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Effective thermal conductivity of a wet porous medium – presence of hysteresis when modeling the spatial water distribution for the pendular regime

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Abstract

This paper deals with the heat transfer between two spherical grains separated by a small gap; dry air is located outside the grains and a liquid water meniscus is supposed to be present between them. This problem can be seen as a micro-scale cell of an assembly of solid grains, for which we are looking for the effective thermal conductivity. For a fixed contact angle and according to the volume of the liquid meniscus, two different shapes are possible for the meniscus, giving a “contacting” state (when the liquid makes a true bridge between the two spheres) and a “non-contacting” one (when the liquid is split in two different drops, separated by a thin air layer); the transition between these two states occurs at different times when increasing or decreasing the liquid volume, thus leading to a hysteresis behavior when computing the thermal flux across the domain.

Keywords: Wet porous media, Evaporation, Effective thermal conductivity, Hysteresis, Contact

1. Introduction

The effective thermal conductivity is an important parameter for the models which describe the evaporation of water in porous media. Many publications deal with heat transfer through granular media, via two-component models or experiments ([1], [2], [8]). On the other hand, it is known that the presence of water affects a lot the thermal properties because the thermal conductivity of water is typically 25 times that of dry air. This has been mentioned by Chen [4] who explicitly emphasized the strong variation of the conductivity for very small quantity of water. Other papers ([3], [5]) introduce the presence of liquid water as a component but without specifying its spatial localisation. The interesting paper of Mitarai & Nakanishi [6] deals with the pendular regime (fig.1) in which the liquid menisci act as a bridge between the grains but their study is restricted to the mechanical properties, not the thermal ones.

When a granular media is constituted by grains which are more or less spherical in shape, the liquid water is located around each contact zone between the grains due to the fact that liquid tends to minimize its surface energy. As stated above, we can expect that even a very small quantity of water increases the effective thermal conductivity by an important factor.

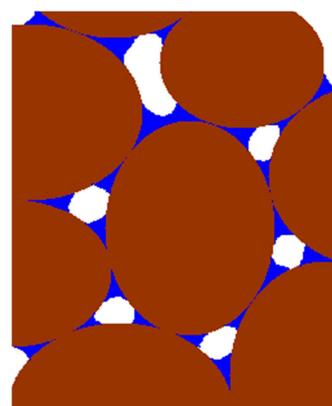


Fig. 1. Real granular medium containing few quantity of water (pendular regime)..

No theoretical model for this three-component medium exists and it is difficult to be discovered by experimental results. However, the values of this effective property can be found by numerical simulations, using the Fourier phenomenological law.

In this paper, we focus on the heat transfer between two spherical solid grains of same radius with the presence of liquid water attached to the solid grains.

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Surface tension is taken into account by computing the exact shape of the liquid meniscus (which must have a constant total curvature) and the role of the contact angle between the liquid-gas interface and the solid surface is also included in our model.

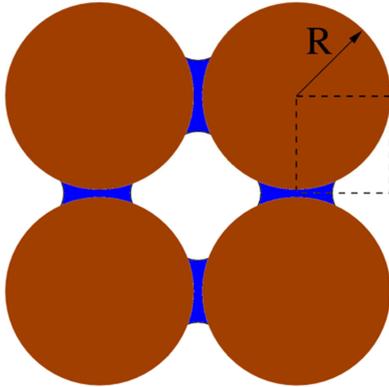


Fig. 2. Simplification of the grains' assembly. The dashed rectangle is the computational domain used in this paper.

Applications concern mainly the drying of materials and agriculture.

2. Micro-scale model

We want to solve the steady-state heat transfer in an elementary cell containing only two spherical solid grains, a few quantity of liquid water, and dry air. Actually, the liquid water should be in thermodynamic equilibrium with its vapor, so the surrounding gas should be a binary mixture of dry air and water vapor. In the present study, the water vapor is neglected and we assume that there is no adsorbed water on the grain surface.

Top and bottom sides are kept at constant temperature whereas the vertical ones are supposed to be isolated (this is related to the model used by [5] in their study of thermal conduction in dry soils). The computational domain can be found using the symmetry planes of the problem knowing the main direction of the heat flux – for example, the bottom symmetry plane comes from the fact that the gravity is neglected. As stated in the introduction, the liquid meniscus is centered along the axis between the two spheres leading to an axis-symmetric problem, so we can reduce the geometrical independent variables to the (r, z) cylindrical coordinates. Each component (solid, liquid water and dry air) has a constant thermal conductivity and the thermal contact between the components is supposed to be perfect.

The shape of the liquid meniscus must have both a constant total curvature (it is a minimum surface) and a prescribed contact angle with the solid. The percentage of liquid water, i.e. the ratio of its volume to that of the available space between the spheres is called humidity.

