INTERNSHIP REPORT

SORBONNE UNIVERSITÉ, PARIS

Numerical study of Rayleigh-Taylor instabilities in porous media with geo-electrics

Author:Supervisor:Neelarun MukherjeeDamien Jougnot, Ph.D.,4th-year Integrated M.Sc. Student,Associate Scientist at CNRSExploration Geophysics,Sorbonne Université,Indian Institute of Technology,7619 METISKharagpur, WBParis, France

Contents

1	Intr	oduct	ion	4		
2	Theoretical Background					
	2.1	RT In	stabilities	6		
		2.1.1	Dimensional Equations	7		
		2.1.2	Non-dimensional Equations	7		
2.2 Effective electrical conductivity		ive electrical conductivity	9			
		2.2.1	General Equations	9		
		2.2.2	Petrophysical relationship between ionic concentration and electrical conductivity			
			of the medium	11		
3	Nu	merica	l Analysis and Methods	14		
	3.1	OpenI	FOAM	15		
	3.2	Geom	etry and Boundary conditions of the system	16		
		3.2.1	Rayleigh Taylor Instability modelling	16		
		3.2.2	Geo-electrical modelling	17		
	3.3	Electr	ical conductivity anisotropy	18		
4	Results					
	4.1 Validation of the code and Results		20			
		4.1.1	Testing the robustness	21		
		4.1.2	Series and Parallel model	22		
		4.1.3	Chessboard tests	24		
	4.2	Sensit	ivity Analysis of Rayleigh Number	25		
		4.2.1	Effect on effective conductivity	25		
		4.2.2	Effect on Anisotropy analysis	26		
	4.3	Applie	cation to Seawater/Freshwater Interface	28		
5	Discussion and Conclusion 3					
	5.1	Discus	ssion	33		

		5.1.1 Rayleigh Taylor instability of the pore fluid	33	
5.1.2 Relationship between concentration field and measured conductivity			33	
		5.1.3 Electrical conductivity anisotropy analysis	34	
	5.1.4 Improvements and ideas for further studies			
	5.2	Conclusion	35	
	5.3 Acknowledgements		36	
6	App	ppendix		
6.1 OpenFOAM codes		OpenFOAM codes	37	
		6.1.1 For Rayleigh Taylor Instability 3	37	
		6.1.2 For calculating the Bulk Electrical conductivity	38	
	6.2	MATLAB code for transferring the field and post processing	39	

Chapter 1

Introduction

The use of geophysical tools for subsurface characterization has become a common practice in environmental studies and geo resources engineering for the last 50 years(e.g., Binley et al. (2015)). There are different non-invasive subsurface geoelectrical imaging methods that were developed over the years such as the DC (Direct Current) method (Schlumberger, 1912; Langer, 1936), Induced polarisation methods (Schlumberger, 1920), electromagnetic methods (Deignan, 2008), seismic methods (Nolet, 1987), etc. The electrical properties of the subsurface are highly influenced by the different properties of the subsurface such as lithology (porosity, permeability, tortuosity, etc.), the pore fluids (water saturation in pore spaces, the concentration of minerals in pore water) and their chemistry (ionic concentration, transport of reactive elements through the pore spaces and stretching of reactive strips). Among all these different petrophysical properties that we can obtain from electric conductivity surveys, those regarding subsurface fluid flows in the porous media are among the most important factors for society. Contaminant transport through groundwater is very important for waste management studies. Density driven flows such as those occurring in solubility trapping, during CO_2 sequestration in petroleum or groundwater aquifers or freshwater-saline water interaction in coastal areas are some phenomena that can be studied and monitored via electrical conductivity measurements. The instabilities discussed can happen at the size that is much smaller than the method resolution. Thus we will be studying what is happening at the sub-resolution scale or mainly pore scale. That is, the model essentially is studied in the mesoscale (Jougnot, 2020; Müller et al., 2010), which is bigger than the pore/micro-scale, but it is smaller than the field measurement scale.

In this geoelectrical modeling study, the measurements are done by injecting current into the subsurface through a pair of electrodes and measuring the potential difference between the other two electrodes between which we have the area under investigation. When scanning the medium with numerous electrical conductivity measurements, it becomes possible to reconstruct the distribution of electrical conductivity in the sub-surface by inversion, and it is referred to as Electrical Resistivity Tomography (ERT) (Binley and Kemna, 2005). The ERT's time-variance can also be used to study the temporal variability of the different physical processes with time-lapse ERT (Revil et al., 2012). The present study deals with the geoelectrical modeling of density-driven instabilities in porous media. In this report, we start by first the Theoretical Background (Chapter 2) of the Rayleigh Taylor instabilities and geoelectrical modeling, the concepts that were used in the study. After that, we discuss the numerical analysis and modeling (Chapter 3) that were implemented. Then we test the validation of the model and the results obtained (Chapter 4) from which it can be studied how the electrical conductivity varies with the evolution of subsurface petrophysical processes during the development of convection.

Chapter 2

Theoretical Background

The main aim is to study the evolution of a porous media's electrical conductivity in which Rayleigh Taylor Instability occurs at the Darcy scale. This study involves both the modeling of Rayleigh Taylor instability in a porous media and then the subsequent change in the effective electrical conductivity in this media.

2.1 RT Instabilities

The physical process that was numerically simulated is Rayleigh Taylor Instability (Rayleigh, 1900; Taylor, 1950). The Rayleigh Taylor Instability or RT Instability is an instability of the interface between 2 fluids where the lighter fluid is pushing the denser fluid. It is a dynamic process whereby the two fluids seek to reduce their combined potential energy. The ensuing convection and mixing have far-reaching consequences in many natural and human-made flows, ranging from supernovae to micro-scale pore geometries. This physical process is widespread in different subsurface phenomenon involving fluids of different densities. We have a miscible fluid, and the density difference is brought about due to the concentration difference between the top and the bottom part of the fluid in a porous media, (Riaz and Hesse, 2006; Neufeld et al., 2010; Vreme et al., 2016; Hidalgo and Carrera, 2009; De Paoli et al., 2019).

We couple the Brinkman-Darcy equations along with the convection diffusion equations with the introduction to the dispersion term in order to study the effect of concentration dispersion (Hidalgo and Carrera, 2009).

2.1.1 Dimensional Equations

The incompressible density-dependent flow and advective–diffusive–dispersive transport equations governs the Raleigh-Taylor instability in a porous media. The classical Brinkman-Darcy Equation is

$$-\nabla p - \left(\frac{\mu}{k}\right)\boldsymbol{u} - \rho g\boldsymbol{e}_{\boldsymbol{z}} = 0$$
(2.1)

where p (Pa) is pressure, μ (Pa s) is viscosity, $k(m^2)$ is permeability, $\rho(\text{kg}/m^3)$ is pore-fluid density, $g(\text{m}/s^2)$ is acceleration due to gravity, u(m/s) is Darcy velocity. The continuity equation is

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \tag{2.2}$$

and

$$\phi \frac{\partial c}{\partial t} = \phi \nabla \cdot (D \nabla c) - \boldsymbol{u} \cdot \nabla c.$$
(2.3)

is the convection-diffusion equation where c(mol) is the concentration and $D(m^2/s)$ is the anisotropic dispersion coefficient. The density contrast arises because of the different concentrations in the heavier fluid and the lighter fluid and the relation between the concentration and the density is given as

$$\rho = \rho_0 (1 + \epsilon_c), \tag{2.4}$$

where $\epsilon_c = \Delta \rho / (rho_0 c_0)$, and the z-axis is taken opposite the direction of gravity (g). The anisotropic dispersion coefficient tensor is

$$D_{ij} = (\phi D_m + \alpha_T ||u||) \delta_{ij} + \frac{(\alpha_L - \alpha_T)(u_i u_j)}{(||u||)}, \qquad (2.5)$$

where, $\Delta \rho$ (Pa) is the difference in density between the two fluids. e_z is the unit vector pointing downwards along the direction of g. D_m is the molecular diffusion coefficient. $\alpha_L(\text{in m})$ and $\alpha_T(\text{in m})$ are longitudinal and transverse dispersivities accordingly. $\delta_{ij}(-)$ is the Kronecker delta, and $|| \cdot ||$ notation is the Euclidean norm.

