SCIENTIFIC NOTEBOOK #766E

P. Shukla, S. Chocron

May 31, 2006

Contents

1 Initial Entries

Scientific Notebook: 766E
Issued to: P. Shukla
Original Issue Date: February 2, 2006

Objective: The scientific notebook documents the work conducted on the development of an explicit simulation of the convection and conduction phenomenon in the backfill of drifts to be excavated in the Yucca mountain repository

Account number: 06002.01.352

Softwares used: Microsoft Excel 2003, Flow-3D v.9.1, Portland Group FORTRAN v5.2, Intel FORTRAN 9.0

Proposed approach for achieving the objectives: First check that analytical and numerical simulations match as a way of validating Flow-3D and getting acquainted with porous models. Second, develop FORTRAN codes that can generate a distribution of particles in a field. Third, explicitly model convection and conduction through the backfill of the drift.

Parameters: Porosity, tortuosity, particle diameter, particle distribution, Forchheimer extension, permeability.

2 February 3, 2006
1-D Simulations

This week was used to wrap up the Flow3-D source code checking, as far as how porosity is implemented. A simple 1-D example was used: the flow of Glyceryne through a 1-D channel 10 meters long.
According to many literature references (Bear, Burmeister, etc...) the drop in pressure should be computed with:

$$\partial P/\partial x = -\rho\left[\frac{\mu}{\rho}\frac{\alpha}{d^2}\frac{(1-\phi)^2}{\phi^3} + \frac{\beta}{d}\frac{(1-\phi)}{\phi^3}V_0\right]V_0 \tag{1}$$

V_0 is the seepage or filter velocity (or volumetric flow divided by cross section of the pipe). Using the following values:

$$\rho = 1261\frac{Kg}{m^3},\ \mu = 1.5\times 10^{-6}\frac{Kg}{ms},\ \phi = 0.38,\ V_0 = 1\frac{m}{s},\ \mathrm{d} = 6\ \mathrm{mm},\ \alpha = 175,\ \beta = 1.75$$

the expected drop in pressure is 4.16 Pa/m

Flow3-D is, by default, using the following equation:

$$\partial P/\partial x = -\rho\left[\frac{\mu}{\rho}\frac{\alpha}{d^2}\frac{(1-\phi)^2}{\phi^2} + \frac{\beta}{d}\frac{(1-\phi)}{\phi}V_0\right]V_0 \tag{2}$$

So the expected drop in pressure with (2) is 0.6 MPa/m

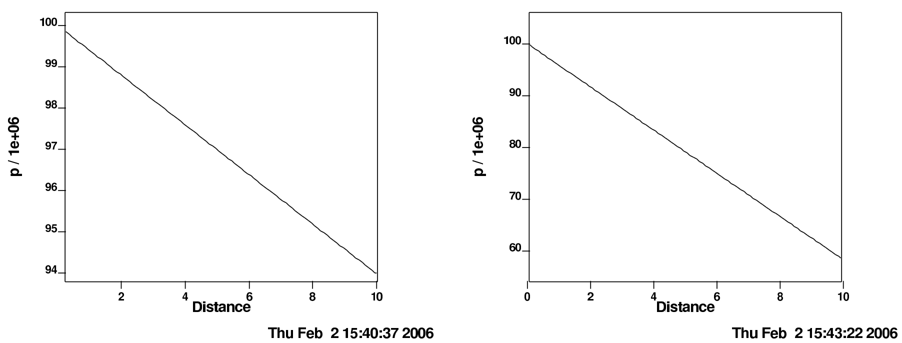


Figure 1: Drop in pressure over 10 m of length: a) With original Flow3-D code b) with the modified subroutine

Two runs were performed in 1-D to confirm the analytically predicted results:

- Run andrei03: Using the original Flow3-D code the result of the drop in pressure is shown in Figure 1 a).
- Run andrei04: Modifying the subroutine drgcl.F to correctly implement Equation (1). The results obtained are shown in Figure 1 b).

Conclusions:

- Flow3-D seems to be confusing filter velocity and microscopic velocity, the user subroutine developed needs to be used.
- Flow3-D has been emailed again (February 2) about this subject.
- Other than that Flow3-D is behaving as expected so it can be used with the modified subroutine.
- Confidence on Flow3-D has been gained.

Immediate future work:

- Rerun the flat plates examples with different porosities and powers applied now we are confident the code that calculates the drag is right.

3 February 10, 2006 Convection Between Two Parallel Plates with Porous Media in Between

1-D Benchmark

This week, with the help of Stuart Stothoff, I finally was convinced that Flow-3D equations for porous media are correct. The misunderstanding on my side came from the fact that Flow-3D displays and uses internally microscopic velocities. The run proposed by Stuart consisted of a pipe 30 meters long with porous material in the middle section (from x=10 to x=20 m).

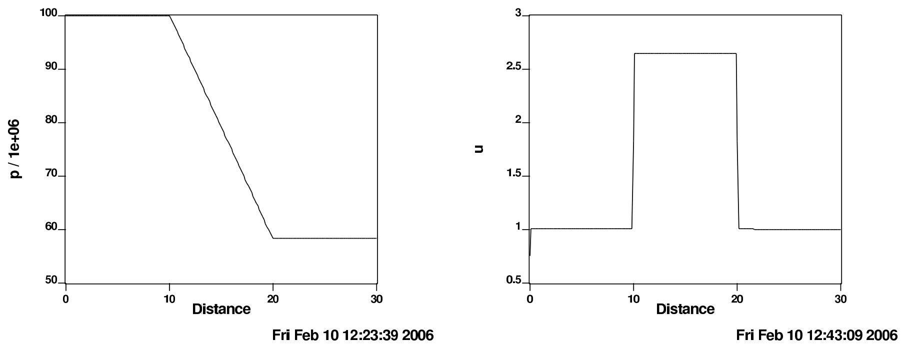


Figure 2: a) Drop in pressure in the pipe, b) velocity profile in the pipe

For a 1-D incompressible steady state flow entering with velocity V_0 in a porous pipe the expected drop in pressure is given by:

$$\partial P/\partial x = -\rho \left[\frac{\mu}{\rho} \frac{\alpha}{d^2} \frac{(1-\phi)^2}{\phi^3} + \frac{\beta}{d} \frac{(1-\phi)}{\phi^3} V_0 \right] V_0 \tag{3}$$

Using the following values:

$\rho = 1261 \frac{Kg}{m^3}$, $\mu = 1.5 \times 10^{-6} \frac{Kg}{ms}$, $\phi = 0.38$, $V_0 = 1 \frac{m}{s}$, d = 6 mm, $\alpha = 175$, $\beta = 1.75$

the expected drop in pressure (done with a hand calculator) is 4.16 Pa/m, which is what Flow-3D predicts implying that it is correctly implemented

Natural convection between two parallel plates

Three runs were performed with porosities of 0.1, 0.35, 0.6. The bottom plate was generating a power of 42.82 W and the top plate was at a constant temperature of 418 K. The distance between the plates was 1.36 meters and the length 3 meters.

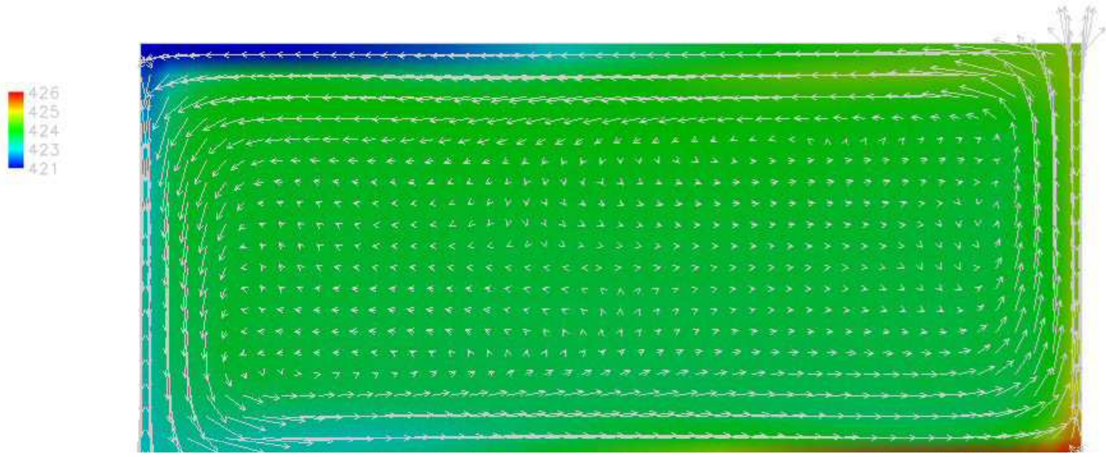


Figure 3: Porosity = 0.1

4 February 15, 2006 Convection Between Two Parallel Plates with Porous Media in Between

Asymmetry Problem

There was some concern about the asymmetry seen in the temperature and velocity fields of last week runs. We decided to let the runs go longer and see if that solved the problem. The stop time was increased to 10^6 seconds. The case with porosity 0.1 seemed to be pretty symmetric at the end of the run but the one with porosity 0.35 still has asymmetries as shown in Figures 4 and 5.

