Fracture Flow

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1 Introduction

Flow through a microscopic fracture coupled with flow through a macroscopic medium is interesting in many geological settings, such as study of coal-seam gas reservoirs. Superficially quite dissimilar, but almost identical as far as MOOSE is concerned is the coupling of surface-water flows with groundwater flows. Both these applications involve coupling physics on an essentially 2D surface with physics in a 3D medium.

In this document I demonstrate that this type of coupling is astonishingly simple in MOOSE. In fact *no extra C++ code needs be written* usually! All that needs be done is to write and benchmark the individual physics *separately* — eg groundwater physics and surface water physics — and then couple them together using a specially designed mesh. All the work then reduces to the mesh creation: a preprocessing stage!

This mesh needs two types of blocks of elements: blocks containing 3D elements; and blocks containing the 2D surface elements. The 2D elements must be faces of a 3D element. In cubit or trelis this step is accomplished by the simple `imprint all` and `merge all` operations. This is necessary so that the 2D physics "feels" the 3D physics, and viceversa, otherwise the two physics will run separately without any coupling. The idea is shown in Figure 1.1.

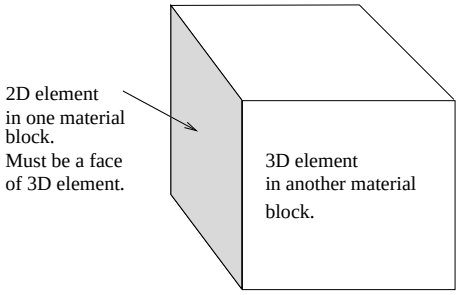

Figure 1.1: Type of mesh needed when coupling 2D surface physics with 3D bulk physics.

2 Solute Diffusion into a Porous Matrix from a Single Fracture

Here I work through in detail a benchmark test described in Section 14.5 of the FEFLOW book[1]. This test is based on analytic results from Tang, Frind and Sudicky[2]. There is also a useful finite element study using a macroscropic-sized fracture in Grisak and Pickens[3] in which the governing equations are carefully explained and an analytical solution presented due to Carslaw and Jaeger which is very similar to the ones found below.

The analytical solutions include the effect of diffusivity within the fracture, as well as radioactive decay of the solute, but, following FEFLOW, I do not consider those effects since I am wanting to concentrate on the fracture-bulk coupling. Hence the governing equation for flow within the fracture and flow within the bulk is the advection-diffusion equation:

$$\frac{\partial}{\partial t}\phi C - \nabla_i\left(\phi D_{ij}\nabla_j C\right) + \nabla_i\left(v_i C\right) = 0\ . \tag{2.1}$$

In this equation:

- t is time with dimensions [T], and x_i with dimensions [L] are the three spatial dimensions
- C is the mass of solute per unit volume of solvent, with dimensions [M.L^{-3}], where M represents mass.
- ϕ is the porosity. This means ϕC is the mass of solute per unit volume of the "rock" [M.L^{-3}]. Below ϕ will be unity within the fracture, since it is assumed to be fully filled with solvent, but less than unity in the bulk.
- D_{ij} is the anisotropic diffusivity tensor [L^2.T^{-1}], which is different in the fracture and in the bulk. The analytical results are only valid for certain D_{ij} as described below
- v_i is the solvent velocity, for instance provided through Darcy flow [L.T^{-1}]. The analytical results are only valid for certain v_i.

At an interface, such as a fracture wall, both

$$C \quad \text{and} \quad n_i(v_i C - \phi D_{ij}\nabla_j C)\ , \tag{2.2}$$

must be continuous. The former is continuity of the concentration, while the latter is continuity of the flux.

[1] H-J G Diersch "FEFLOW Finite Element Modeling of Flow, Mass and Heat Transport in Porous and Fractured Media" Springer 2014

[2] DH Tang, EO FRind and EA Sudicky "Contaminant transport in fractured porous media: Analytical solution for a single fracture" Water Resources Research 17 (1981) 555-564

[3] GE Grisak and JF Picken "Solute transport through fractured media 1. The effect of matrix diffusion" Water Resources Research 16 (1980) 719–730

2.1 Physics of a microscopic fracture

Now consider a medium containing a single fracture, as depicted in Figure 2.1. The fracture sits in the region $-a \le x \le a$.

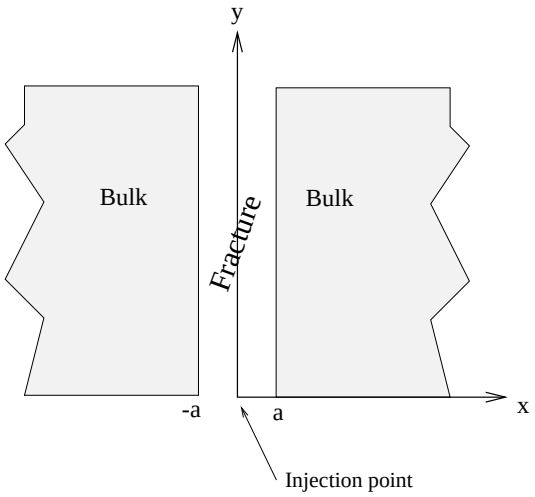

Figure 2.1: A single fracture sits in the region $-a \le x \le a$. As described in the text, solute will be injected at $y = 0$.

