Modelling of gas flow through porous granular media

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Abstract

As part of the Cophylab collaboration, the aim of this project is to better understand the physics of gas flow through cometary surface material. In this work specifically, a combined Darcy-Knudsen flow model for the description of gas flow in porous granular media was analyzed by means of simulations, using the finite element method. Experimental data of dry granular materials from a previous project was used as input for the computer model and the results were compared in order to validate the model.

While the simulation results mostly agree with the measurements for materials with spherical grains, some discrepancies suggest potential areas for the improvement of the experimental setup for future analysis of volatile samples as well as for the refinement of the simulation model.

Introduction

Description of single species gas flow **J** through porous material by means of a combined Darcy-Knudsen model:

$$\boldsymbol{J} = -\left(\frac{D_K}{RT} + \frac{nB}{\mu}\right)\nabla p$$

- Knudsen diffusion coefficient D_K for Knudsen regime with mean free path lengths much larger than average pore size
- Permeability B for viscous regime (dynamic viscosity μ) with bulk flow behavior with small mean free path
- Ideal gas law for relation between pressure p and particle density n: p=nRT

Other relevant sample parameters:

- Porosity ϵ: Void fraction of sample volume
- Tortuosity τ: Measure of sinuosity, interconnectedness and surface properties (roughness) of pores

[1] Schweighart et al., [2] Mason et al.

Measurement of D_K, B, ϵ and knowledge of τ allows for calculation of average pore size d_p (*[1] Schweighart et al.*):

$$d_p = \frac{3\tau^2 D_K}{\epsilon}\sqrt{\frac{\pi M}{8RT}}$$

The analytical description of the intrinsic relation between D_K, B and ϵ is complex and can thus only be given approximately for specific grains - monodisperse spheres:

- $B = \frac{\Phi^2 d_S^2 \epsilon^3}{150(1-\epsilon)^2}$

  ϕ...sphericity, ds...equivalent sphere diameter

  [3] Pinto et al.

- $D_K = \frac{d_S \epsilon^2}{3\Psi q(1-\epsilon)}\sqrt{\frac{8RT}{\pi M}}$

  Ψ=13/6, q...geometric correction factor (tortuosity)

  [4] Asaeda et al.

Experiment and Simulation

In the experiment, the pressure differences across various samples in a vacuum chamber (see fig. 1) were measured for different preset mass flow levels. From the results the parameters D_K and B were computed. By measuring the sample volume and mass, ϵ was determined in accordance with *[1] Schweighart et al.*

The boundary conditions (mass flow and pressure level on one side) together with the experimentally determined parameters served as input data for the computer simulations. Using the FEM method, the sample was modelled as a cylinder matching the dimensions of the experiment (see fig. 2). The physics was controlled by the governing equations (($\boldsymbol{u}$ flow velocity, ρ mass density)

$$\boldsymbol{u} = -\left(\frac{B}{\mu} + \frac{D_K}{p}\right)\nabla p$$

…modified Darcy equation taking Knudsen flow into account

$$Q_m = \frac{\partial}{\partial t}(\epsilon\rho) + \nabla \cdot (\rho\boldsymbol{u})$$

…continuity equation with vanishing source term $Q_m = 0$

and the boundary conditions (up- and downstream pressures agree with those in respective compartment volumes, given inflow and pump performance, implemented through appropriate functions).

Steady-state and transient simulations were performed with parameter variations, to test different aspects of the model. In transient studies, the initial cylindrical model geometry was also adapted to investigate the influence of tapering through the sieve present in the experiment. Furthermore, effects of inhomogeneity at the cylinder wall (higher porosity), which arise because particles cannot be cut through by the wall, were analyzed in an alternative campaign. This was realized by defining a layer of the same dimension as an individual grain at the wall with an altered porosity.