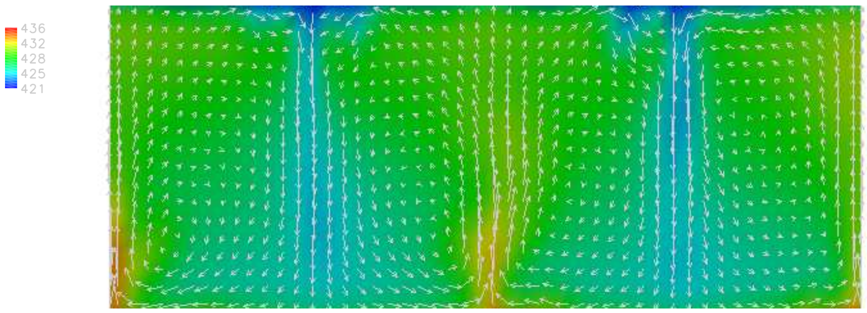


Figure 4: Temperature distribution for Porosity = 0.1

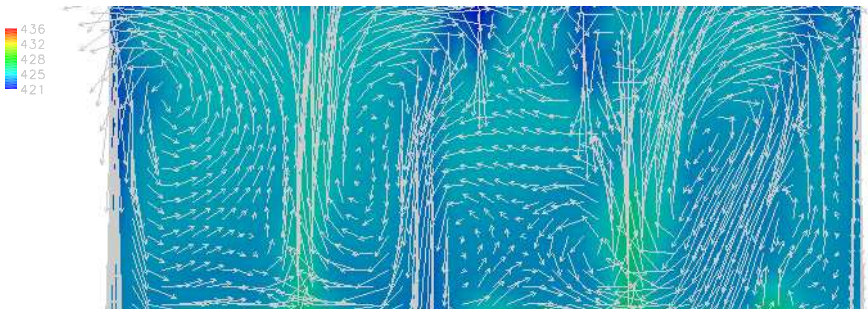


Figure 5: Temperature distribution for Porosity = 0.35

Since we are already using very large stop times to reach the steady state I think that increasing it even more is only going to harm us in the future.

This is a very easy and straightforward run with a coarse mesh that should not take a lot of computation time. My opinion is that the geometry of natural convection between two parallel plates is inherently unstable and, as such, very sensitive to any numerical oscillation that might occur. To prove this point I changed the geometry and run the problem that follows.

Natural convection in porous media between two concentric cylinders

The geometry of this problem consists of two concentric cylinders, the inner one (radius 0.5 m) at a temperature of 450 K and the outer one (radius 2 m) at 418 K. A porous media, with porosity 0.35, is placed between the cylinders. The steady state in this configuration is reached after only 2000 seconds. The temperature and Reynolds distribution are shown in Figure 6.

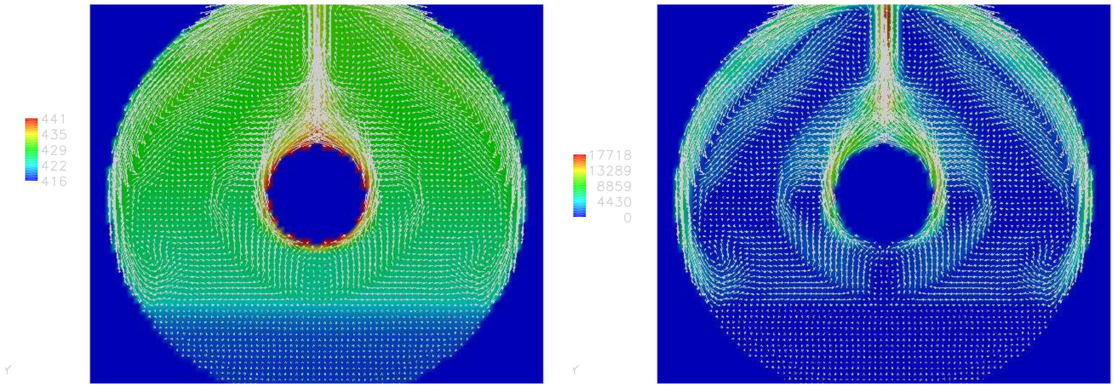


Figure 6: Temperature and Reynolds distribution for two concentric cylinders. Porosity = 0.35

The result is symmetric, as expected, and stable (does not oscillate with time).

5 February 20, 2006 Parameters used by Flow-3D

Brief discussion of the parameters

Equation (3) found in Mohanty's paper [1] gives permeability as:

$$K = \frac{\bar{D_p}^2 \phi^3}{72\tau(1-\phi)^2} \left[\frac{(\gamma C_{D_p}^3 + 3C_{D_p}^2 + 1)^2}{(1 + C_{D_p}^2)^2} \right] \tag{4}$$

If, for simplification, we assume all the particles are the same size ($C_{D_p} = 0$) then the equation is rewritten as:

$$K = \frac{D_p^2 \phi^3}{72\tau(1-\phi)^2} \tag{5}$$

Usually in the literature the permeability coefficient is written as:

$$K = \frac{D_p^2 \phi^3}{\alpha(1-\phi)^2} \tag{6}$$

Where α is a non-dimensional coefficient. The value of α is experimental and its usual value is around 180 or 175. In the case of Mohanty's paper we can identify:

$$\alpha \equiv 72\tau \tag{7}$$

Since in Mohanty's paper (table 5.1) an average value of tortuosity is $\tau \approx 2.125$ then $\alpha = 72 \times \tau = 153$, which is the value used in the simulations and "in family" with the 180 usually found in the literature. If an average particle diameter of $\bar{D}_p \approx 0.3m$ is used then, the parameter **oadrg** $\equiv \frac{\alpha}{\bar{D}_p^2} = 1700\ m^{-2}$.

Flow-3D uses the following equation to calculate the drop in pressure across a cell with a porous material:

$$\partial P/\partial x = -\rho \left[\frac{\mu}{\rho} \frac{\alpha}{d^2} \frac{(1-\phi)^2}{\phi^3} + \frac{\beta}{d} \frac{(1-\phi)}{\phi^3} V_0 \right] V_0 \tag{8}$$

This equation can be rewritten in terms of the permeability as:

$$\partial P/\partial x = -\rho \left[\frac{\mu}{\rho} \frac{1}{K} + \frac{\beta}{d} \frac{(1-\phi)}{\phi^3} V_0 \right] V_0 \tag{9}$$

β is also a semiempirical parameter which has a usual value in the literature of 1.75. β allows to better predict flows at high Reynolds numbers, but this correction is not being used in Mohanty's paper. The constant **obdrg** used by flow-3D is simply $obdrg = \beta/D_p$ so **obdrg** is zero in the runs.

Summary

Flow-3D uses three main input parameters for flow in a porous media:

- **opor** : the porosity ϕ
- **oadrg** $= \alpha/D_p^2$, related to permeability through $K = \frac{D_p^2\phi^3}{\alpha(1-\phi)^2} = \frac{\phi^3}{\mathbf{oadrg}(1-\phi)^2}$
- **obdrg** $= \beta/D_p$, corresponds to the Forchheimer extension, see Burmeister [2], page 48.

6 February 27, 2006 Parametric study for concentric cylinders

Analytical predictions

The Rayleigh number for an isothermal horizontal cylinder in an infinite porous media is given by (Mohanty [1] or Burmeister [2], page 441):

$$Ra_d = \frac{Kg\rho\beta\Delta Td}{\mu\alpha} \tag{10}$$

Convective flow is supposed to start for Rayleigh numbers of 40 or more. A simple parametric study using Equation 10 and varying the diameter d of the particles of the porous media and the porosity produces the table shown in Figure 7.

gravity	$g=$	9.81 m/s2		
internal radius	$r_i=$	1.4 m	$\alpha=$	153
diffusivity backfill	$\alpha_m=$	3.42E-04 m2/s		
viscosity air	$\mu=$	1.86E-06 Kg/ms		
density air	$\rho=$	1.225 kg/m3		
Th. Cond. Backfill	$\kappa=$	0.27 W/mK		

d=1 mm			**d= 10 mm**			**d= 100 mm**		
Porosity	**Permeability (m^2)**	**Ra**	**Porosity**	**Permeability (m^2)**	**Ra**	**Porosity**	**Permeability (m^2)**	**Ra**
0.005	8.25225E-16	0	0.005	8.25225E-14	0	0.005	8.25225E-12	0
0.01	6.66865E-15	0	0.01	6.66865E-13	0	0.01	6.66865E-11	4
0.02	5.44435E-14	0	0.02	5.44435E-12	0	0.02	5.44435E-10	29
0.03	1.87555E-13	0	0.03	1.87555E-11	1	0.03	1.87555E-09	99
0.04	4.53885E-13	0	0.04	4.53885E-11	2	0.04	4.53885E-09	240
0.08	3.95369E-12	0	0.08	3.95369E-10	21	0.08	3.95369E-08	2093
0.1	8.06907E-12	0	0.1	8.06907E-10	43	0.1	8.06907E-08	4272
0.2	8.16993E-11	4	0.2	8.16993E-09	433	0.2	8.16993E-07	43254
0.3	3.60144E-10	19	0.3	3.60144E-08	1907	0.3	3.60144E-06	190670
0.4	1.16195E-09	62	0.4	1.16195E-07	6152	0.4	1.16195E-05	615164
0.5	3.26797E-09	173	0.5	3.26797E-07	17302	0.5	3.26797E-05	1730150
0.6	8.82353E-09	467	0.6	8.82353E-07	46714	0.6	8.82353E-05	4671405
0.7	2.49092E-08	1319	0.7	2.49092E-06	131876	0.7	0.000249092	13187588
0.8	8.36601E-08	4429	0.8	8.36601E-06	442918	0.8	0.000836601	44291842
0.9	4.76471E-07	25226	0.9	4.76471E-05	2522559	0.9	0.004764706	252255882

Figure 7: Rayleigh number for different porosities and particle diameters

Also shown are the values used for the other parameters. Highlighted in that figure are the porosities where the convection should start for the particle diameter considered. Some numerical simulations were performed to check if Flow-3D was able to predict the "transition" porosities.