2.1.2 Non-dimensional Equations

For analysis purposes, it is convenient to write governing equations in a dimensionless form. For the non-dimensional form, we use a non-dimensional number, namely the Rayleigh Number (Ra), based on which the instability's physics depends on.

$$Ra = \frac{k\Delta\rho gH}{\phi D_m \mu} \tag{2.6}$$

where H(in m) is the length scale of the media.

So basically, by changing any of these parameters, we will get a different Rayleigh number. Now, obviously, we can get the same Rayleigh number for several sets of these parameters. Thus, we can safely conclude that all of these sets of parameters will essentially give us exactly the same physics. Also, the simulation time is very much decreased according to the time scale defined in the non-dimensional case. The different scaling factors are as follows:

Velocity scale,

$$U = \frac{k\Delta\rho g}{\mu},\tag{2.7}$$

Domain pressure scale,

$$P = \delta \rho g H, \tag{2.8}$$

Time scale,

$$t' = \frac{\phi H}{U}.\tag{2.9}$$

H is defined as the length scale, which is equal to the length dimension of the system. Based on these scales the non dimensional system of equations are derived from equations 2.1, 2.2, 2.3, 2.4 and 2.5. The non-dimensional governing equations are

$$-\nabla p + Da(\nabla^2 u) - u + ce_z = 0, \qquad (2.10)$$

$$\nabla \cdot u = 0 \tag{2.11}$$

and

$$\frac{\partial c}{\partial t} = \left(\frac{1}{Ra}\right) \nabla \cdot (D\nabla c) - u \cdot c, \qquad (2.12)$$

where, Da is the Darcy number. The anisotropic diffusion coefficient is

$$D = (1 + \frac{\alpha_T U}{\phi D_m})||u||\delta_{ij} + \frac{(\alpha_L - \alpha_T)U}{\phi D_m} \frac{(u_i u_j)}{(||u||)}.$$
 (2.13)

2.2 Effective electrical conductivity

Among the different geo-electrical methods, the Direct Current (DC) resistivity method allows us to find the spatial distribution of conductivity and monitor the soil's changes in conductivity. These properties are highly affected by the lithology, pore fluid chemistry, fluid dynamics in the porous media (Glover, 2015). In the measurement scale of DC conductivity studies, the spatial variation of resistivity is monitored using four-electrode measurements, two of them are used to inject current into the subsurface, and the other two are used to measure the potential difference of the part of which we want to check the resistivity of. The study aims to find out the effective electrical conductivity at the mesoscopic scale (Müller et al., 2010; Jougnot, 2020) in a medium where the Rayleigh Taylor instability in achieved by injecting direct current through it and check the changes in the effective conductivity of the subsurface as it changes as the instability progresses. The mesoscopic scale is the scale that is located between the measurement scale and the pore/micro scale. In Müller et al. (2010), this scale was used in a seismic study, but this scale can be used in all kinds of geophysical methods. In hydro-geophysics, this mesoscale cannot be directly correlated to the Representative Elementary Volume (REV), but these mesoscale properties such as porosity, water content, wettability, concentration gradient, among other mesoscopic heterogeneities can strongly affect the flow and transport in a porous media. In the study, we mainly focus on a single cell or a mesh in our electrical tomogram as we will see that it cannot be ignored when conducting field-scale measurements (see also Jougnot et al. (2018); Ghosh et al. (2018)).

2.2.1 General Equations

For the numerical analysis of this method, we designed a numerical scheme to simulate the evolution of the effective electrical conductivity of the Rayleigh Taylor Instability in a porous media. The measurement of DC Resistivity is based on Ohm's Law. It consists in injecting an electrical current in a geological medium and measure the resulting electrical potential differences to determine its electrical conductivity. In this case, the mesoscopic scale is the main focus of the geoelectric study. The governing equation to get the potential distribution in the media with an applied external potential and injected current (Binley and Kemna, 2005) is given as,

$$\nabla \cdot (\sigma \nabla V) = -I. \tag{2.14}$$

where σ is the electrical conductivity distribution in the media. V is the electric potential map in the media and I is the intensity of the single current source from an electrode. To discuss and study the conductivity of different petrophysical phenomena, the concept of "geometrical factor" is fundamental. The geometrical factor (K_g) is a numerical multiplier defined by the regular spacings between electrodes, which is used in conjunction with the

current-to-voltage ratio or conductance (Siemens, S) measured in electrical conductivity surveys to give an apparent conductivity (σ_a) such that $\sigma_a = \frac{G}{K_g}$. Note that this apparent conductivity is a kind of average of the electrical conductivity distribution at the scale of the measurement.

The conductivity actually depends on the media's geometry or, more specifically, the measurement length (l). For example, for a cylindrical case such as fig. 2.1,



Figure 2.1: Determining the Geometrical factor

the *E* is the externally applied electric field, *I* is the current intensity (A) through the cylinder and *J* is the current density (A/m²). *a* is the measurement cross-section area. The conductance, *G* (S) is defined as

$$G = \frac{a}{l}\sigma,\tag{2.15}$$

and the geometrical factor, ${\cal K}_g$ is defined as

$$K_g = \frac{a}{l}.\tag{2.16}$$

2.2.2 Petrophysical relationship between ionic concentration and electrical conductivity of the medium

The pore fluid's conductivity depends mostly on concentrations and mobilities of ion species present in the fluid (i.e., the charge carriers) (Glover, 2015). Suppose we consider an ionic species *i* with charge $Z_i e$ where Z_i is the valency of the charge carrier and *e* is the electronic charge ($e \approx 1.6022 \times 10^{-19}C$). In an electric field \vec{E} (Vm^{-1}) the force on this charge is $Z_i e \vec{E}$. μ_i is defined as the mobility ($m^2 V^{-1} s^{-1}$) of an electronic charge carrier in a medium which mainly depends on the type of the charge carrier (mainly the size of the ion), the medium and the temperature. The current density \vec{J} (Am^{-2}) is defined as the charge that passes unit area per second and n_i is the number of charge carriers passing per second per unit volume and D_i (in $m^2 s^{-1}$) is the diffusion coefficient of the charged species, then,

$$\vec{J} = n_i Z_i e \mu_i \vec{E}, \tag{2.17}$$

and the ionic mobility can be derived as

$$\mu_i = \frac{Z_i e D_i}{k_b T},\tag{2.18}$$

where k_b is the Boltzmann's constant ($\approx 1.3806 \times 10^{-23} m^2 kg s^{-1} K^{-1}$) and T is temperature (in K).By combining the equations eq. (2.17) and eq. (2.18), we may obtain the electrical conductivity of for an ion in solution, often termed as the Nernst Einstein relationship (Einstein, 1905):

$$\sigma_i = \frac{D_i Z_i^2 e^2 N n_i}{k_b T},\tag{2.19}$$

where N ($\approx 6.022 \times 10^{23}$) is the Avogadro's number. Now considering steady state such that the driving electric force $Z_i eE$ is exactly balanced by the viscous drag on the hydrated ions $6\pi\eta r\vec{v}$ (according to Stoke's law), where V_i (in m/s) is the velocity of the ion, it's hydrated radius is r_i (in m) and the viscosity of the fluid, η (in *Pas*). Thus the ionic mobility can be written as:

$$\mu_i = \frac{Z_i e}{6\pi\eta r}.\tag{2.20}$$

From this expression of mobility combined with the general expression of conductivity, $\sigma_i = n_i Z_i e \mu_i$, we obtain the conductivity of the ion in solution:

$$\sigma_i = \frac{n_i Z_i^2 e^2}{6\pi\eta r}.\tag{2.21}$$

Thus the conductivity is directly proportional to (i)the number of charge carriers per unit volume, (ii) the square of the net charge each carrier carries and (iii)inversely proportional to the radius of the hydrated ions and (iv) inversely proportional to the viscosity of the pore fluid.

