

APC 523 Final Project Writeup

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Question: What is the relationship between temperature and fluid concentration of a parcel of soil?

1.1 Introduction

In soil, diffusion drives the transport of heat energy, of gasses, of solutes, and of water throughout a sample area. Researchers have been investigating examples of such processes like finding how gasses like methane move through melting permafrost, how hydrocarbons might move in porous rock, how sequestered CO₂ might flow, how structural materials are affected by fluids, or hydrologic processes, among other examples. In addition, changes in physical soil characteristics and the environmental conditions of the soil can have a significant impact on the diffusivity flux of a fluid [1].

Diffusion is represented by a parabolic partial differential equation (Eq. 6). Solving this analytically is extremely challenging, so numerical methods are implemented to solve such a system. Multigrid methods (see Section 1.3) can be leveraged to break down the problem space so that higher resolutions can be investigated at better computational efficiency. Modeled in two dimensions, diffusion can be tracked both across a physical space and throughout time.

For this model, a soil sample will experience an influx of fluid, which will then diffuse across the cross section. Two aspects of the system will change as a function of time and temperature (also a function of time). First the porosity of the base material will vary with temperature, and second, the intensity of fluid into the material will change over time. The fluid forcing can even be stopped after a desired amount of time, leaving the fluid concentration to dissipate into traps throughout the material. This model is purposely designed to be flexible for user-chosen fluid forcing and material. Examples have been selected to demonstrate the model performance for this project.

1.2 Representation of the Soil System

On one side of a normalized grid there is a concentration gradient (can be taken as ∞ for simplicity). The opposite side has a boundary of zero (so in physical terms, one side of our “sand box” has infinite fluid, the other zero). The fluid will enter the system so that it moves towards the side with zero concentration. For this model, boundary conditions are set on the soil parcel sides so that the fluid is contained in the grid. If the fluid reaches the bounds, it may end up moving back towards the center.

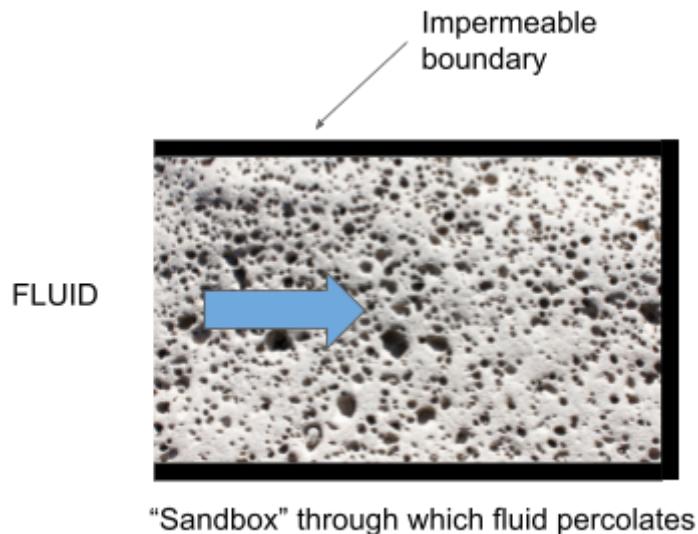


Figure 1. Representation of fluid diffusion through a soil sample.

As stated previously, the soil and its void spaces are temperature sensitive. This changes the diffusion of the soil and consequently the fluid concentration with respect to position and time.

1.2.1 Time Dependency

For a particular parcel of material, its porosity can be described by:

$$\phi = \frac{V_v}{V_T} \quad (1)$$

which depends on the void volume V_v and the total soil volume V_T . The total parcel can be thought of as consisting of two phases, ϕ_1 and ϕ_2 [3]. They are related by

$$\phi_1(T(t)) + \phi_2(T(t)) = 1 \quad (2)$$

in which we hold volume constant.

Each of these parcels volume fractions (the void, and the soil matrix) are sensitive to temperature, based on the coefficient of thermal expansion for the soil type. This parameter is different for each material. We can then write the dependence of porosity on temperature as:

$$\frac{d\phi}{dT} = \frac{\frac{dV_v}{dT}}{\frac{dV_T}{dT}} \quad (3)$$

$T(t) = g(t)$, where g is an arbitrary function that describes temperature as a function of time.

Both the void and the total volume will depend on temperature independently as a material property, giving an effective porosity that also changes as temperature changes. However, the total volume must be held constant.