Flow-3D Prediction for d=1 mm

According to the previous table transition should happen around a porosity of 0.4. Indeed Figure 8 does not show any convection and very small Reynolds numbers, while Figure 9 does show the asymmetry expected in the temperature if convection happens.

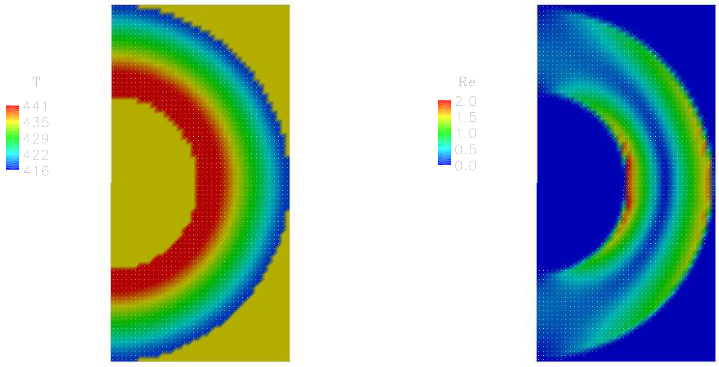


Figure 8: Porosity 0.4, diameter = 1 mm

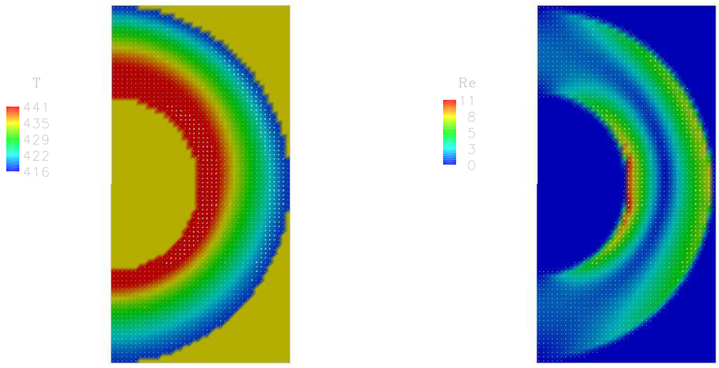


Figure 9: Porosity 0.5, diameter = 1 mm

Not shown is a computation that was performed at a porosity of 0.2 showing no convection.

Flow-3D Prediction for d=10 mm

According to the table above for particles of 10 mm transition should happen around a porosity of 0.1. Two computations were performed at 0.08 and 0.2 porosity and only the last one shows convection.

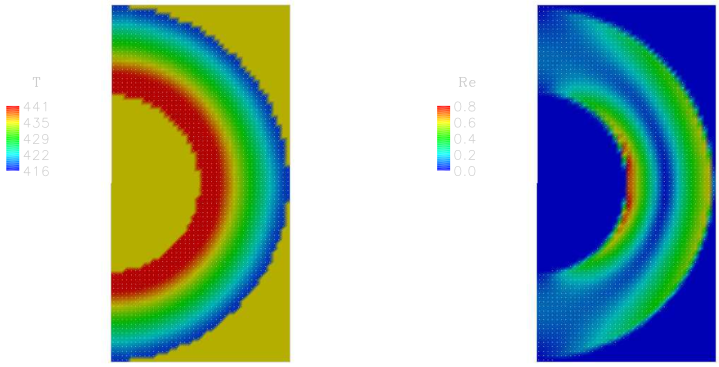


Figure 10: Porosity 0.04, diameter = 10 mm

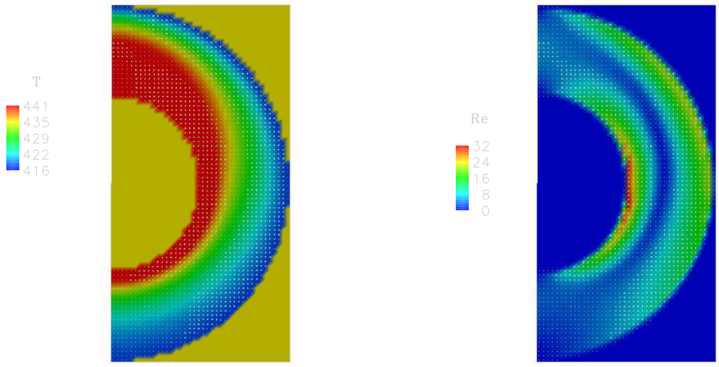


Figure 11: Porosity 0.2, diameter = 10 mm

Flow-3D Prediction for d=100 mm

For the particles with diameter 100 mm the predicted transition is around 0.04 porosity. Two computations performed at 0.01 and 0.08 porosity are shown in Figures 12 and 13. The last one shows some plumes raising from the hot cylinder.

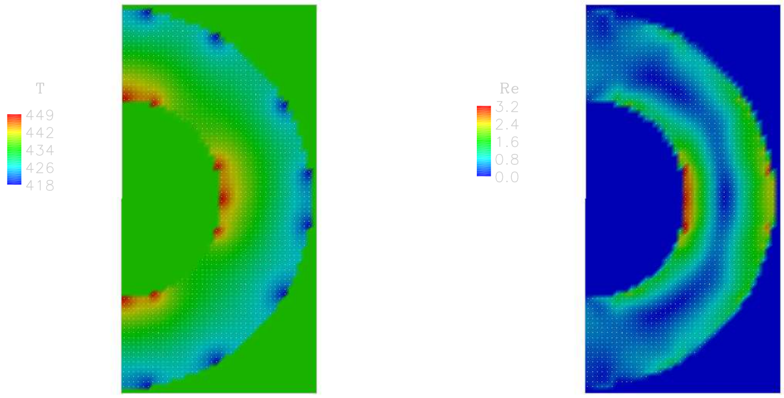


Figure 12: Porosity 0.01, diameter = 100 mm

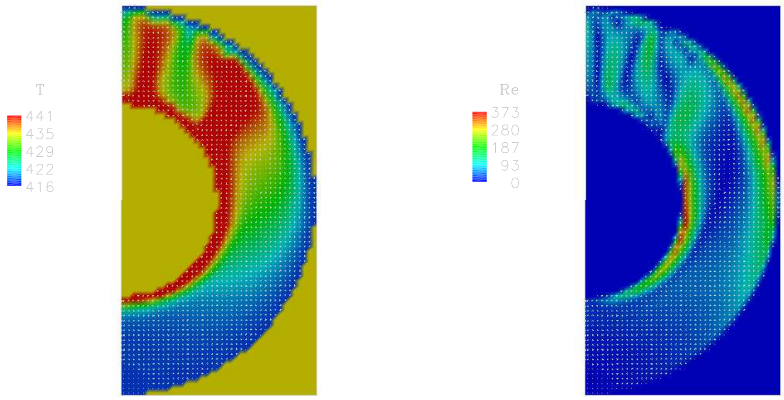


Figure 13: Porosity 0.08, diameter = 100 mm

Conclusions and future work

From my perspective Flow-3D seems to be doing a good job in predicting when convection starts, although the accuracy in that prediction should be discussed. Are we expecting it to predict correctly up to ± 0.1 or ± 0.01 or the Rayleigh number? I started with the cylindrical geometry because it seems more stable than the rectangular. Next step will be to repeat these calculations with two parallel plates. Any comments?