The input geometrical parameters are:

R : the radius of the two solid spheres

ϵ : the gap between the spheres

V : the volume of the liquid water

θ : the contact angle between the liquid interface and the solid.

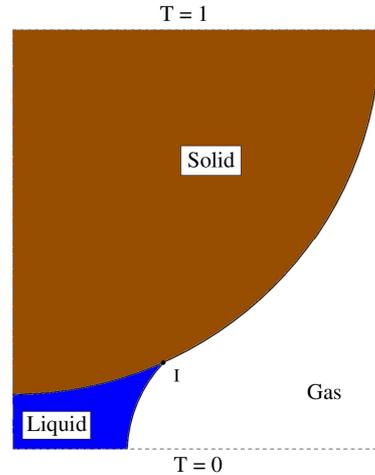


Fig. 3. Sketch of the cylindrical computational domain (taking into account all the symmetries). Boundary conditions are of homogeneous Dirichlet type on top and bottom sides, and of Neumann type on the external vertical side.

In this study, the radius R is equal to 1 (that is, all other geometrical lengths are expressed in terms of R), whereas ϵ and θ are kept constant (resp. 0.1 and 30 degrees), so the only input variable is V . The output variable of the problem is the (vertical) thermal flux Φ across the domain, which is related to the effective thermal conductivity of our composite medium. Note that in a complete model, the liquid volume V should be related to the gas pressure but this is out of the scope of this study.

3. Equilibrium shape of the liquid meniscus

The geometrical shape of the liquid meniscus is obtained by integrating a differential algebraic system of equations, stating that:

- the total curvature C is constant (but unknown);
- the contact angle at the solid surface has the prescribed value of θ ;
- the volume of the liquid meniscus is V .

Actually, the solution is obtained numerically by a shooting method over the two parameters C and the starting position of the point (r_0) in the “contacting” state, or z_0 in the “non-contacting” state); these two parameters are varied until the prescribed values (θ and V) are found. The family of the curves obtained, in both states, are drawn in the next figures.

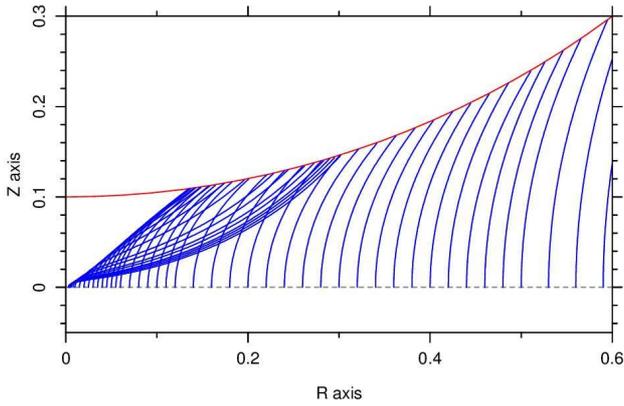


Fig. 4-a. This represents the family of the liquid meniscus when the volume varies, in the “contacting” state. Each curve is the boundary of the half of a bridge linking the two grains.

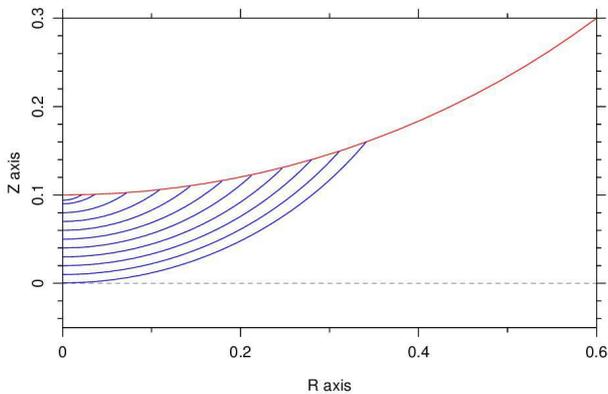


Fig. 4-b. This represents the family of the liquid meniscus when the volume varies, in the “non-contacting” state. Each curve is the boundary of a sessile drop, and the same symmetric drop is on the top of the other grain (not represented).

4. Numerical computation of the heat flux

Solving our problem numerically appears unavoidable: some authors (resp. [1], [7]) have used analytical solutions but they are respectively restricted to an asymptotic behavior (so, adapted to a local geometrical zone) or to too crude approximations.

The steady-state heat transfer is solved using a Finite Volume scheme applied on a regular structured mesh of rectangular cells. The matrix of the linear system is stored in a sparse way and the UMFPack linear sparse solver (from SuiteSparse [ref]) is used. Some tries have shown that a 500 by 500 mesh is required to obtain a good accuracy (fig. 5). Each numerical computation takes about few seconds on a laptop (Intel Core i7 @ 2.7 GHz).