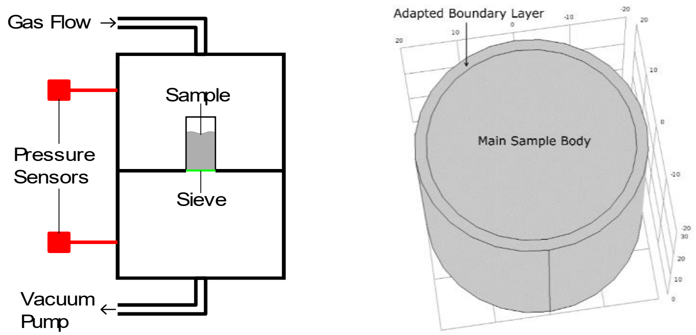

Figure 1 and 2: Hover mouse for details

Results

For stationary simulations, the downstream pressure was used as a boundary condition, whereas for transient simulations the pump performance (empirical function representing the flow to the pump as a function of pressure) was implemented. The up- and downstream pressure (top and bottom sample boundary) from the simulations were compared with the measurements for all samples. Fig. 3 shows the results for the top side of glass bead samples as an example. The discrepancies are most significant for samples with angularly shaped grains (e.g. Asteroid and Lunar analogues).

The simulations with an adapted geometry to account for the tapering effect of the sieve in the experiment (e.g. in Fig. 4), showed that the pressure difference across the sample increases up to 5% for a constriction in the bottom sixth of the sample from 40 mm to 36 mm. In the case of a tighter constriction down to 32 mm, the differences can go above 15%. They are smaller by a few percent for constricted samples with finer grains.

The investigation of the altered wall layer showed that an increased porosity, due to the lack of grains that would project behind the wall (see Fig. 5), reduced the pressure drop across the sample as the gas flows through this layer with less resistance. This reduction is negligible (max. 3%) for the glass bead sample with the smallest grains (63 µm), considerable (max. 30%) for medium grains (250 µm) and massive (max. 89%) for large grains (3.8 mm).

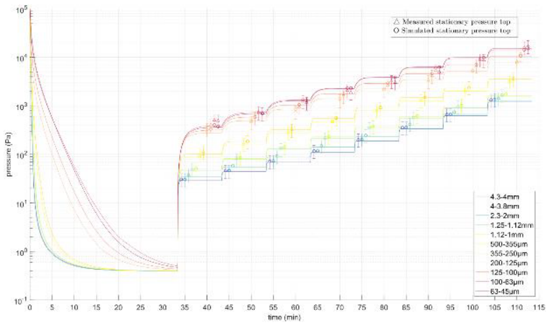

Fig. 3: Hover mouse for details

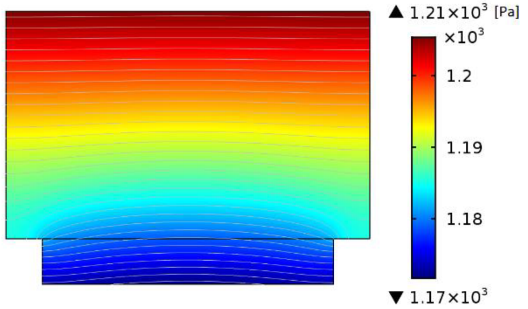

Fig. 4: Hover mouse for details

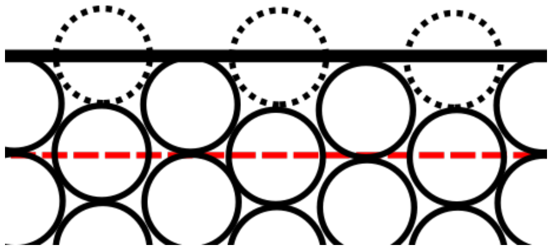

Fig. 5: Hover mouse for details

Conclusions

As the physical model presented here describes materials macroscopically, one of the main goals of this work was to validate, whether simulations assuming homogenous sample properties could describe the real experiment sufficiently. Within the accuracy of the measurements, the simulation and experimental results match well for samples with spherical grains, however there are significant discrepancies for samples with irregularly shaped grains, especially for lower gas flow levels.

Possible explanations for these differences are:

- Use of a simplified simulation model (for main transient simulations) neglecting geometric effects such as sample constriction and additional resistance due to the sieve
- Inhomogeneity effects due to finite dimensions of the sample as well as the interaction of gas and material with the sieve were initially not considered
- Assumption of isothermal processes might not be valid

Considering these points, a refinement of the physical model can be achieved by:

- Usage of more accurate pressure sensors and inclusion of temperature measurements in experiments
- Use of complementary software to analyze material packing properties for better modelling of samples
- Consideration of geometric and inhomogeneity effects, as well as variable temperature in all future simulation models

References and Acknowledgments

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More information about the CoPhyLab project can be found on the CoPhyLab webpage.