et al., 2011) that it is not sufficient to base the calculation of the REV simply on porosity, as the calculations based on pressure drop give larger REVs than the ones based on porosity. One REV was chosen for each snow type (Table 2) after performing preliminary calculations on one sample of each type. All the simulations were performed along the vertical and the horizontal axes of the samples, which are both principal axes of the snow (Löwe et al., 2013; Riche and Schneebeli, 2013). The sample was always cut in order to have the shortest length parallel to the flow direction.

A CFD code based on the finite volume technique (Ansys, 2009) was applied to solve the 3D Navier–Stokes equations. The computational domain consisted of a square duct containing a sample of snow. The boundary conditions consisted of uniform inlet velocity, temperature and outlet pressure, no-slip velocity, constant wall temperature at the solid–fluid interface, and symmetry of the sample at the lateral duct walls. The square duct, which measured 5 times the length of the sample, was added to ensure a fully developed velocity profile at the entrance of the snow sample (Fig. 1).

At low fluid velocities, the pressure drop over a spatially averaged isotropic porous medium is given by Darcy's law (Dullien, 1992):

$$\nabla p = -\frac{\mu}{K} u_D \tag{1}$$

where p is the pressure, K is the permeability, μ is the dynamic viscosity of the fluid and u_D its superficial velocity, $|\overline{u}_D| = \frac{1}{V}\int_V u dV$, with volume V larger or equal to REV. However, this equation remains true only at very low Reynolds number Re (Re → 0). At higher fluid velocities, Eq. (1) gets separated into two different regimes (Amaral Souto and Moyne, 1997; Lasseux et al., 2011; Skjetne and Auriault, 1999):

- Weak inertia takes place when Re = O($\delta^{1/2}$), where δ is the small scale separation parameter, $\delta = d/L$. d is a characteristic length scale of the pores (here the equivalent pore diameter, $d = 6\varepsilon/\text{SSA}$ (Dullien, 1992)) and L is a characteristic length of the macroscopic flow. At the weak inertia regime, the correction to Darcy's law is a cubic term in velocity given by:

$$\nabla p = \frac{-\mu}{K} u_D - \frac{\gamma \rho^2}{\mu} u_D^3 \tag{2}$$

where ρ is the fluid density and γ is a dimensionless factor.

- Strong inertia starts at Re = O(1) and is described by:

$$\nabla p = \frac{-\mu}{K} u_D - F \rho u_D^2 \tag{3}$$

where F is the Dupuit–Forchheimer coefficient. Since determination of the transitional Re between weak and strong inertia is difficult,