7 March 8, 2006
Parametric study for parallel planes

Analytical predictions

The Rayleigh number was miscalculated in the last report (progress briefing no. 5). Since the thermal expansion coefficient for an ideal gas is $\beta = 1/T$, I inadvertently simplified ΔT and β, leading to a bad calculation of the Rayleigh number. The Rayleigh number for both, an isothermal horizontal cylinder in an infinite porous media and porous media in between two planes is given by (Mohanty [1] or Burmeister [2], page 441):

$$Ra_d = \frac{Kg\rho\beta\Delta T d}{\mu\alpha} \tag{11}$$

gravity	g=	9.81	m/s^2	α=	153	n.d.
internal radius	r_i=	1.4	m	Tmax=	450	K
diffusivity backfill	α_m=	3.42E-04	m^2/s	Tmin=	418	K
viscosity air	μ=	1.86E-06	Kg/ms	ΔT=	32	K
density air	ρ=	1.225	kg/m^3	Tavg=	434	K
Th. Cond. Backfill	κ=	0.27	W/mK			

	d=0.001 m		d=0.01 m		d=0.1 m	
Porosity	**Permeability (m^2)**	**Ra**	**Permeability (m^2)**	**Ra**	**Permeability (m^2)**	**Ra**
0.005	8.25E-16	0	8.25E-14	0	8.25E-12	0
0.01	6.67E-15	0	6.67E-13	0	6.67E-11	0
0.02	5.44E-14	0	5.44E-12	0	5.44E-10	1
0.03	1.88E-13	0	1.88E-11	0	1.88E-09	4
0.04	4.54E-13	0	4.54E-11	0	4.54E-09	9
0.08	3.95E-12	0	3.95E-10	1	3.95E-08	77
0.1	8.07E-12	0	8.07E-10	2	8.07E-08	157
0.2	8.17E-11	0	8.17E-09	16	8.17E-07	1595
0.3	3.60E-10	1	3.60E-08	70	3.60E-06	7029
0.4	1.16E-09	2	1.16E-07	227	1.16E-05	22679
0.5	3.27E-09	6	3.27E-07	638	3.27E-05	63784
0.6	8.82E-09	17	8.82E-07	1722	8.82E-05	172218
0.7	2.49E-08	49	2.49E-06	4862	2.49E-04	486178
0.8	8.37E-08	163	8.37E-06	16329	8.37E-04	1632879
0.9	4.76E-07	930	4.76E-05	92998	4.76E-03	9299756

Figure 14: Rayleigh number for different porosities and particle diameters

Convective flow starts, according to a perturbation analysis that can be found at the end of [2], for Rayleigh numbers of 40 or more. A simple parametric study using Equation 11 and varying the diameter d of the particles of the porous media and the porosity produces the table shown in Figure 14.

The table is valid for two concentric cylinders as well as for two parallel planes

Also shown are the values used for the other parameters. Note that now ΔT is shown in the table. The porosities where the convection should start for the particle diameter considered are highlighted. Twelve runs were performed using porosities of 0.02, 0.1, 0.5 and 0.9 with particle diameters of 1 mm, 10 mm and 100 mm. The objective of the runs was to check if Flow-3D can capture properly the onset of convection. More runs, as described below, were performed around the onset value of convection to determine more accurately where it starts.

Flow-3D Prediction for d=1 mm

The distance between the two parallel planes is 1.36 m. The bottom plate is at a temperature of 418 K (145 C) and the top plate at 450 K (177 C). The length of the plates is 10 m. According to Figure 14 transition should happen around a porosity of 0.7. The computation performed with $\phi = 0.5$ did not show any convection, while the one with $\phi = 0.9$, see Figure 15, does show maximum Reynolds numbers of around 100. A finer study (runs drift47 through drift51) in increments of 0.05 from a porosity of 0.6 to 0.8 shows that convection only starts for $\phi = 0.8$ or a Rayleigh number of 163. Although this number is somewhat larger than the expected Ra=40, I still think it is actually a remarkably good prediction.

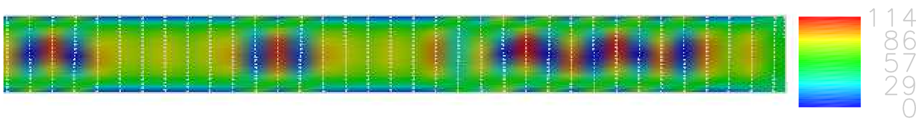


Figure 15: Porosity 0.9, diameter = 1 mm

Flow-3D Prediction for d=10 mm

According to the table above for 10 mm particles transition should happen around a porosity of 0.3. The "coarse" (large steps in ϕ) computations showed that convection was happening at $\phi = 0.5$ and a finer study done later (runs drift51 through drift55) shows convection barely starts at $\phi = 0.25$, with Reynolds numbers of 1 and it is definitely happening at $\phi = 0.3$, very close to the expected Ra=40 value.

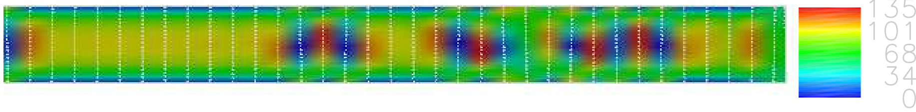


Figure 16: Porosity 0.5, diameter = 10 mm

Flow-3D Prediction for d=100 mm

For the particles with diameter 100 mm the predicted the theoretical transition is between 0.04 and 0.08 porosity. The first set of runs showed convection starting around $\phi = 0.1$. Refined computations from $\phi = 0.02$ to $\phi = 1$ in steps of 0.02 (runs drift57-61) show that the onset actually happens at 0.04, where Reynolds numbers of around twenty could be seen.

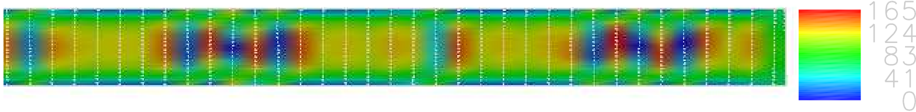


Figure 17: Porosity 0.1, diameter = 100 mm

Summary, Conclusions and future work

Table 1 compares the predictions given by the theory and Flow-3D. The code does a very good prediction for particles of 10 mm diameter and, although it is a little bit off for 1 and 100 mm particles, it gives reasonable prediction for the other sizes.

From these results, I think Flow-3D is a reliable code as far as flow in porous media. Probably the next step should be to implement in Flow-3D a distribution of porous media with different porosities and permeabilities. Since there are a lot of ways to implement this maybe it would be good to have a discussion. I also would like to have some more time to study the origin of the Rayleigh number (which comes from a perturbation solution)

Diameter	**Analytical**	**Flow-3D**
1 mm	0.6-0.7	0.75-0.8
10 mm	0.2-0.3	0.25-0.3
100 mm	0.04-0.08	0.02-0.04

Table 1: Comparison of porosities when convection is supposed to start predicted by the theory and by Flow-3D for different particle diameters

to understand better the problem and, on the top, to have an idea of the charateristic times involved.

8 April 11, 2004 Approach to explicitly model the porous media distribution of natural backfill with Flow-3D

Approach

Explicitly accounting in the simulations for the individual particles and chanels is impossible even with large computers because the models need to be 3-D for the fluid to be able to flow through the interstices of the rubble.
An easy way to simulate the natural backfill is to use an average homogeneous porous media as we have done so far. A step further is to use an inhomegenous porous media, meaning the characteristics of the porous media depend on the position.
What characterizes a porous media in a computation cell is its porosity ϕ, and the parameter a_0, which for spherical particles of diameter D_P is known to be:

$$a_0 = \frac{180}{D_p^2} \tag{12}$$

Computational Procedure

If we consider the parameters tortuosity, skewness,standard deviation and porosity $(\tau, \gamma, \sigma_p, \phi)$ fixed to some given value as well as $\bar{D}_p$ we can build a computation field as follows:

1. Fix $\tau, \gamma, \sigma, \phi$ and $\bar{D}_p$
2. Generate the mathematical distribution of particle diameters with its average value $\bar{D}_p$ (Do we also want a distribution of porosities?)
3. Divide the flow field in $n \times m$ bins.
4. Use a Monte Carlo procedure with the D_p distribution to assign to each bin a particle diameter. This is equivalent to assign a permeability K to the bin given by,

$$K = \frac{{D_p}^2 \phi^3}{72\tau(1-\phi)^2} \tag{13}$$

The term

$$\left[\frac{(\gamma C_{D_p}^3 + 3C_{D_p}^2 + 1)^2}{(1 + C_{D_p}^2)^2}\right] \tag{14}$$

is not included in Eq. (13) because it is already being taken into account when determining D_p from the distribution of diameters. For Flow-3D purposes assigning K is done through a_0, the parameter that determines the porous material:

$$a_0 = \frac{\alpha}{D_p^2}, \quad where, \quad \alpha = 72\tau \tag{15}$$

Each bin will have its particular porous media, from one bin to another the diameter of the particle is different

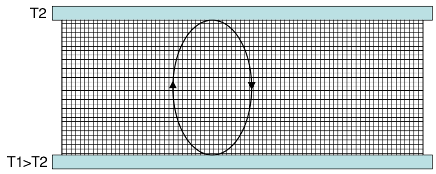


Figure 18: Two plates with a distribution of inhomogenous porous media in between

Some concerns

- We need to decide the size of the bins. My first idea is to have all the bins the same size and try smaller and smaller sizes to see the difference in the convection pattern
- Is the smaller the better? We should have 3 to 5 cells across the bin.
- Does it make sense to have the bin being smaller than the diameter of the particle?
- What would an explicit simulation of the particles give us that the average approach does not?

9 April 21, 2006
Study of Forchheimer extension on the onset and level of convection between two parallel plates

Introduction

D'arcy's law can be extended to high Reynolds numbers to account for turbulence effects by means of the Forchheimer extension. In Flow-3D notation, for an incompressible steady-state flow in 1-D (no gravity):

$$\partial P/\partial x = \underbrace{-\frac{\alpha}{d^2}\mu\frac{(1-\phi)^2}{\phi^3}V_0}_{D'arcy}\underbrace{-\rho\frac{\beta}{d}\frac{(1-\phi)}{\phi^3}V_0^2}_{Forchheimer} \tag{16}$$

Where V_0 is the macroscopic velocity of the fluid.