The diffusion equation in two dimensions is given by Fick's Second Law [2]:

$$\frac{d\phi}{dt} = -D \left(\frac{d^2\phi}{dx^2} + \frac{d^2\phi}{dy^2} \right) + q(t) \quad (4)$$

where q is a forcing/source term and J is our fluid flux and ϕ is the fluid concentration, which changes with location (x and y). D is the effective diffusion. This value of diffusion is dependent upon porosity, among other factors like constrictivity and tortuosity that will keep constant in this analysis, giving us:

$$D = K \phi(T(t)) \quad (5)$$

Where K is a constant based on the diffusion coefficient of the gas in air and the soil tortuosity (i.e $K = D_0 \tau$).

Plugging in this function for D , the final two dimensional partial differential equation to represent diffusion can be written as:

$$\frac{d\phi}{dt} = -K\phi(T(t)) \left(\frac{d^2\phi}{dx^2} + \frac{d^2\phi}{dy^2} \right) + q(t) \quad (6)$$

Diffusion through the material depends upon microstructural properties. As mentioned, we characterize the material as consisting of two phases (ϕ_1 and ϕ_2). In our code, we start with a 0.5 volume fraction, meaning half the material is void space and half is in the matrix phase. We have set an arbitrary relationship between time and temperature, where temperature increases as time goes on. For simplicity, we make this an external temperature variation that we adjust directly with time (thus, we essentially have porosity changing with respect to time). However, it may be possible to add feedback mechanisms into the model, for example higher fluxes would lead to temperature increases due to friction between the fluid particles and the matrix. In such a case we can add another parameter that relates temperature change with regard to concentration. This is a broadly adaptable relationship—other time-temperature relations can be used as replacement. In a natural system, this can be considered a model of sun hitting a porous medium, climate change, or other outside heating, depending on the timescale and temperature used.

In the present model, a bounded parcel of soil is considered. Upon increasing temperature, we then use the coefficient of thermal expansion (α) to change the soil microstructure. This coefficient is material specific and is an empirical constant. In this model, we consider only one constant value of α through time (in reality, different coefficients exist in different temperature regimes). The matrix phase (ϕ_2) expands, taking up more space. Since the conservation relationship $\phi_1 + \phi_2 = 1$ must hold, ϕ_1 must decrease proportionally. We set the end cutoff to be 0, which is the extreme limit case (this means after some heating time, enough heating will have occurred that there is no void space left). Our diffusion depends on the porosity. As porosity falls, diffusion will as well. For simplicity, percolation thresholds are ignored, and the void phase is considered connected at all volume fractions [3]. Besides porosity, diffusion also depends on the constant K, which we use as a broadly encompassing constant of several terms, such as the fluid properties, the soil tortuosity, etc. Multiplying these terms together into a dynamic diffusion allows for the model to update over time iterations as temperature increases.

1.3 Multigrid Implementation

The multigrid method is a technique that solves differential equations using a hierarchy of discretizations. For a two-dimensional, square-shaped area, with n levels of discretizations, the coarsest grid is 2×2 , and subsequently finer levels have $2^2 \times 2^2$, $2^3 \times 2^3$, ..., $2^n \times 2^n$ grid points. The goal of the algorithm is for the numerical solution to converge in as few iterations as possible. Our procedure is recursive in nature, and it consists of the following eight steps:

1. Start with an initial guess, and start on the finest grid.
2. Use three Jacobi iterations for smoothing and reducing high frequency errors.
3. Compute the residual errors after the three Jacobi iterations.
4. Perform restriction by downsampling the residuals to the next coarsest grid.
5. Perform prolongation by interpolating a correction computed on a coarser grid into a finer grid.
6. Correct fine grid solution by adding prolonged coarser grid solution onto the finer grid.
7. Use an additional three Jacobi iterations for further smoothing.
8. Repeat steps 2 through 7 until the max number of iterations or a numerical convergence is reached.

For the Jacobi iterations, the guiding equation is:

$$\varphi_{i,j}^{(n+1)} = \varphi_{i,j}^{(n)} + \Delta t \cdot D \left[\frac{\varphi_{i+1,j}^{(n)} + \varphi_{i,j+1}^{(n)} - 4\varphi_{i,j}^{(n)} + \varphi_{i-1,j}^{(n)} + \varphi_{i,j-1}^{(n)}}{h^2} \right] + \Delta t \cdot q \quad (7)$$

A multigrid algorithm is carried out in each time step of our simulation such that the restriction and prolongation operations are only happening in space but not in time. Diffusion constant, D , is a function of temperature, which is a function of time.

Currently, the code is not parallelized, but the multigrid scheme lends itself to easy parallelization if faster runtime is desired.