In practice, the most common and useful empirical formula for the conductivity of an aqueous solution of NaCl given by Sen and Goode (1992) which is,

$$\sigma_f(T, C_f) = (d_1 + d_2T + d_3T^2)C_f - \left(\frac{d_4 + d_5T}{1 + d_6\sqrt{C_f}}\right)C_f^{3/2}$$
(2.22)

where $d_1 = 5.6$ [S l $m^{-1}mol^{-1}$], $d_2 = 0.27$ [S l $m^{-1}mol^{-1}$] / ${}^{o}C$, $d_3 = -1.51 \times 10^{-4}$ [S l $m^{-1}mol^{-1}$] / ${}^{o}C^2$, $d_4 = 2.36$ [S $m^{-1}/(mol \ l^{-1})^{3/2}$], $d_5 = 0.099$ [S $m^{-1}/(mol \ l^{-1})^{3/2}/{}^{o}C$], $d_6 = 0.214$ [$(mol \ l^{-1})^{-1/2}$], T is in ${}^{o}C$ and C_f is the salinity of the bulf pore fluid [$mol \ l^{-1}$].

In a geological media, the charge transport happens through the pore fluid. Indeed, if the rock material is composed of insulating materials like the silicates or the carbonates which have a conductivity range approximately from 10^{-14} Sm⁻¹ to 10^{-10} Sm⁻¹ which is quite negligible in contrast to the conductivity of the pore fluid which varies around 10^{-3} Sm⁻¹ to 1 Sm⁻¹. Thus, the conductivity of the domain is mainly dominated by the pore fluid's conductivity and how well these pore spaces are connected throughout the rock and the rock's microstructure. Thus the conductivity of the rock mainly depends on the following factors:

i. The conductivity of the pore fluid.

ii. The porosity of the rock.

iii. The pore fluid saturation that is the degree to which the pore spaces are filled with the conductive fluid.

iv. The connectivity and tortuosity of the pathways of the pore spaces inside the rock. Archie et al. (1942) refers to the conductivity of a medium in a saturated condition as

$$\sigma = \frac{1}{F}\sigma_f,\tag{2.23}$$

where σ is electrical conductivity (Sm^{-1}) of the porous medium and σ_f is electrical conductivity (Sm^{-1}) of pore water, F is the Formation factor (-) and n is the saturation exponent(-). The formation factor, F quantifies the tortuosity of the medium (see Jougnot et al. (2009, 2018)). The Formation factor is related to porosity by the relation: $F = \phi^{-m}$ (Archie's first law), where m is called a cementation exponent. m and n depend on the pore space and the water phase geometry. The equation 2.23 is based on the assumption that the pore water salinity is homogeneously distributed in the wetting phase at the considered scale (see Jougnot et al. (2018)). In the present study, we consider that the ionic concentration simulated solving the RT instability corresponds to a given electrical conductivity combining Eq. 2.22 and 2.23 for each cell of the numerical simulation.

From the concentration map from the Rayleigh Taylor simulation, we get the concentration of the fluid phase in the simulation C_f for each point in the medium mesh. From the concentration data, $C_f(x, y)$, we convert the concentration values to corresponding conductivity values, $\sigma_f(x, y)$ by applying Eq. 2.22. Now, we can determine the porosity of the medium, ϕ and the formation factor, F and the value of the cementation exponent, m, for the type of porous media that in under consideration for our case (For eq., F = 1.3for consolidated sand and F = 2 for a sandstone). Now we have the values of $sigma_f(x, y)$ and F, thus, from equation 2.23, we can get the value of $\sigma(x, y)$.

Chapter 3

Numerical Analysis and Methods

Most of the numerical modeling and simulation has been done extensively in OpenFOAM. Two modified solvers were mainly used in the simulation, one for solving the Rayleigh-Taylor Instability and the other for solving the potential distribution in the subsurface. The post-Processing of the results from the Rayleigh Taylor instability simulation, conductivity modeling, and the preprocessing for mapping the concentration field to the conductivity field is done in MATLAB. The work process can be described as in Fig.3.1 with an example for a random concentration distribution from the simulation.



Figure 3.1: Flowchart of the steps for the numerical simulations

3.1 OpenFOAM

OpenFOAM (for "Open-source Field Operation And Manipulation") is a C++ toolbox for the development of customized numerical solvers. It's a free open-source software used mainly for Computational Fluid Dynamics (CFD). For the simulations, OpenFOAM version 5 is used.

Our coupled equations for the Rayleigh-Taylor Instability involved a Brinkman-Darcy Equation (Eq.2.10) coupled with a convection-diffusion equation (Eq.2.12) with concentration dispersion (Eq.2.13). The "laplacianFoam" solver solves the Laplace Equation for unsteady, isotropic diffusion. The main governing equation for the laplacianFoam solver is

$$\frac{\partial T}{\partial t} - \nabla \cdot (D_T \nabla T) = 0, \qquad (3.1)$$

where T is the scalar field which is to be solved for and D_T is the diffusion coefficient. The laplacianFoam solver is modified to solve the Diffusion equation, and the Brinkman-Darcy Equation is coupled along with it such that the solver solves for the concentration field along with the Darcy velocity in a coupled manner. The Brinkman-Darcy equation is a steady-state equation, unlike the convection-diffusion equation.

Now for analyzing the change in the subsurface's effective conductivity as the instability progresses, the Poisson's Equation (Eq.2.14) for calculating potential distribution in the media with the injected current is used. In this study, there is no source or sink inside the media, and all the current going through the media is essentially from an external source, and all the current goes back to the sink current electrode assuming no leakage. Therefore our principle equation is essentially a modified Laplace's Equation which is

$$\boldsymbol{\nabla} \cdot (\boldsymbol{\sigma} \nabla V) = 0. \tag{3.2}$$

Nevertheless, before that, we had to map the concentration field obtained from the Rayleigh-Taylor Instability simulation to a conductivity field. The conductivity of the medium has been mapped from the concentration field of the pore fluid described in Section: 2.2.2

In this example, the top denser layer's conductivity has a value of 1000 S/m and less dense fluid have a conductivity of 0.001 S/m. The effective conductivity (σ_{eff}) is simulated after importing the mapped conductivity field to another solver. The solver used is electrostatic foam which solves for electrostatic equations using a couple of Poisson's Equations. This solver is modified to solve the Eq.3.2, which solves for the overall potential field of the domain. However, before measuring the model's effective conductivity on the original Rayleigh Taylor Instability model, some validation tests were performed to check the robustness of the numerical simulations. A detailed description of the procedure will be discussed in the results section (Section 4.1). For the testing, some help of OpenFOAM's post-Processing utility has been used as the probe feature. Using the probe utility, the potential value at any part of the domain can be obtained along any line. The measured values of potential at the potential electrodes (P1 and P2), are shown in figure 3.3 has been obtained by using the probes. Also, they are used to obtain some potential values and resistivity values to calculate the current passing through the media. The C1 and C2 are the current electrodes from where the external current has been injected into the media.

3.2 Geometry and Boundary conditions of the system

3.2.1 Rayleigh Taylor Instability modelling

The basic geometry that has been used in the Rayleigh-Taylor Instability is in considering the length scale of 1m. Some basic OpenFoam boundary conditions that are used here are fixedGradient, zeroGradient, cyclic and fixedValue. The fixedGradient boundary condition gives a fixed gradient condition that the patch field's value is calculated that the there is no change in the gradient of the field. The zeroGradient boundary condition applies a zero-gradient condition from the internal patch field onto the patch faces. The cyclic boundary condition enforces a cyclic condition between a pair of boundaries. The fixedValue prescribes the value of a field on a certain boundary of the domain. This value could be constant or dependent on time and space coordinates.