Burmeister [2] writes the same equation in terms of permeability K and the inertia coefficient C as:

$$\partial P/\partial x = \underbrace{-\frac{\mu}{K}V_0}_{D'arcy}\underbrace{-\rho\frac{C}{K^{1/2}}V_0^2}_{Forchheimer} \tag{17}$$

Where

$$K = \frac{d^2\phi^3}{\alpha(1-\phi)^2} \qquad and \qquad C = \frac{\beta}{\alpha^{1/2}\phi^{3/2}} \tag{18}$$

The parameters required by Flow-3D input deck are $a_0 = \alpha/d^2$ and $b_0 = \beta/d$, where usually $\alpha \approx 180$ and $\beta \approx 1.75$. To stay consistent with Mohanty [1] we need to use $\alpha = 72\tau$ as explained in previous briefings.

Computation setup

Two parallel planes 20 m long and 1.36 m apart have porous material in between. The boundary conditions used this time were different than the previous runs:

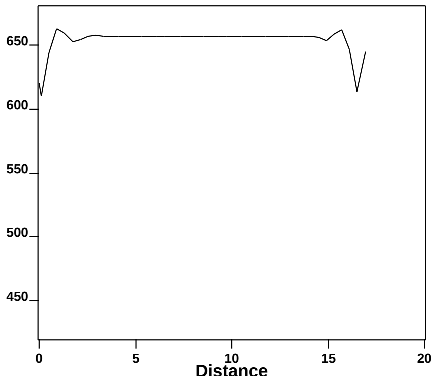
1. Top plate has a constant temperature of 420 K (147 C)

2. Bottom plate has a constant power of 256 W/m^2. The power was calculated on the basis that the heat output of the cask is 1.45 kW/m, the length is 5.125 m and the radius is 0.9 m.

Computations were performed for two different particle diameters, 0.1 and 0.01 m, to check where the onset of convection was. The final temperature of the bottom plate can be used to assess the "level of convection". If the temperature is similar to the pure conduction temperature (around 660 K) then no significant convection contributes to the cooling of the lower surface.

Particles with d=10 cm

A total of 10 runs were performed, 5 runs with the Forchheimer extension off ($\beta = 0$) and 5 runs with $\beta = 1.75$. The runs swept the following range of porosities: $\phi = (0.02, 0.04, 0.06, 0.08, 0.1)$.



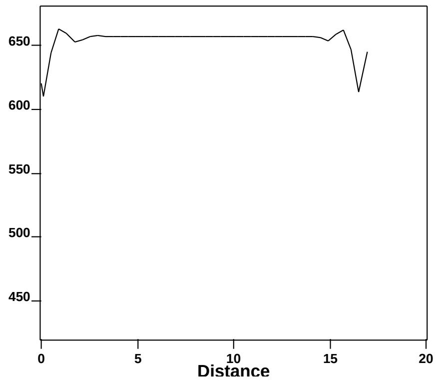


Figure 19: a) Temperature profile in the lower plate with Forchheimer extension off, run drift64 b) with Forchheimer on, run drift69. Porosity for both is $\phi = 0.02$. No convection.

Figure 19 (temperatures in the vertical axis are in Kelvin) shows that no convection is happening when the porosity is 0.02, but, as shown in Fig. 20 convection starts with porosity $\phi = 0.04$. Convection onset does not depend on the Forchheimer extension since it is only important at high Reynolds numbers and, of course, at the onset of convection Re numbers are very small.

At high porosities ($\phi = 0.1$) the level of convection becomes important and the turbulent term is expected to be more significant. Figure 21 compares

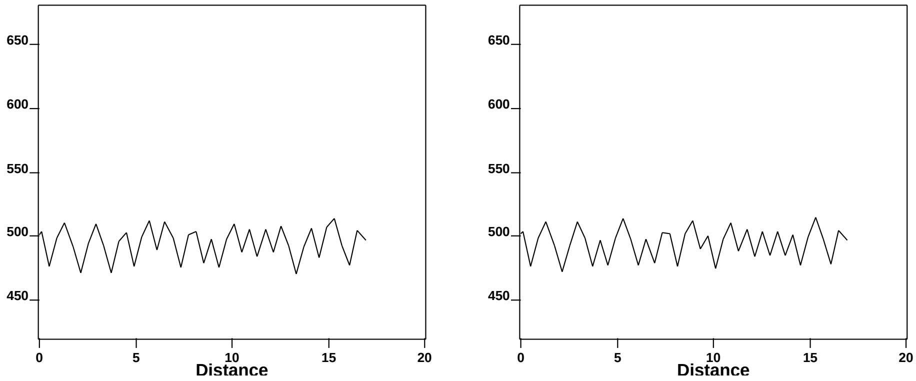


Figure 20: a) Temperature profile in the lower plate with Forchheimer extension off, run drift65 b) with Forchheimer on, run drift70. Porosity for both is $\phi = 0.04$. Convection takes the temperature down.

the temperature of the bottom plate with and without the turbulent term. Clearly the influence is very small. The Reynolds numbers on these computations were on the order of 100.

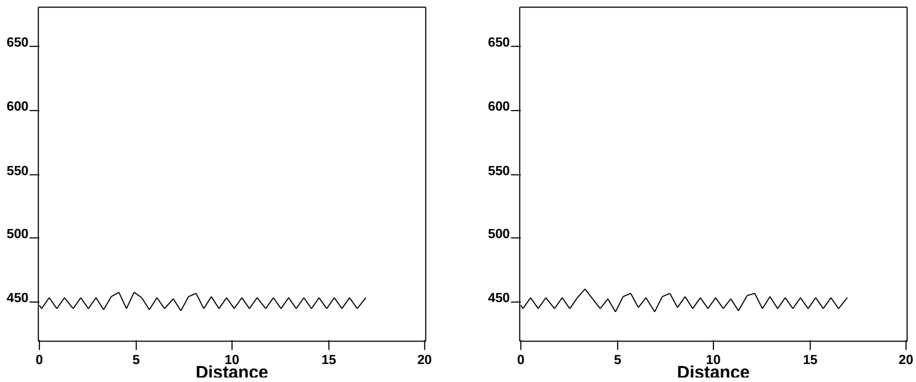


Figure 21: a) Temperature profile in the lower plate with Forchheimer extension off, run drift68 b) with Forchheimer on, run drift73. Porosity for both is $\phi = 0.1$. Again Forchheimer extension is hardly noticeable.

The Forchheimer extension will become important when:

$$\frac{\alpha}{d^2}\mu\frac{(1-\phi)^2}{\phi^3}V_0 \approx \rho\frac{\beta}{d}\frac{(1-\phi)}{\phi^3}V_0^2 = \mu\frac{\beta}{d^2}Re_d\frac{(1-\phi)}{\phi^3}V_0 \qquad (19)$$

$$Re_d \approx \frac{\alpha}{\beta}(1-\phi) \approx 100(1-\phi) \tag{20}$$

Where Re_d is the Reynolds number based on the diameter of the particle. If we want to know the Reynolds number based on the characteristic length of the problem, which is the distance beween the plates then:

$$Re_L \approx 1000(1-\phi) \tag{21}$$

$$V_0 \approx \frac{\mu d}{\rho} 100(1-\phi) \approx 0.1(1-\phi) \qquad if \quad \phi << 1 \qquad V_0 \approx 0.1 mm/s \tag{22}$$

Note that if the higher the porosity the more important the Forchheimer extension.

Particles with d=1 cm

A similar exercise (runs drift74 to drift87) to the one presented in the previous section was done with 1 cm particles leading to a similar conclusion: the Forchheimer extension does not affect the onset of convection and, even when convection happens, its influence on the convection level is small, see Fig. 22.

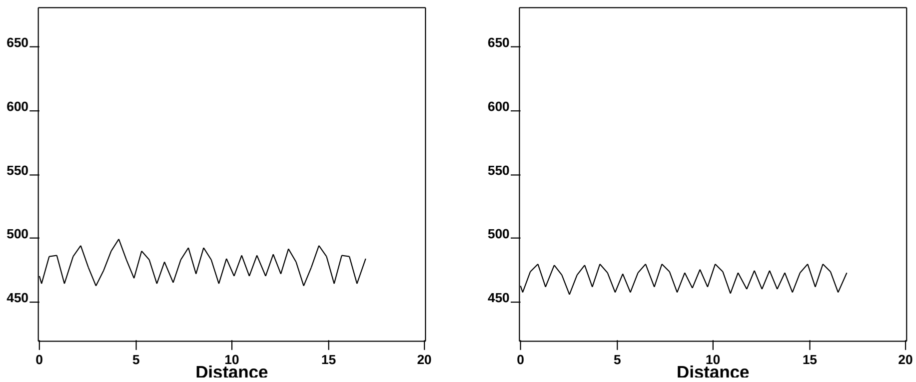


Figure 22: a) Temperature profile in the lower plate with Forchheimer extension off, run drift79, particle size 1 cm b) with Forchheimer on, run drift87. Porosity for both is $\phi = 0.4$. Forchheimer extension begins to make a difference, but it is still a small one.