1.4 Results and Discussion

The multigrid implementation allows for computationally efficient calculations of diffusion throughout the entire soil grid. Different initial conditions are supplied to see the behavior of a fluid plume based on its origin source. The three conditions explored in the project are (1) fluid being supplied across the entire left side of the parcel, (2) fluid being injected at a particular point on the edge and (3) fluid being injected at the center. Figures at different time points for the different fluid sources are shown below. All of the simulations shown have the same time dependency for the intensity of fluid injection ($q = \sqrt{time/2}$) and the supply of fluid is terminated at its point of origin at $t = 80$. Therefore, we expect to see a gradual increase in concentration until $t = 80$ after which it is expected for the concentration to dissipate, particularly close to the point of origin (see right figure for all cases).

1. Influx from full edge

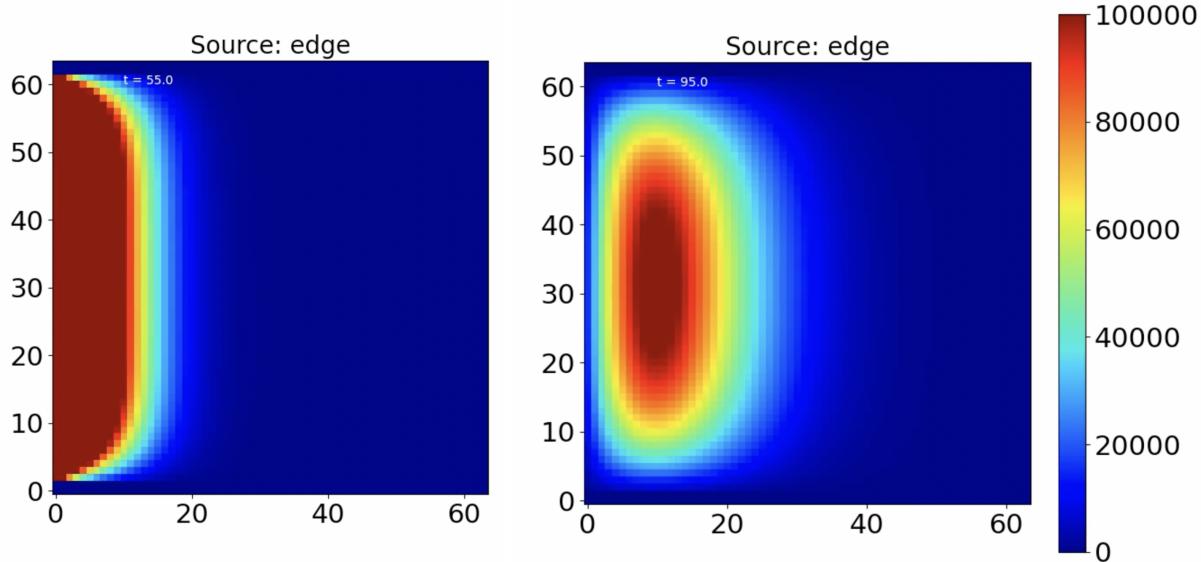


Figure 2. Edge origin diffusion at $t=55$ (left) and $t=95$ (right).