The geometry for the simulation is essentially a square with a side length of 1m but with a "cyclic" boundary condition between the right and left walls which makes the geometric domain to be a layer with an infinite length and the width being 1m in order to simulate a reservoir like scenario. The pressure boundary condition is such that it has a "fixed-Gradient" with a gradient of -1 at the top, which is accounting for the continuation of pressure throughout the media and not a sudden change at the top boundary. The pressure boundary condition for the lower boundary is 0 Pa to keep a reference concerning which all the pressure in the domain has been calculated. The velocity boundary conditions are "zeroGradient" at both the top and the bottom surfaces. The initial condition for the concentration boundary condition is maintained such that the higher concentration pore fluid is occupying the top half of the domain, as shown in fig:3.2.



Figure 3.2: Concentration field at t=0

3.2.2 Geo-electrical modelling

The modeling has been done similar to the Schlumberger survey geometry with four electrodes, two current electrodes (C1 and C2) at two extremes and two inner potential electrodes (P1 and P2) for measuring the potential values at two extremes of the studydomain as shown in the figure 3.3, similar to the experimental paper (Jougnot et al. (2018)) It has to be kept in mind that the potential electrodes should be outside the heterogeneous domain in the homogeneous region to ensure less error due to measurement. The zone of investigation is essentially between the electrodes P1 and P2. Thus we map the concentration field at each time step from the RT Instability study to conductivity maps and import the field between the electrodes P1 and P2. The C1 and C2 electrodes are close to the potential electrodes. The distance between the potential electrodes is 1m and the distance between C1 and P1 and between C2 and P2 id 0.2m. The distance between C1, P1 and C2, P2 is the approximate distance for which we got an almost minimum error in determining the effective conductance. The outer part outside our main investigation area has been kept at a higher conductivity (σ_{ex}) to have a lower error in the model. The value of σ_{ex} was investigated that the model gives a fairly good result for a conductivity contrast from 100 S/m to 1×10^7 S/m as explained in section 4.1.1.



Figure 3.3: Geoelectric modeling configuration. C1 and C2 are the current electrodes, and P1, P2 are the potential electrodes. C1 and C2 inject current in the medium. P1 and P2 measure the potential at the selected positions.

The potential boundary condition is given as 1V to the left wall of the system and 0V to the right wall of the system so that the net potential difference between the two extremes of the system is 1V, which helps to inject the current in the system from C1 to C2.

3.3 Electrical conductivity anisotropy

The anisotropy test is necessary to test the relation of the effective conductivity to the concentration field's spatial distribution. Since the simulation is mainly a gravity-driven instability, the concentration distribution is dependent on the orientation of the media, and hence the effective conductivity will also be sensitive to the orientation. To study this effect, the effective bulk conductivity has been calculated for the same simulation but the porous media has been rotated by 90° around it's center i.e. imposing transverse electrical transport concerning the main flow direction. The fig.3.4 illustrates the anisotropy simulation setup. The anisotropy factor, λ is a dimensionless quantity (Linde and Pedersen,



Figure 3.4: Numerical study of the anisotropy in the effective electrical bulk conductivity for a.the original simulation orientation and b.a rotation of the set of electrodes with respect to the medium by 90°

2004) and is calculated as

$$\lambda = \sqrt{\frac{\sigma^{sim}}{\sigma_{90^o}^{sim}}},\tag{3.3}$$

where σ^{sim} and $\sigma^{sim}_{90^{o}}$ are the longitudinal and the transverse simulated electrical conductivities with respect to the fluid flow direction, respectively. For isotropic conditions, $\lambda \approx 1$. We can get an idea about the degree of anisotropy from the amount of deviation of λ from 1.

Chapter 4

Results

4.1 Validation of the code and Results

Three extensive examples are given to illustrate the accuracy of the proposed numerical method to monitor the evolution of conductivity in the subsurface with different subsurface configuration. The first example deals with checking the robustness and the error that creeps in for a given value of conductivity (σ_{given}) in the media and whether it is the same as the numerically obtained value of conductivity (σ_{sim}) for different conductivity contrasts between the extra medium. The second example deals with a layered (series and parallel) model and checks whether the model follows the "Rule of Mixtures". The third example is finding the effective conductivity for a randomly distributed conductivity map and check whether the σ_{sim} values fall under the theoretically-known boundaries. The 'Rule-of-mixture' equations are widely used to bind the modulus and strength of fiber-reinforced composites based on the fiber filler's weighted contributions and matrix. The electrical properties are also treated similarly. The effective conductivity in a mixture of components having different conductivities flows the "Rule of Mixtures" or, more specifically, the "Voigt and Reuss Bounds" (Voigt, 1889; Reuss, 1929), also known as the Weiner Bounds (Wiener, 1912). The Voigt and the Reuss bounds are essentially weighted arithmetic and harmonic mean constituting the components constituting the media whose effective conductivity that we need to find out.

Suppose the two conductivity present in the wetting phase of the medium are σ_1 and σ_2 . And the wetting phase of the medium constitutes of f part of σ_1 and (1-f) part of σ_2 . Thus the effective conductivity bounds are given as, Voigt Bound (Upper bound):

$$\sigma_{voigt} = f\sigma_1 + (1 - f)\sigma_2 \tag{4.1}$$

Reuss Bound (Lower bound):

$$\sigma_{reuss} = \left(\frac{f}{\sigma_1} + \frac{1-f}{\sigma_2}\right)^{-1} \tag{4.2}$$

4.1.1 Testing the robustness

The robustness is to be tested by calculating ho much the numerically calculated results deviate from the original value of conductivity. In order to test that, a conductivity of the media (σ) of 1 S/m is given as an input to the domain, and it is to be checked how much the simulated value of measured conductivity deviates from 1 S/m. In the proposed geometry for the conductivity as in section 3.2.2, the conductivity value between the potential electrodes is taken to be 1 S/m as shown in fig.4.1.

The σ_{ex} i.e., the conductivity of the extra space where the potential and the current



Figure 4.1: a.Schematic representation for testing the robustness of the solver.

σ _{ex} (S/m)	σ _{sim} (S/m)
1.5	1.00103064
100	1.0049250
1000	1.00501426
1×10^5	1.00503101
1×10^7	1.00509447
1×10^{8}	0.94019567
1×10^{9}	0.57695958
1×10^{10}	0.53800158
1×10^{12}	0.53694042

Figure 4.2: The different values of σ_{sim} for different values of σex .

electrodes are placed. The value of σ_{ex} has been changed for a range of values whereas the internal conductivity is kept constant at 1 S/m. And it was checked till what conductivity contrast, the model can accurately obtain the value of σ_{sim} such that $\sigma_{sim} \approx \sigma(=1S/m)$. Suppose the potential measured by P1 electrode is V1 V and P2 electrode is V2 V. And according to the boundary conditions as explained in section 3.2.2, the potential at the left boundary of the system is 1V and the right boundary is 0V. The solution algorithm that is used for the check is explained in fig 4.1.

From the table given in fig. 4.2, it can be seen that the accuracy decreases as the contrast increases but the the the error in computation remains pretty small ($\approx 0.1\%$) till $\sigma_{ex} = 1 \times 10^7 S/m$. But for a very high contrast the error also increases pretty much more than 50%. Also, this test has been done at a mesh size of 200 × 200. The error will decrease for a much finer mesh. From this experiment we can conclude about the conductivity contrast that we can assume for our original case.