In Grisak and Pickens both the fracture and the bulk are discretised with 3D finite elements and Eqn (2.1) is solved with ϕ, D and v being different in the fracture and the bulk. Here I want to take a different approach, which is identical to FEFLOW as Tang, Frind and Sudicky. Assume

- $v_x = 0$ in the fracture;
- a^2/D_{xx} is tiny compared with any other timescale in the problem.

Then the solute concentration in the fracture will obey

$$\frac{\partial C}{\partial x} \approx 0 \ . \tag{2.3}$$

This is the standard "small aperture" approximation. To avoid having to mesh the fracture[4] with 3D elements, *all the solute mass between* $0 \le x \le a$ *is placed on the surface at* $x = a$. The DE governing solute movement on this surface is therefore

$$\frac{\partial}{\partial t}\phi a C - \nabla_i \left(\phi D_{ij} \nabla_j a C\right) + \nabla_i \left(v_i a C\right) = 0 \ . \tag{2.4}$$

Here ϕ, D and v are parameters relevant for the fracture. Of course one may trivially divide by[5] a and the same solution within the fracture will be obtained, however Eqn (2.4) will correctly

[4] I am going to consider just the region $x > 0$ in the MOOSE simulation. If I were considering the full 3D domain, $-\infty < x < \infty$, then all the solute mass between $-a \le x \le a$ would be placed on a surface at $x = 0$, and then the bulk translated by a to create a sandwich. This means that there would be a factor of $2a$ instead of a in Eqn (2.4)

[5] or $2a$ in the case of the previous footnote

count mass at a finite-element node, so may be used straightforwardly in MOOSE when coupled with Eqn (2.1) in the bulk.

2.2 The analytical solution

Tang, Frind and Sudicky derived the analytical solution under the following assumptions.

- In the fracture $v_x = 0$, and a^2/D_{xx} is inconsequential compared with any other timescale in the problem, so the fracture may be treated as described above.
- The concentration is initially zero everywhere, and at time $t \geq 0$ the concentration of solute is fixed at the fracture entry:
$$C(x = a, y = 0, t) = 1 \, . \tag{2.5}$$
- The boundary at $y = 0$ is impermeable, and the domain is semi-infinite as suggested in Figure 2.1.
- In the fracture v_y is constant. Also I (and FEFLOW) assume $D_{yy} = 0$ in the fracture in order to simplify the formulae below. Hence solute simply advects up the fracture with a constant velocity.
- In the bulk $v = 0$, and also all components of D are zero except $D_{xx} \neq 0$.

These assumptions mean that solute will advect in the y direction within the fracture. It will leak to the bulk in the x direction, but will not diffuse in the x direction within the bulk. This is depicted in Figure 2.2

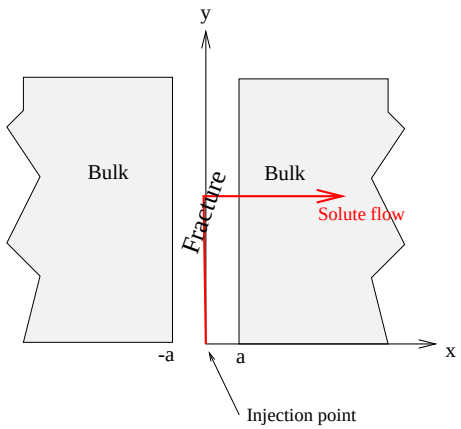

Figure 2.2: Showing the solute flow direction is vertical within the fracture and horizontal within the bulk.

Define
$$\tau = t - \frac{y\phi^{\text{frac}}}{v} \, , \tag{2.6}$$

which is positive for points in the fracture behind the advecting front, and negative for those that haven't been touched by solute yet. Then the analytic solution is

$$C = \begin{cases} \text{erfc}\left[\frac{1}{2\sqrt{\tau}}\left(\phi^{\text{bulk}}\sqrt{D_{xx}^{\text{bulk}}}\frac{y}{av_y^{\text{frac}}} + \frac{x-a}{\sqrt{D_{xx}^{\text{bulk}}}}\right)\right] & \text{for } \tau > 0 \\ 0 & \text{for } \tau \leq 0 \end{cases} \tag{2.7}$$

This formula is correct, but note that there is a typo in both Tang, Frind and Sudicky, and the FEFLOW manual which means the solution for $x = a$ (at the fracture surface) is wrong unless the porosity of the fracture is unity, which is fortunately the case studied in the FEFLOW benchmark. Here erfc is the complimentary error function.