2. Influx from point on edge

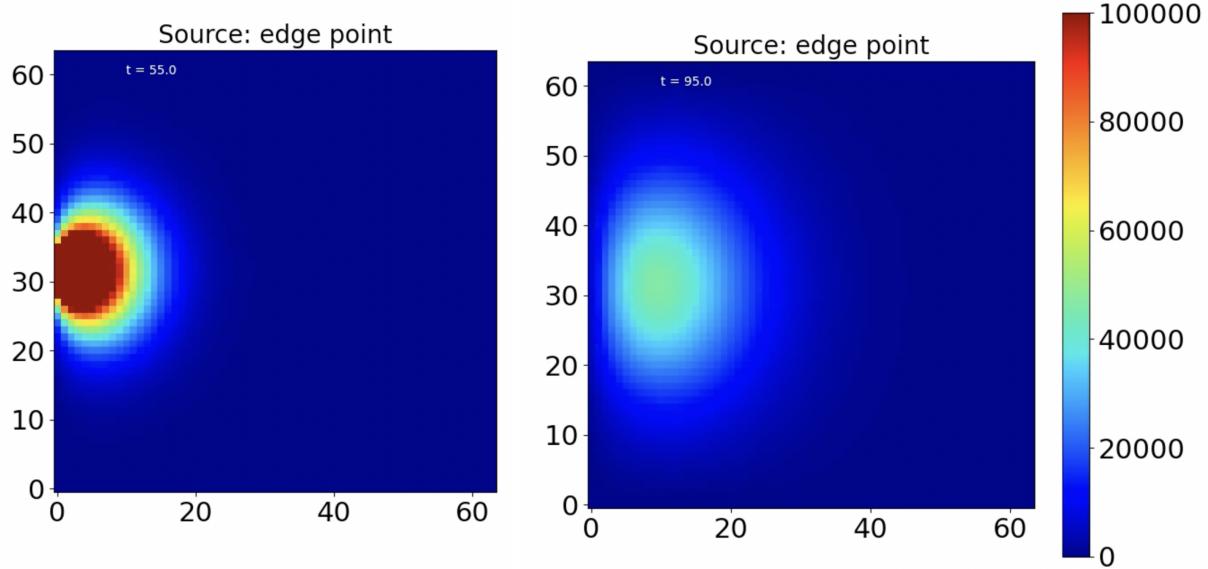


Figure 3. Edge point origin diffusion at $t=55$ (left) and $t=95$ (right).

3. Influx from center point

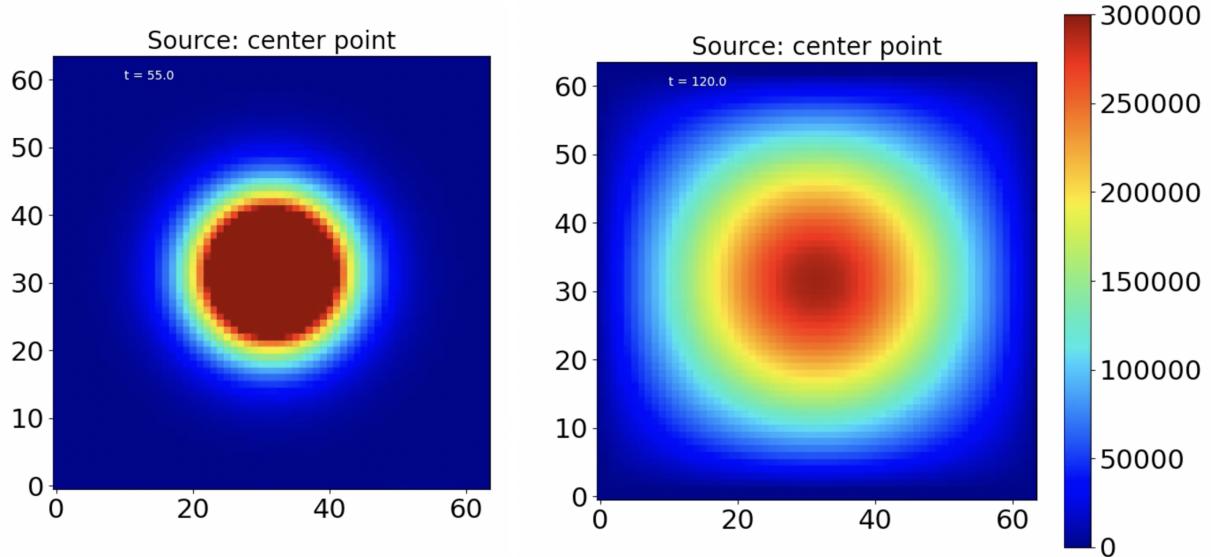


Figure 3. Center point origin diffusion at $t=55$ (left) and $t=120$ (right).

Notice that for both edge and edge-point origin cases, the extent of diffusion grows in between t=55 and t=95. See the associated powerpoint or mp4 files for the entire simulation. As expected, the concentration across all cases begins to decrease once the fluid input forcing is turned off. Interestingly, in both scenarios in which the fluid is injected at the boundary, the concentration maximizes at about 100000 and dissipates quite quickly, while the center source case peaks at a concentration of 300000 and dissipates slower.

1.5 References

1. Stępniewski W., Sobczuk H., Widomski M. (2011) Diffusion in Soils. In: Gliński J., Horabik J., Lipiec J. (eds) Encyclopedia of Agrophysics. Encyclopedia of Earth Sciences Series. Springer, Dordrecht. https://doi.org/10.1007/978-90-481-3585-1_273
2. Neira, J., Ortiz, M., Morales, L., & Acevedo, E. (2015). Oxygen diffusion in soils: understanding the factors and processes needed for modeling. Chilean journal of agricultural research, 75, 35-44.
3. Torquato, Salvatore. (2002). Random Heterogeneous Materials: Microstructure and Macroscopic Properties. Springer New York, NY.