4.1.2 Series and Parallel model

According to the "Rule of mixtures"/"Voigt and Reuss bounds"/"Weiner bounds", the extremes of the effective conductivity of a mixture of different conductivities is obtained by the weighted arithmetic mean and the weighted harmonic mean of the conductivities mixed in the wetting phase and the weights being the volume fraction of each one of them, f. So, by arranging the different layers having contrasting conductivities in a series or a parallel configuration, we can check whether the effective conductivities for different values of f does match with the calculated values of the bounds. Some of the configurations are

shown in fig.4.3.



Figure 4.3: The configurations used for the test.



Figure 4.4: The Voigt and Reuss bounds and the plots for the parallel and series configuration.

From fig.4.4, it can be seen that all the points fall along the exact bounds for all the

range of volume fraction. Thus we can safely conclude that the model works fine with very negligible deviation.

4.1.3 Chessboard tests

In order to test the model and whether the calculated effective conductivities stay within the calculated bounds, the model is tested on a 8x8 chessboard-like conductivity field with random conductivity blocks at random squares. The conductivity field on the chessboard contains all the possible volume fraction of conductivity regions from 0 to 1. Also for each value of f, there are more than one conductivity configuration possible on the chessboard. That is why for each value of volume fraction, the model is tested for two different configurations as it can be seen in fig.4.5 and fig.4.6. It can also be seen that all



Figure 4.5: The different chessboard configurations: a: f=0.25, b: f=0.5, c: f=0.5, d: f=0.75

the conductivity points does lie inside the bounds for all the chessboard configurations. From the figure, it can be noticed that there is a sudden conductivity drop around f = 0.6. This can be attributed to the percolation threshold () for electrical conductivity. The percolation threshold can be defined as the given volume fraction for a particular component in a mixture that allows the percolation of the higher conductivity part. It is the value of f for which the mixture changes from a low conductive material to a high conductive material.



Figure 4.6: Effective conductivity for the chessboard model and the Reuss and Voigt Bounds

4.2 Sensitivity Analysis of Rayleigh Number

4.2.1 Effect on effective conductivity

As it was discussed in section 2.1.2, the Rayleigh number plays a big role in determining the overall physics of the model. So, the model is tested for a series of Rayleigh numbers to check the variation of evolution of the instability for the different Rayleigh numbers. With the variation in Rayleigh number, there is a variation of mixing length, the average velocity of the fingers, and the finger number density (FND). Because of the change in physics due to the change in Rayleigh numbers, the conductivity also changes. The test is carried on for a series of Rayleigh numbers 1000, 2000, 5000, 7000 and 10000. So for each one of the Rayleigh number the same modeling and simulation procedure has been taken as shown in fig.3.1. The evolution of effective conductivity has been plotted in fig.4.7. For the figure, it can be seen that the effective conductivity decreases with time for any



Figure 4.7: Conductivity evolution for a range of Rayleigh numbers.

given Ra, and decreases with Ra at any given time. For an increase in Rayleigh number, the finger number density increases, the wavelength decreases, and the mixing length increases faster. Mixing length is defined as the interface's width from concentration 10% to concentration 90% of the maximum concentration. From fig4.7, we can get an idea about when the instability starts from the effective conductivity measurement.

4.2.2 Effect on Anisotropy analysis

As discussed in Section:3.3, the anisotropy analysis has also been done for the range of Rayleigh numbers 1000, 2000, 5000, 7000 and 10000. With the start of the instability, the system shows a very high anisotropy, but with the increase in mixing length, the system tends towards a more isotropic system ($\lambda \approx 1$).

Figure 4.9a and b clearly show how the anisotropy evolves with time for different Rayleigh numbers. The behavior of the anisotropy factor is almost similar for all the values of Rayleigh numbers. In Fig. 4.9a, the variation of the initial part, when the instability starts, has been shown. It can be seen that initially, the rate of decrease of anisotropy factor is much more for the lower values of Rayleigh numbers, and then the rate of decreases



Figure 4.8: Concentration field for two different Rayleigh numbers at different times of evolution.



Figure 4.9: a. Evolution of the anisotropy coefficient with Rayleigh numbers 2000 to 10000, b. For Rayleigh numbers 2000 and 7000 for a longer time to homogenize. The time mentioned is the nondimensional time.

increases as the instability evolves. For example, in Fig.4.9a, at time = 0.2, the value of λ for Ra = 1000 is minimum and Ra = 10000 is maximum, whereas, for time = 1.8, Ra = 1000 has the maximum value of λ and Ra = 1000 has the minimum value. From Fig.4.9b, which gives an overall picture for two values of Rayleigh numbers 2000 and 7000, it can be seen that the higher Rayleigh number reaches isotropic conditions faster than a lower Rayleigh number. Also, it can be noticed that there is a sudden drop of effective conductivity from t = 2.2 to t = 2.3 for Ra = 2000 and from t = 2.9 to t = 3.0 for Ra = 7000. This is because, at that time, the first finger from the higher concentration zone

reaches the opposite side (See fig.4.8). Thus the connectivity of the higher conductive fluid is established from one side to the other. Also, it can be intuitively said that the velocity of the evolution of instability fingers is faster for a higher Rayleigh number, and it slows down with the decrease of Rayleigh number, which is also evident from fig.4.8.

4.3 Application to Seawater/Freshwater Interface

In this section, the simulation procedure described to study the effective conductivity of Rayleigh Taylor instabilities is applied to a porous media involving more denser saltwater over low-density freshwater. The model that is programmed here can be directly applied to saltwater-freshwater fingering instabilities observed in a porous media when saltwater overcoming in coastal aquifers and also in salt lakes where we find the similar kind of a scenario where we have a layer of higher density fluid over lower density fluid thus triggering the Rayleigh Taylor Instability in such cases. There have been many numerical studies that are going on regarding these density-driven fingering instabilities in porous media (Johannsen et al. (2006)). So far, people have used intrusive methods that do not apply to the field or any very difficult to apply on the field. Here we propose to simulate what will be the effective response of the time-varying instabilities and what would be the effective electrical response of it as ERT (Electrical Resistivity Tomography) can be used effectively on the field.

As discussed in Section: 2.2.2, the net bulk conductivity is calculated from the ionic concentration in the fluid phase or the wetting phase. However, in a practical scenario, researchers often try to get to the ionic concentration field from the measurement of the effective electrical conductivity of the media at the resolution scale from the different petrophysical relationships (Eq.2.22, Eq.2.23). The application of ionic concentration is driven density difference, which is the triggering factor for the Rayleigh Taylor Instability in a porous media, which can be seen in saline-water freshwater interaction in coastal regions between seawater and groundwater.

In the case of a saline water-freshwater interaction, for the Rayleigh Taylor instability, we need to determine the value of Rayleigh number (Eq.2.6) determine the physics. To apply the model, we need to get the specific petrophysical properties and electrical parameters for the media and the pore fluids (saline water and fresh water). For the media, we considered a consolidated section of sand. The hydrodynamic properties of sand are

taken from Jougnot and Linde (2013). The hydrodynamic and electrical properties of the pore fluids (seawater and freshwater) are calculated from Jougnot and Linde (2013); Lide (2006); El-Dessouky and Ettouney (2002) and Sharqawy et al. (2010). It is assumed that the freshwater is 100 times less saline than the seawater from the observations. Now

	Parameter	Saltwater	Freshwate	r Un	its				
ĺ	Salinity	0.5100	0.00493	mo	1/1				
	Density	1.0202	0.8896	kg	/1				
	Dynamic Viscosity	1.060×10^{-3}	1.001×10^{-1}	$^{-3}$ kg/	m s				
	Param	eter	Value	Units					
	Temperat	ure (T)	20	°C	1				
	Permeabi	lity (k)	1.54×10^{-11}	m^{-2}					
	Porosity	$V(\phi)$	0.403	(-)					
	Formation f	actor (F)	3.569	(-)					
	Cementation ex	xponent (m)	1.40	(-)					
	Saturation ex	ponent (n)	1.6	(-)					
	Molecular diffus	ivity of NaCl	1.6×10^{-9}	m ² s ⁻¹					
	11		1	11					

Table 4.1: Hydrodynamic parameters of the pore fluids (top); Other physical parameters (bottom)

it can be seen that the viscosity is also contrasting for the seawater and the freshwater. Which may trigger a viscosity driven Saffman-Taylor instability (Saffman and Taylor, 1958) over the density driven Rayleigh Taylor instability. But in case of the seawater and the freshwater considered here, the density contrast is much more than the viscosity contrast. Thus the density driven instability will be much more dominant in this case. From all the values given in Table 4.1, we can get the Rayleigh number value of 5090.79 (from Eq.2.6). The non-dimensional time scale is calculated to be around 35 hours (from Eq.2.9). That is, t' = 1 in the simulation means t = 35 h dimensionally.