Conclusions

This study has shown that the Forchheimer extension does not affect the onset of convection. When convection is ongoing at porosities of around 0.4 the Forchheimer extension has a small effect on the convection level, making it slightly larger.

I think we should still explore a "mesoscale" approach (implementing "patches" of rock with distributed sizes in the flow field). Convection is clearly very important as a cooling mechanism of the drip shield, and, even if whole scale convection is not possible due to low porosity, convection cells that could develop locally would help the cooling mechanism.

10 May 5, 2006 - Random particle generation

Random Particle Generation

A FORTRAN code (part.f90) was written to generate a particle distribution. The important features of the codes are:

- The particle distribution to be sorted is an input of the code
- The distribution is read and the minimum and maximum possible particle radius is determined. Figure 23 shows the (made-up) distribution in terms of particle size and phi ($= -log_2(D_p)$).
- The code first divides the space into seed points or a grid where possible particle centers could be placed. The distance between the seed points is the minimum radius.
- The code then randomly selects one of the seed points checking that it does not lay inside another particle or closer than the minimum radius
- The code checks the distance between the seed point and the boundaries to avoid interference, if the distance is r_{min} then the minimum radius particle is automatically assigned.
- The code randomly selects a radius for the particle and check if it interferes with boundaries or other particles
- If there is interference the code resamples and iterates. The iterations limit is arbitrarily set to 5 million.
- The code goes on until it reaches the desired number of particles or the maximum number of iterations. Flow-3D has a limit of 500 particles but they can provide us with a "special" version with more particles if we need it.

Three examples of the particles obtained with the previous method and distribution are shown in Fig. 24

Another made-up distribution, with smaller particles, was also tried to further check the FORTRAN code. The distribution is shown in Fig. 25. The smallest particle used had a 5 mm diameter. With smaller particles it is possible to better fill the field and obtain lower porosities.

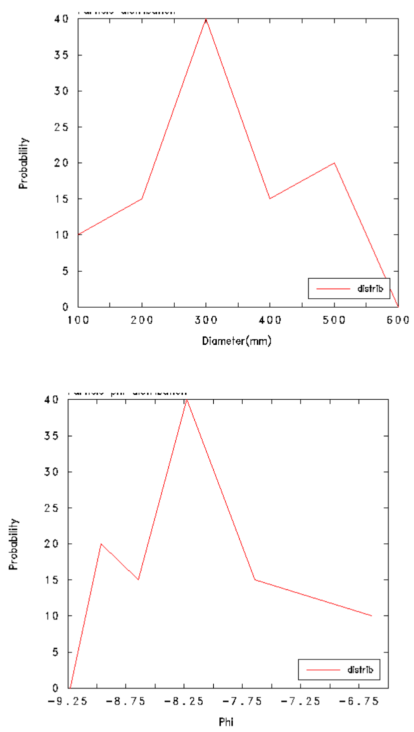


Figure 23: a) Made-up distribution used as input b) Phi-distribution

An example of the field obtained for the last distribution is shown in Fig. 26. Also shown are the temperature of the particles and the velocity vectors. “Black meanders” are consequently preferred paths for the fluid. Important details in the computation procedure (run driftzz) are:

- The temperature at the top is a boundary condition set to 420 K. The bottom has a power condition of 256.4 W/m^2 which correspond to the 1.45 kW/m^2 number provided by Mohanty (in fact in need to double check this).
- The fluid in between is air treated as an ideal gas.
- The distance between the planes is 1.36 m.
- The mesh was 300 $\times$ 200, it took 18 hours to reach the point shown in Fig. 26 and still is running to confirm quasi-steady state.

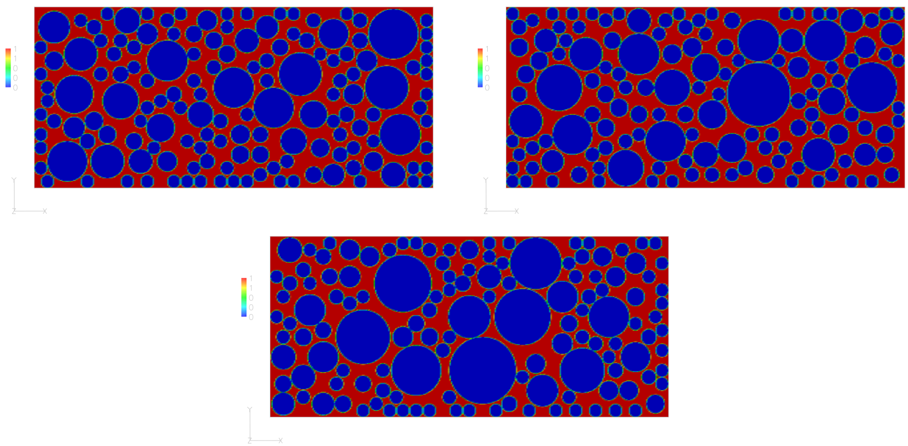


Figure 24: Using the distribution shown in Fig. 23 we can obtain different particle fields like the ones shown in this image. The number of particles is around 140 and was limited by the number of iterations needed to place the particles.

The fluid temperature is shown in Fig. 27. The level of convection is high making the temperature of the bottom plate drop to around 480 K (217 C).

Conclusions

A random particle generator, based on a given particle distribution, has been written and proved to work. The next step should be to decide how many particles we want to use (do we need to ask for a special version of the code?) and what would be considered a realistic distribution.

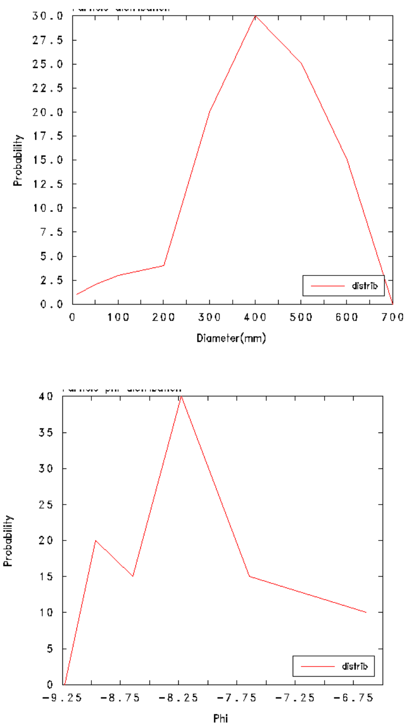


Figure 25: a) Distribution with smaller particles used as input wit b) Phi-distribution

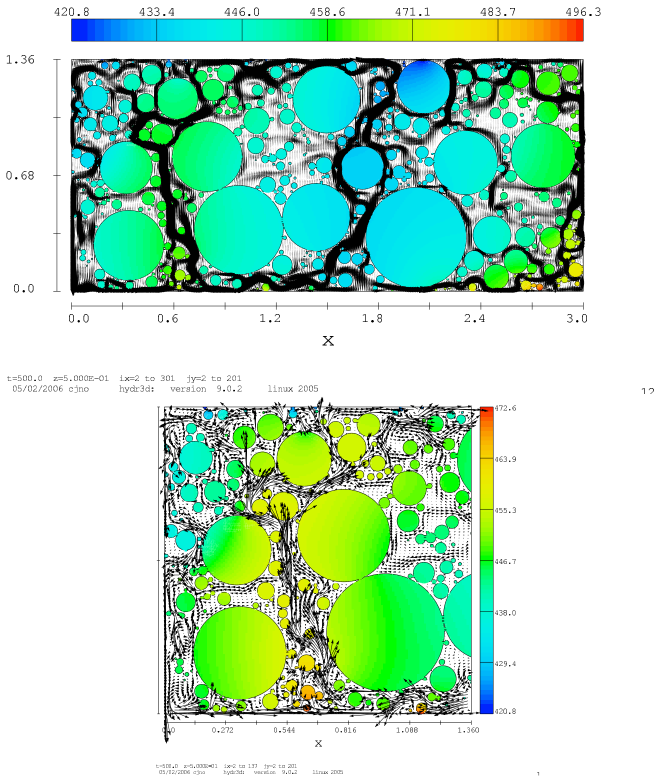


Figure 26: a) Particles and temperature field obtained with a distribution that has smaller particles. Also shown are velocity vectors. Resulting porosity is 0.453. The number of particles is 499 b) Detail of the left image