2.3 Comparison with MOOSE

In a similar way to FEFLOW, the following simulation parameters are used in MOOSE

Domain	
Mesh width (x)	1 m
Mesh height (y)	1 m
Number of quad elements	25×50 (this is $x \times y$)
Fracture	
Porosity, ϕ^{frac}	1
Half-aperture, a,	0.1 m
Velocity, v_y^{frac}	0.8 m.s^{-1}
Bulk	
Porosity, ϕ^{bulk}	0.2
Diffusivity, D_{xx}^{bulk}	0.01 m^2.s^{-1}

The simulation is run for 1 s.

Figure 2.3 depicts the solute concentration at $t = 1$ s, and comparisons with the analytical results are shown in Figure 2.4. The timestep has a large influence on the result. The results depicted below use $\Delta t = 0.002$ s, and by decreasing the timestep the results agree more closely with the analytical results. In the test suite this simulation is marked "heavy". There is a non-heavy test that uses $\Delta t = 0.1$ s that is run automatically every time MOOSE is updated. Better agreement would probably be obtained by lumping the mass and using upwinding, however, such features concern the individual physics (2D fracture flow, or 3D bulk flow) and have nothing to do with the coupling that is being tested here.

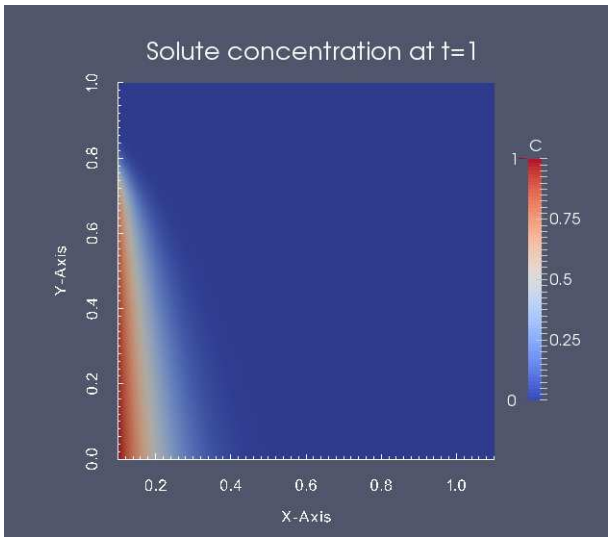

Figure 2.3: Contour of the solute concentration at $t = 1\,\mathrm{s}$

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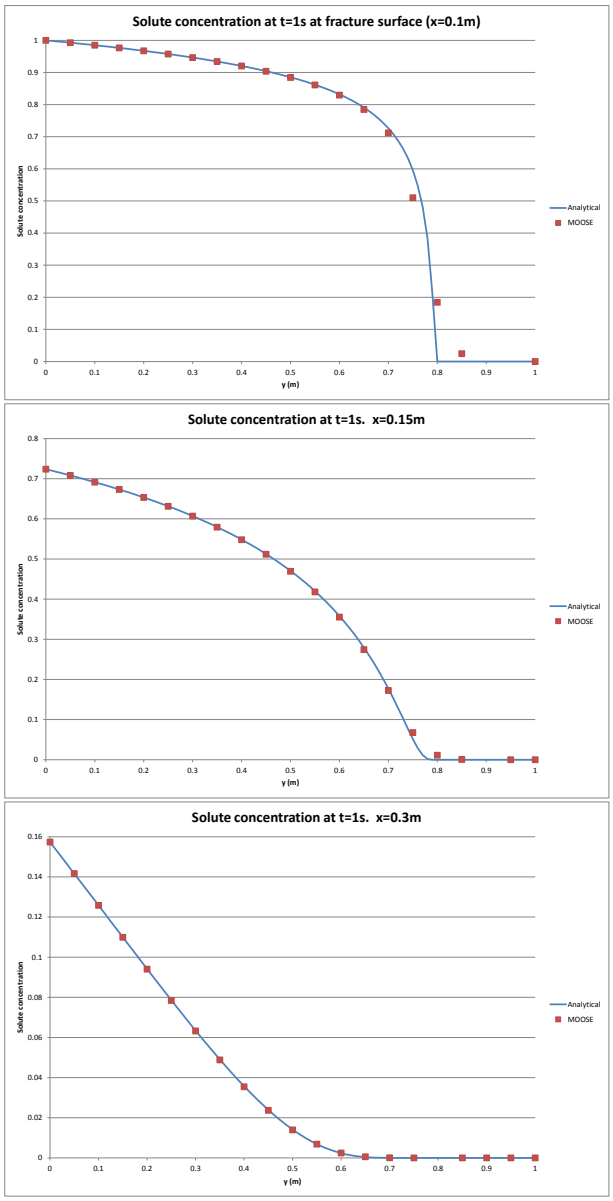

Figure 2.4: Comparison of MOOSE simulation results with the analytical results. The agreement around the sharp front is improved by using finer spatial resolution or smaller Δt.