From Fig.4.10 and the corresponding plots in fig.4.11, it can be easily understood how the net conductivity varies, and the anisotropy changes as the instability progress between the denser saltwater at the top and the lighter freshwater at the bottom. From the figures, it can be concluded about the extent of mixing between the saltwater and the freshwater. Also, in all the physical processes involving density-driven instability in nature, this kind of numerical model will help to get a time-lapse model of effective conductivity. Thus it is possible to compare the field results with the simulation results to get a better validation of the numerical model. The results can also be directly compared with the ERT prospecting in near-surface phenomenon, thus opening up several possibilities for comparing field scale tomography results with the simulation results. Nevertheless, there are still numerous scopes of improvement in the numerical model. Also, we need to



streamlines. The time mentioned in the non dimensional time. Figure 4.10: The concentration evolution during the Rayleigh Taylor Instability and the consequent evolution of the conductivity field and current





consider the anisotropic nature of the electrical conductivity at the resolution scale while performing inversion on their ERT data. The anisotropy analysis suggests a strong impact of pore scale and sub-resolution effects of the instability on the up-scaled bulk electrical conductivity. The anisotropy analysis shows quite a change in value as the instability progresses.

Chapter 5

Discussion and Conclusion

5.1 Discussion

5.1.1 Rayleigh Taylor instability of the pore fluid

The instability of a dense fluid layer supported by a light one has generally known as Rayleigh-Taylor (RT) instability. It can occur under gravity and, equivalently, under an acceleration of the fluid system toward the denser fluid. We considered a 2D porous media and how the instability progresses with time for a set of miscible fluids having a density contrast to trigger the Rayleigh Taylor Instability. Under our consideration, the fluids are the seawater and the groundwater and how they will interact if we have higher denser seawater at the top and a much lower denser freshwater at the bottom in a reservoir scenario. The Rayleigh number instability modeling has been done in an entirely nondimensional way, and the Rayleigh number defines the physics of the instability in the porous media singlehandedly. From Eq.2.6, it can be seen the Rayleigh number depends on the different hydrodynamic parameters of the two fluids involved, and by varying any one of these, we can define a new physics, and the model will simulate the corresponding flow-physics.

5.1.2 Relationship between concentration field and measured conductivity

In Section 2.2.2, it has been discussed how the conductivity field is mapped from the concentration field. Figure. 4.7 can be explained as such that for all the values of Rayleigh numbers, the conductivity gradually decreases. Also, from the Rayleigh number tests, we can see how the conductivity changes with the increase in Rayleigh number (Fig. 4.7). Overall the effective conductivity decreases with time as the instability progresses, but the

rate of decrease of the effective conductivity increases for an increase in Rayleigh number. This particular phenomenon of the decrease of effective conductivity with the instability's progress can be explained from Fig. 4.4, where we see how the bounds are defined for the different configurations. The series configuration defines the lower bounds, and the parallel configuration defines the upper bounds. Thus the parallel configured system has more conductivity than a series system.

At t=0, the concentration field is arranged in a parallel mode of connection. As the instability progresses, there is a transition from the parallel connection to homogeneity as the fluids of the two concentration mixes. Now, as the instability progresses i.e., the lighter fluid starts pushing, the denser fluid and vice-versa and the fingers are generated, we can consider that to be analogous to a series configuration as the fingers reach the opposite sides (check Fig. 4.8 to see the transition). This explains the conductivity drop as the instability progresses. Thus, by monitoring the conductivity, we can comment on the reservoir's concentration distribution and how much the instability has progressed.

5.1.3 Electrical conductivity anisotropy analysis

From the previous section, it can be concluded that the medium's net conductivity is dependent on the orientation of the medium. We can also say that the orientation changes the nature of the value of effective conductivity from a parallel nature to a series one by just a rotation of 90° about the center (Check Fig.4.3). The orientation dictates the connectivity between the faces concerning fluid transport in the medium. The method has been discussed in detail in Sec.3.3. We also did the anisotropy test for all the Rayleigh number values to monitor how the anisotropy factor changes with the instability evolution with time for the different physics. (Fig.4.9). From the diagrams, we can see that the anisotropy coefficient starts with a very high number initially, but it gradually decreases towards one as the instability progresses, and the mixing starts. This is logical because, for a homogeneous media, the anisotropy factor is theoretically equal to one, and as the mixing progresses, the system gradually starts to move towards homogeneity. Thus the factor approaches 1. We can also comment on the mixing rate from the anisotropy factor for the different Rayleigh numbers because the anisotropy factor gives an idea bout how fast the mixing is progressing, which also depends on the velocity of the fingers.

5.1.4 Improvements and ideas for further studies

Over the last few decades, there has been different illustrations and studies about variable density flows in groundwater hydrology which includes seawater intrusion, fresh-saline water interfaces and saltwater upcoming in coastal aquifers, subterranean groundwater discharge, dense contaminant plume migration, DNAPL studies, density-driven transport in the vadose zone, flow through salt formations in high-level radioactive waste disposal sites, heat and fluid flow in geothermal systems, palaeohydrogeology of sedimentary basins, sedimentary basin mass and heat transport and diagenesis, processes beneath sabkhas and salt lakes and buoyant plume effects in applied tracer tests (see Simmons (2005), Simmons et al. (2001), Diersch and Kolditz (2002)). For further research this model can also be developed for a 3D spatial scenario so that the bulk conductivity can be measured in all the 3 directions as the evolution of the subsurface processes in time lapse similar to 4D monitoring of a groundwater reservoir.

One major societal problem that gives rise to the phenomenon of contaminant and reactive transport through near-surface reservoirs flows through the porous media as DNAPL (dense non-aqueous phase liquid), which results in plumes developing from landfills and reactive waste disposal sites. The model can be applied to monitor density-driven contaminant transport or reactive mixing in the groundwater.

CO $_2$ storage is also a significant application where we can observe Rayleigh Taylor instabilities, but since CCS is not a much near-surface phenomenon, boreholes can be dug. The mixing rate of supercritical CO₂ and the evolution of the instability can be monitored between boreholes using the bulk conductivity model.

5.2 Conclusion

The complexity of variable density problems generally increases as one moves from situations where light fluid overlies dense fluid to potentially unstable situations where dense fluid overlies less dense fluid. In unstable cases, transport can be characterized by rapid instability development where finger instabilities sink under the gravitational influence, enhancing solute transport and mixing. These are several emerging challenges in hydrogeology, which involves monitoring density-driven near-surface and subsurface flows. In fact, monitoring density-driven flows in the subsurface from field data and correlating that with the simulation data to understand the transport physics of subsurface flows better because field data does not always provide a very clear picture of the physics. From fieldscale data, it becomes challenging to analyze and get how the concepts of heterogeneity, concentration dispersion, etc. affect the flow regime, mixing length, the mixing rate, etc. That is why this model is devised to implement the physics and see how the density-driven instabilities affect the net conductivity inside an aquifer. This conductivity model devised in an open-source software OpenFOAM can be used in any kind of near-surface pore-scale fluid transport phenomenon. This suggests a strong impact of the pore scale and sub-resolution effects on the bulk electrical conductivity in terms of magnitude and anisotropy. The model can also be up-scaled and downscaled to any resolution necessary. The mode has been tested via a widespread variation of conductivity maps and tested to validate the calculated bulk conductivity stays within the Voigt and Reuss bounds. The results can also be later validated with field-scale measurements and get an idea of real-time subsurface conditions by matching the simulated data from the model with the measured data. This opens up a range of opportunities to investigate the link between the electrical signals and a variety of pore scale subsurface processes such as reactive transport, mixing processes in porous media, and other biogeochemical reactions.