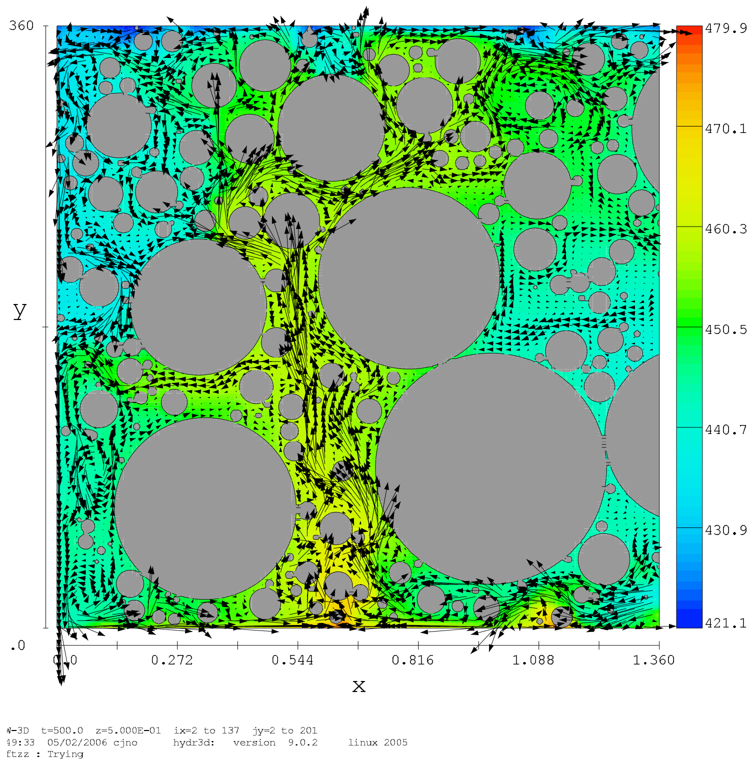


Figure 27: Fluid temperature detail

11 May 11, 2006 - Comparison of analytical and numerical results

Natural convection between two concentric cylinders with porous material in between given the heat flux in the inner cylinder

Theory

The Nusselt number for this configuration is found in [1], Eq. (9). The Rayleigh number based on the internal radius is $Ra_L = gK\beta\Delta T r_i/\nu\alpha$. The Nusselt number for this configuration is given by

$$Nu \approx 0.44 Ra_{r_i}^{1/2} \frac{ln(r_o/r_i)}{1 + 0.916(r_i/r_o)^{1/2}} \tag{23}$$

To estimate the temperature of the inner cylinder ($r_i = 1.6\ m$) the equations and constants were implemented in an Excel file (Temp concentric2.xls) where the temperature was iterated and solved. The outer cylinder radius is 2.76 m

Particle Diameter Dp		0.01	m
Porosity phi		0.6	
alpha constant al		153	
Permeability Kp		8.82E-07	m2
Conductivity backfill kb		0.27	W/mK
Avg Compressib.	β=	0.002192	1/K
density air	ρ=	0.77423	kg/m3
Kinematic Viscos	ν=	2.40E-05	m2/s
diffusivity air	α_m=	4.82E-05	m2/s
WP power		7430	W
WP length		5.125	m
Power per leng		1450	W/m
Power per area		165	W/m2
Tout		418	
Ti estimated		494	
Tavge		456.0	
Ra		1.75E+03	
Nu		7.732	
Solved Twp		494.6	K

Figure 28: Table showing the important parameters used in the analytical model and the results

The analytical model gives a temperature for the inner cylinder of 495 K as shown in Fig. 28.

Numerical simulation

Flow-3D v9.2, modified for ideal gas, was used to simulate natural convection between two parallel cylinders, see Fig. 29. The important input parameters follow (run driftb01):

- The inner cylinder generates a heat flux equal to 165 W/m^2, the outer cylinder is set to a constant temperature of 418 K (144.8C).
- The porous media in between has a porosity of 0.6 and a particle diameter of 1 cm. The a constant that describes the porous object for Flow-3D was set to

$$a = \frac{\alpha}{D_p^2} = \frac{153}{0.01^2} = 1530000 \Rightarrow K = \frac{D_p^2\phi^3}{\alpha(1-\phi)^2} = 8.82 \times 10^{-7} m^2 \quad (24)$$

- Porous media conductivity is 0.27 W/mK.
- Thermal interaction between the porous media and the fluid was allowed through a input variable called OSPOR which is the pore surface per unit of volume of porous media. The value used was 10.

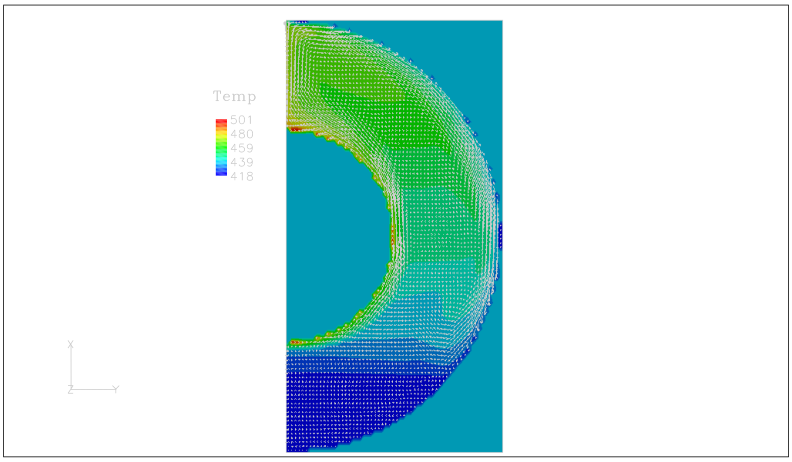


Figure 29: Results from Flow-3D simulation, temperature plot (in Kelvin), run driftb01

Comparison and concerns

The theory gives inner cylinder temperature of 495 K while Flow-3D gives an area-averaged temperature of 497 K so the comparison is very good. Nevertheless I still have some concerns with this run:

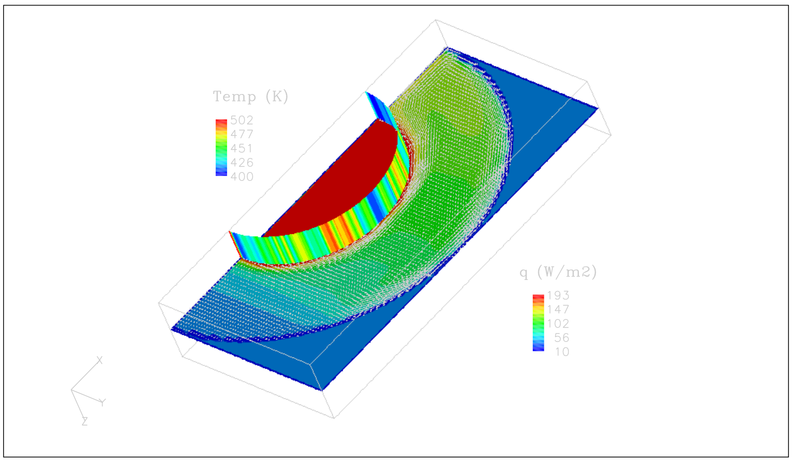


Figure 30: Fluid temperature and surface showing heat flux for run driftb01

- The heat flux was double checked with the postprocessor by creating a surface where flux is known and integrating the flux over the surface, see Fig. 30. The area-averaged (or integrated) heat flux was not 165 W/m^2 as requested in the input, but varied with time and stayed around 100 W/m^2. This is an unexpected behavior of Flow-3D that has been reported and is under study.

- A similar run (drift92) but without porous material in the cavity (only air) gave an averaged temperature of the inner cylinder of 490 K while the theoretical prediction is 515 K (using equation in page 428, [2]). With half the power applied to the inner cylinder I was getting the right power in the postprocessing part, at least for the inner cylinder.

In summary the results are promising but I still feel I have not completely under control what Flow-3D is doing as far as applying heat flux conditions or even temperature conditions to obstacles.

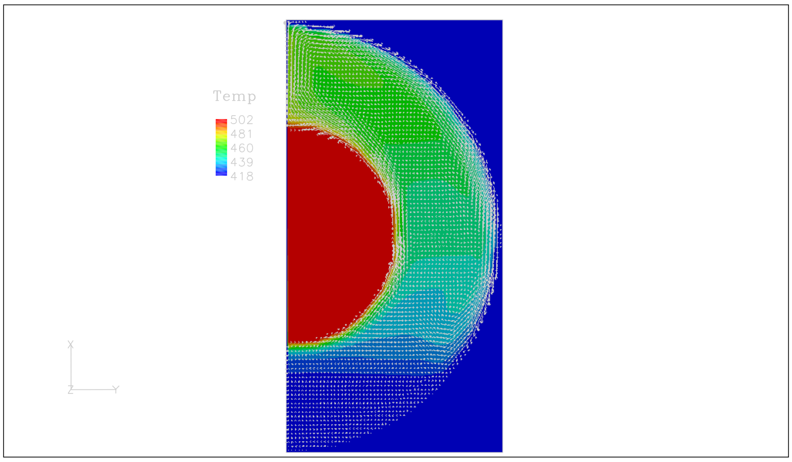


Figure 31: Porous media and cylinders temperatures in Kelvin for run driftb01

Natural convection between two parallel planes with porous material in between, given heat flux in bottom plate

Theory

The theory is explained in [2], page 444. Natural convection will happen in a saturated porous medium of thickness L enclosed between two plates and heated from below when the Rayleigh number based on the thickness $Ra_L = gK\beta\Delta TL/\nu\alpha$ is bigger than 39.5. The Nusselt number for this configuration is given by $Ra_L/40$ when $Nu_L = Ra_L > 40$.
To estimate the temperature of the bottom plate the equations and constants were implemented in an excel file (Temp concentric2.xls) where the temperature was iterated and solved.

The analytical model gives a bottom temperature of 569 K as shown in Fig. 32.