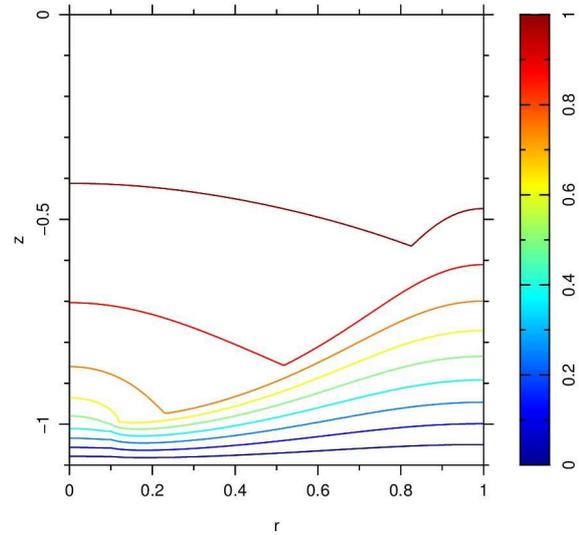


Fig. 5. The contour curves of the temperature obtained after a numerical computation on a 500x500 mesh.

5. Heat flux with respect to the water liquid volume.

During the evaporation/condensation of water in a wet granular medium, the liquid volume in each elementary cell changes with time. It is interesting to know the variation of the effective thermal conductivity with respect to the liquid volume. By using the Fourier law on our computational domain, the effective thermal conductivity is proportional to the heat flux. This heat flux depends of course on the water liquid volume because, as stated in the introduction, the thermal conductivity of the water is much more important than that of the dry air. Further, we expect a jump in the heat flux curve because there are two possible geometrical configurations for the liquid meniscus (the “contacting” state and the “non-contacting” one, as described in figures 4a and 4b).

Below, the heat flux is presented in figure 6-a, for humidity (or liquid volume) ranged from 0 to 20%. As expected, a hysteresis behavior is highlighted by our numerical computations and is more visible in figure 6-b which presents an enlarged view of the previous one.

6. Conclusion and perspectives.

A strong hysteresis behavior for the effective thermal conductivity has been shown when changing the humidity of a granular medium. It is due to a switch between two different geometrical configurations of the liquid meniscus attached to the two solid spheres. The presented results are preliminary and work is in progress to obtain more advanced ones especially when other parameters are varying (contact angle θ , gap between the grains ϵ).

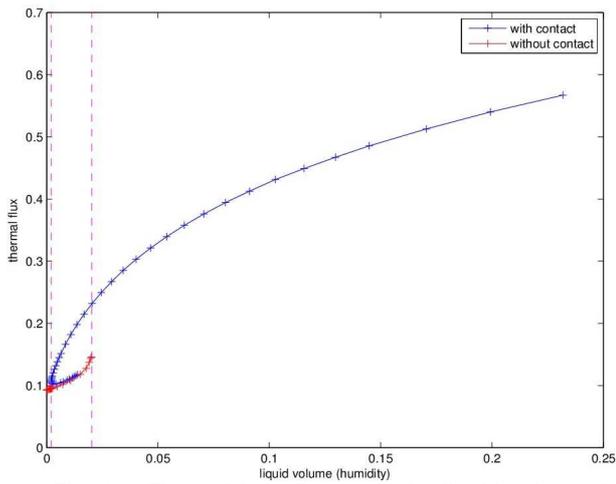


Fig. 6-a. Thermal heat flux w.r.t. the liquid volume, for the “contacting” state (blue) and the “non-contacting” state (red). Note the great increase in the heat flux due to the presence of water: about a factor 5 when humidity is only 20%.

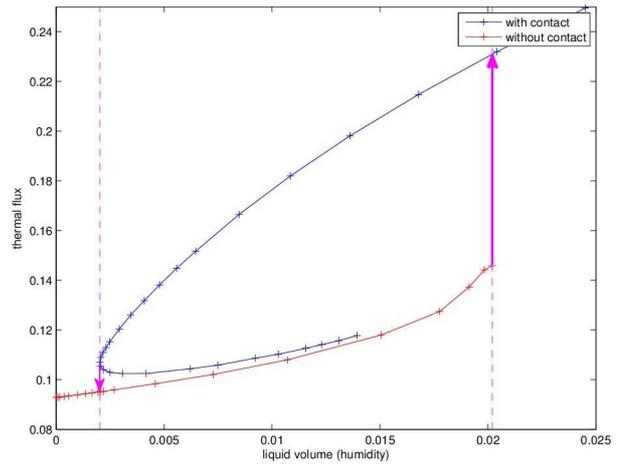


Fig. 6-b. This zoom of figure 6-a shows with more evidence the hysteresis behavior when liquid volume is increasing or decreasing. The jump in the heat flux occurs at the magenta dashed line; this jump is more pronounced in the decreasing case, i.e. during evaporation cycle of water. The arrows show the direction in the hysteresis cycle.

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