5.3 Acknowledgements

I gratefully acknowledge the guidance and support from my supervisor Dr. Damien Jougnot for the internship. Despite performing the whole project remotely from India due to the COVID-19 pandemic scenario, I learned a lot during the whole process from doing the work and from Dr. Jougnot, who was helpful with all my doubts. Thank you very much for this opportunity.

Chapter 6

Appendix

6.1 OpenFOAM codes

6.1.1 For Rayleigh Taylor Instability

```
Solver: darcyConcFoam.C
#include "fvCFD.H"
#include "simpleControl.H"
int main(int argc, char *argv[])
{
   #include "setRootCase.H"
   vector g0(0,-1.00,0);
    dimensionedVector zy("g",dimensionSet(0,1,-2,0,0,0,0),g0);
   #include "createTime.H"
   #include "createMesh.H"
   #include "createFields.H"
   simpleControl simple(mesh);
   Info<< "\nCalculating temperature distribution\n" << endl;</pre>
   while (simple.loop())
   {
      Info<< "Time = " << runTime.timeName() << nl << endl;</pre>
      while (simple.correctNonOrthogonal())
      {
         volVectorField gradc(fvc::grad(c));
```

solve

```
(
           - fvm::laplacian(p) - gradc.component(vector::Y)
        );
        U = -(fvc::grad(p)) + zy*c ;
    phi = linearInterpolate(U) & mesh.Sf();
        solve
    (
      fvm::ddt(c)
   + fvm::div(phi, c)
   - fvm::laplacian((1/Ra), c)
   - (1/Ra) * a * fvm::laplacian(mag(U) ,c, "laplacian(Dc,c)")
   - ((1/Ra)*(1-a))/((mag(U)+delS))*fvm::laplacian((U*U),c, "laplacian(Dc,c)" )
    );
}
       runTime.write();
      Info<< "ExecutionTime = " << runTime.elapsedCpuTime() << "s"</pre>
        << " ClockTime = " << runTime.elapsedClockTime() << " s"
        << nl << endl;
}
Info<< "End\n" << endl;</pre>
return 0;
```