Numerical simulation

Flow-3D v9.2, modified for ideal gas, was used to simulate natural convection between two parallel plates. The important input parameters follow (run driftb10):

Distance between planes (Lp)			1.36 m
Ttop			447 K
Avg Compressib.		β=	0.00196799 1/K
density air		ρ=	0.69497791 kg/m3
Kinematic Viscos		ν=	2.68E-05 m2/s
diffusivity air		α_m=	5.37E-05 m2/s
Power per area			165 W/m2
		g=	9.81 m/s2
Ra		1.97E+03	
Nu		49.205	
	Ti estimated		569
	Tav		508.0
	Solved Twp		569.3

Figure 32: Table showing the important parameters used in the analytical model and the results

- The bottom plate is a boundary condition of heat flux equal to 165 W/m^2, the top plate is set to a constant temperature of 418 K (144.8C). Lateral boundary conditions are symmetry conditions.
- The distance between the plates is 1.36 m.
- The porous media in between has a porosity of 0.6 and a particle diameter of 1 cm. The a constant that describes the porous object for Flow-3D was set to the same than the one for the cylinder
- Porous media conductivity is 0.27 W/mK.

Comparison and concerns

The theory gives a bottom plate temperature of 569 K while Flow-3D gives an area-averaged temperature in the bottom of 555 K, see Fig. 33. This might seem a reasonable result, but note in Fig. 32a) that the top temperature I had to use in the model is not the boundary condition temperature but the area-averaged temperature in the top. If I use 418 K as the top temperature in the analytical model the temperature predicted in the bottom is 528 K. Some concerns:

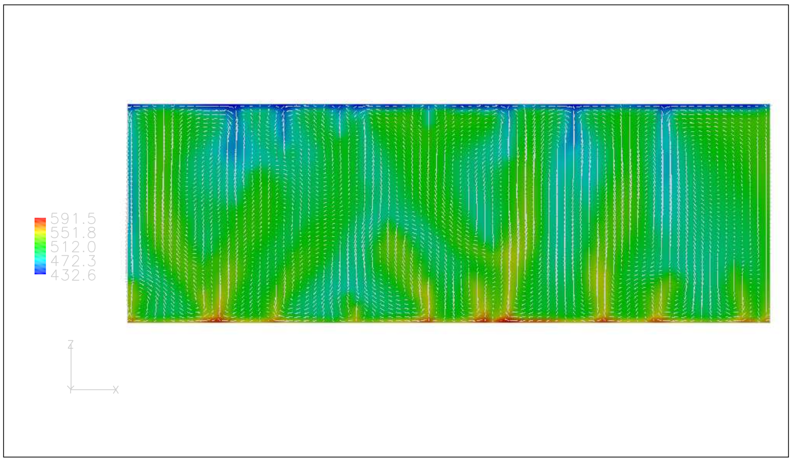


Figure 33: Fluid temperatures in Kelvin for run driftb10

- By default Flow-3D does not produce any thermal interaction between porous media and fluid. So the run showed in Fig. 32b) solved independently the conduction problem for the porous medium. If allow that interaction to happen (by setting a constant called OSPOR, as in run driftb05) the result is even less satisfactory.
- I also tried to play with heat transfer coefficients between boundaries and fluid and between boundaries and porous media but the results were not good.
- Putting some rugosity in the boundary did not make things better.
- Simplifying the run by setting top and bottom temperatures in the boundaries and comparing heat flux for analytical and numerical results was not successful either
- Did some correspondance with Flow-3D but still did not solve the problems.

In summary the two plane problem, either with a heat flux or constant temperature boundary condition was not solved satisfactorily. Probably I would need to talk a lot with Flow-3D to get it to match the analytical predictions.

Conclusions

Natural convection is being a tricky problem in Flow-3D. Sometimes it looks like the code is not enforcing the boundary conditions in power or temperature. Conversations are going on with Flow-3D. Still I think we should continue exploring the explicit particles simulations and, little by little continue benchmarking Flow-3D with some known analytical solutions.

12 May 30, 2006 - More on Benchmarking, Natural Convection in Vertical Planes

Introduction

In the last briefing (no. 10) the comparison of theory and numerical results was satisfactory for the natural convection between cylinders although some points remained to be clarified. For natural convection between parallel planes the result was clearly less than satisfactory for both convection with and without porous media in between.
In this briefing a step back was taken to compare analytical and numerical results for natural convection in the presence of a vertical wall. This case is the simplest both analytically and numerically so Flow-3D is expected to match the model's results. In fact both analytical and numerical results match very well.

Natural convection close to a vertical plate at constant temperature

The local Nusselt number for this configuration is found in [2], pg. 396, in the equation right before Eq. (10-22):

$$\frac{Nu_x}{Ra_x^{1/4}} = 0.51\left(1 + \frac{20}{21Pr}\right)^{-1/4} \tag{25}$$

This equation was implemented in the Excel file Temp concentric2.xls with a temperature of the fluid far away from the wall of 300 K, and a wall temperature of 400 K. The properties used for the air were:

- Average compressibility: $\beta = 1/T_{wall} = 0.0025K^{-1}$
- Average density of the air: $\rho = P/(RT_{wall}) = 0.883kg/m^3$ where the pressure P is atmospheric and R is the gas constant for the air $R = 287J/kg/K$
- Kinematic Viscosity: $\nu = \mu/\rho = 2.23 \times 10^{-5} \quad m^2/s$
- Air diffusivity: $\alpha = k/(\rho c_p) = 4.48 \times 10^{-5} \quad m^2/s$

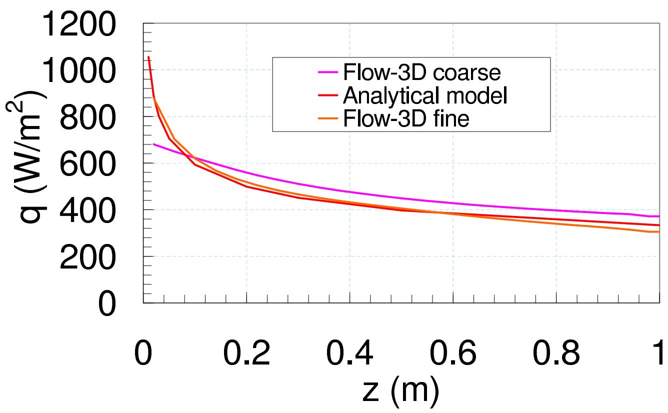


Figure 34: Comparison of the heat flux, for a wall at constant temperature, obtained with the analytical model and Flow-3D with fine mesh (bench01) and coarse mesh (bench03)

Figure 34 compares the results obtained with the Nusselt number shown in Eq. 25. The match between theory and numerical simulations is excellent confirming that Flow-3D is very good prediction natural convection in this configuration.

Natural convection close to a vertical plate with constant heat flux

The local Nusselt number for this configuration is found in [2], pg. 399:

$$Nu_x = \frac{hx}{k} = -\frac{(Gr_x/5)^{1/5}}{\theta(0)} \tag{26}$$

The boundary condition in this case for Flow-3D was a constant heat flux of 800 W/m^2. Figure 35 compares the results obtained with the Nusselt number shown in Eq. 26. Again the comparison is very satisfactory

Conclusions

Flow-3D performs very well in the vertical wall with natural convection. The next step should be to repeat these runs with air in porous media and check if heat fluxes and temperature profiles are still the ones predicted by the theory. Still some feedback from Flow-3D is being expected about an inquiry of how

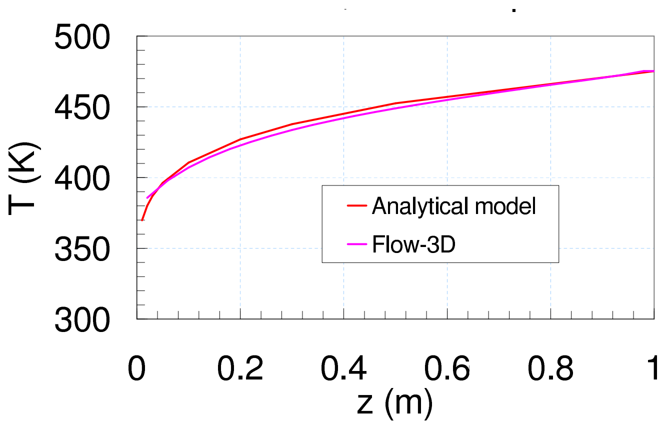


Figure 35: Comparison of the heat flux, for a wall with constant heat flux, obtained with the analytical model and Flow-3D (bench02)

heat flux is dealt with in the presence of porous media, to see if we can clarify why the parallel plate and concentric cylinder runs are not giving the expected heat transfer values.

References

[1] Sitakanta Mohanty, George Adams, A model for estimating heat transfer through drift degradation-based natural backfill materials, ARMA/USRMS, 2005

[2] Louis C. Burmeister, Convective heat transfer, John Wiley & Sons, 1993, 2nd. edition

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 766E

Document Date:	05/31/2006
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	■"Non-Sensitive" ☐ Sensitive ☐"Non-Sensitive - Copyright" ☐ Sensitive - Copyright
Date Generated:	10/01/2006
Operating System: (including version number)	Windows
Application Used: (including version number)	
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	1 CD
File Types: (.exe, .bat, .zip, etc.)	wpd
Remarks: (computer runs, etc.)	File folders