6.1.2 For calculating the Bulk Electrical conductivity

}

Solver: poissonFoam.C

6.2 MATLAB code for transferring the field and post processing

%run it section-wise, not together.

```
%% input
mx = 600; my = 720; m = mx*my ; % mesh size
deltaT = 0.1;
iniT = 0;
finT = 3.2;
Ra = 5090.79; %change reynolds no
count = iniT:deltaT:finT;
%% postprocess RTI
%/reading the concentration distribution files
for i = 1:(finT/deltaT + 1)
    %mes(i) = fopen(['---folderpath---\RTI_Ra',num2str(Ra),'\',num2str((i-1)/10),'\c'],'r');
    mes(i) = fopen(['---folderpath---\RTI_salfre1\',num2str((i-1)/10),'\c'],'r');
    %datac(:,i) = textread(['---folderpath---\RTI_salfre1\',num2str(Ra),'\',num2str((i-1)/10),'\c'], '%s',
    datac(:,i) = textread(['---folderpath---\RTI_salfre1\',num2str((i-1)/10),'\c'], '%s', 'delimiter'
```

```
end
P = datac(26:(26+(mx*mx)-1),:);
for j = 1:(finT/deltaT + 1)
    S = P(:,j);
    Q = sprintf('%s*', S{:});
    c(:,j) = sscanf(Q, '%f*');%each column of c is each matrix of c
    c(:,j) = c(:,j) ;
    eval(['A' num2str(j) '= reshape(c(:,j),[mx,mx]);']);%each column in a saperate matrix of its own
                 %%generate the images
                                             % info_access: G = eval(['A' num2str(j);]);
    figure(j)
    pcolor(eval(['A' num2str(j);])');
    shading interp; axis image;colorbar;
    title('Concentration Field')
    F(j) = getframe(gcf);
    close;
end
writerObj = VideoWriter('Concentration.avi');
writerObj.FrameRate = 2;
% open the video writer
open(writerObj);
% write the frames to the video
for i=1:length(F)
    % convert the image to a frame
    frame = F(i) ;
    writeVideo(writerObj, frame);
end
% close the writer object
close(writerObj);
%% postprocess RTI + Preprocess ERT
%dimensionalise everything and map to conductivity field
T = 20; %temperature
d1 = 5.6;
d2 = 0.27;
d3 = -1.51e-4;
d4 = 2.36;
d5 = 0.099;
d6 = 0.214; %sen and goode 1992
```

```
phi = 0.403; %porosity
m =1.40; %cementation exponent
ff = phi<sup>(-m)</sup>; %formation factor
ex = 1e4 * ones(600, 60);
                                              %making a extra space dimension of 600X60 mesh size measured
for j = 1: (finT/deltaT + 1)
    G = eval(['A' num2str(j);]);
    %G = G';
                                               %comment out for anisotropy calculation
    % G = (G + 0.01) .* 0.5; %will change later
    G = (d1 + d2*T + d3*(T<sup>2</sup>)).*G - ((d4 + d5*T)./(1 + d6 .* sqrt(G))) .* G.<sup>(1.5)</sup>;%senandgoode | con
    %find the conductivity of medium
    G = G .* (1/ff);
    eval(['B' num2str(j) '=[ex G ex] + 0.00001;']);
    figure(j)
    pcolor(log(eval(['B' num2str(j);]))); shading interp;
    axis image;colorbar;
    title('Conductivity Field (in log(S/m))');
    F(j) = getframe(gcf);
    close;
end
writerObj = VideoWriter('Conductivity.avi');
writerObj.FrameRate = 2;
% open the video writer
open(writerObj);
% write the frames to the video
for i=1:length(F)
    \% convert the image to a frame
    frame = F(i);
    writeVideo(writerObj, frame);
end
% close the writer object
close(writerObj);
\% write the conductivity field on a file : i/p in <code>OpenFOAM</code>
for i = 1:(finT/deltaT + 1)
    G = eval(['B' num2str(i);]);
    eval(['L' num2str(i) '= zeros(mx*my,1);']);
    M = zeros(mx*my,1);
```

```
for j = 1:mx
        M(1+(j-1)*my:(j-1)*my+my) = G(j,:);
    end
    eval(['L' num2str(i) '= M;']); % thus we have all the linear matrices suitable for openFOAM
    %convert them to saperate sigma1 files with headers and tailnote
    J(:,i) = M;
end
J = num2cell(J);
messig = fopen(['---folderpath---\poissonERT_test\constant\sigma1'],'r');
sigmaread = textread(['---folderpath---\poissonERT_test\constant\sigma1'], '%s','delimiter', '\n');
for i = 1: (finT/deltaT + 1)
    %make the conductivity files
    sigma1 =[sigmaread(1:25);J(:,i);sigmaread(432026:432054)];
    %copy to files
    filePh = fopen(['---folderpath---',num2str(i),'\constant\sigma1'],'w');
    %D = eval(['sigma' num2str(i);]);
    fprintf(filePh,'%s\n',sigma1{:});
    fclose(filePh);
end
\% run the ERT in OpenFOAM till the value of i
%% postprocess of ERT
sigma_ex = 1e4 ; A = 1;
1 = 0.04; %change the value acc to width for current measurement
VO =0;
%close all;
format longE;
% take measurement electrode data
for i = 1:(finT/deltaT + 1)
    casename = ['RTIERT',num2str(i)]; % change the case name accordingly
    mes11 = fopen(['---folderpath----',casename,'\postProcessing\P11\1\line_v.xy'],'r');
    formatSpec = '%f %f';
    sizeA1 = [2 Inf];
    P11 = fscanf(mes11,formatSpec,sizeA1);
    fclose(mes11);
    mes12 = fopen(['---folderpath---', casename, '\postProcessing\P12\1\line_v.xy'], 'r');
    formatSpec = '%f %f';
```

```
sizeA1 = [2 Inf];
P12 = fscanf(mes12,formatSpec,sizeA1);
fclose(mes12);
P1_values = [P11,P12];
P1_values = P1_values';
P1 = median(P1_values(:,2));
mes21 = fopen(['---folderpath---',casename,'\postProcessing\P21\1\line_v.xy'],'r');
formatSpec = '%f %f';
sizeA1 = [2 Inf];
P21 = fscanf(mes21,formatSpec,sizeA1);
fclose(mes21);
mes22 = fopen(['---folderpath---',casename,'\postProcessing\P22\1\line_v.xy'],'r');
formatSpec = '%f %f';
sizeA1 = [2 Inf];
P22 = fscanf(mes22,formatSpec,sizeA1);
fclose(mes22);
P2_values = [P21,P22];
P2_values = P2_values';
P2 = median(P2_values(:,2));
% measure do(V)
dataV = fopen(['---folderpath---',casename,'\postProcessing\singleGraph1\1\line_v.xy'],'r');
formatSpec = '%f %f';
sizeA1 = [2 Inf];
Vy1 = fscanf(dataV,formatSpec,sizeA1);
Vy1 = Vy1';
fclose all;
V1 = Vy1(:,2);
y1 = Vy1(:, 1);
% figure ;
% plot(y1,V1);
% xlabel('y', 'FontSize',10, 'FontWeight', 'bold');
% ylabel('V','FontSize',10,'FontWeight','bold');
```

```
% title('V(y) variation');
% grid on;
dataV = fopen(['---folderpath---',casename,'\postProcessing\singleGraph2\1\line_v.xy'],'r');
formatSpec = '%f %f';
sizeA1 = [2 Inf];
Vy2 = fscanf(dataV,formatSpec,sizeA1);
Vy2 = Vy2';
fclose all;
V2 = Vy2(:,2);
y_2 = Vy_2(:, 1);
% calculate eff sigma
V1m = mean(V1);
V2m = mean(V2);
I_meas = (V1m - V2m)*sigma_ex*(A/l) ;
delta_V = (P2-P1);
R_meas = delta_V / I_meas ;
%sigma_check_p = (1-vf) * 1 + (vf)*0.001
%sigma_check_s = ((1-vf)/1 + vf/0.001)^-1
sigma_meas (i,:) = (1.000105)/(A * R_meas)
%sigma_check = vf * 0.001 + (1-vf)*1
% read data map (V,sigma)
mx = 720; my = 600; m = mx*my ; %change for a change inmesh size
dataV = textread(['---folderpath---',casename,'\1\V'], '%s','delimiter', '\n');
P = dataV(26:(26+m-1));
S = sprintf('%s*', P\{:\});
Vl = sscanf(S, '%f*');
datasig = textread(['---folderpath---',casename,'\constant\sigma1'], '%s','delimiter', '\n');
Q = datasig(26:(26+m-1));
R = sprintf('%s*', Q{:});
sigmal = sscanf(R, '%f*');
```

```
V = reshape(V1, [mx,my]);
    V = V';
    sigma = reshape(sigmal , [mx,my]);
    sigma = sigma';
    % plot streamlines
    % calculate potential gradients
    [Vx,Vy]=gradient(V(:,61:660));
                                             %change the val acc to mesh size
    % figure(3)
    % pcolor(Vx); shading interp;
    % figure(4)
    % pcolor(Vy); shading interp;
    Ix=sigma(:,61:660).*Vx;
    Iy=sigma(:,61:660).*Vy;
    Size_V=size(V(:,61:660));
    nDisp=5;
    Disp_Ix=Ix(1:nDisp:Size_V(1),1:nDisp:Size_V(2));
    Disp_Iy=Iy(1:nDisp:Size_V(1),1:nDisp:Size_V(2));
    [x,y]=meshgrid(61:nDisp:660,1:nDisp:Size_V(1));
    figure(i)
    quiver(x,y,Disp_Ix.*1e10,Disp_Iy.*1e10,3,'r');
    colorbar
    axis image
    set(gca,'YDir','normal')
    title('Current intensity, J [A m^{-2}]')
    F(i) = getframe(gcf);
end
writerObj = VideoWriter('Current Streamlines.avi');
writerObj.FrameRate = 2;
% open the video writer
open(writerObj);
% write the frames to the video
for i=1:length(F)
```

```
\% convert the image to a frame
```

```
frame = F(i);
    writeVideo(writerObj, frame);
end
% close the writer object
close(writerObj);
 % open your file for writing
 fid = fopen('eff_sigma.txt', 'wt'); %name changed for the anisotropy analysis
 % write the matrix
  if fid > 0
     fprintf(fid,'%d\n',sigma_meas');
     fclose(fid);
  end
  %% Testing the aniotropy
\% step1: transfer the files to the respective folders
% now continue
%count = iniT:deltaT:(finT-0.1)
%sig0 = textread(['---folderpath---',num2str(Ra),'\eff_sigma.txt'], '%s','delimiter', '\n');
sig0 = textread(['---folderpath---\eff_sigma.txt'], '%s', 'delimiter', '\n');
S = sprintf('%s*', sig0{:});
sig0 = sscanf(S, '%f*');
%sig90 = textread(['---folderpath---',num2str(Ra),'\eff_sigma90.txt'], '%s','delimiter', '\n');
sig90 = textread(['---folderpath----\eff_sigma.txt'], '%s','delimiter', '\n');
S = sprintf('%s*', sig90{:});
sig90 = sscanf(S, '%f*');
lambda = sqrt(sig0./sig90);
figure(911);
```

```
plot(count',lambda,'d--'); %change
```

Bibliography

- Archie, G. E. et al. (1942). The electrical resistivity log as an aid in determining some reservoir characteristics. *Transactions of the AIME*, 146(01):54–62.
- Binley, A., Hubbard, S. S., Huisman, J. A., Revil, A., Robinson, D. A., Singha, K., and Slater, L. D. (2015). The emergence of hydrogeophysics for improved understanding of subsurface processes over multiple scales. *Water Resources Research*, 51(6):3837–3866.
- Binley, A. and Kemna, A. (2005). DC Resistivity and Induced Polarization Methods, pages 129–156. Springer Netherlands, Dordrecht.
- De Paoli, M., Zonta, F., and Soldati, A. (2019). Rayleigh-taylor convective dissolution in confined porous media. *Phys. Rev. Fluids*, 4:023502.
- Deignan, T. M. (2008). Low and High Frequency Electromagnetics in Landfill Investigations, pages 361–372.
- Diersch, H.-J. and Kolditz, O. (2002). Variable-density flow and transport in porous media: approaches and challenges. *Advances in water resources*, 25(8-12):899–944.
- Einstein, A. (1905). Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen. Annalen der Physik, 322(8):549–560.
- El-Dessouky, H. T. and Ettouney, H. M. (2002). Appendix a thermodynamic properties. In Fundamentals of Salt Water Desalination, pages 525 – 563. Elsevier Science B.V., Amsterdam.
- Ghosh, U., Borgne, T. L., Jougnot, D., Linde, N., and Méheust, Y. (2018). Geoelectrical signatures of reactive mixing: A theoretical assessment. *Geophysical Research Letters*, 45(8):3489–3498.
- Glover, P. (2015). 11.04–geophysical properties of the near surface earth: Electrical properties. Treatise on geophysics, pages 89–137.
- Hidalgo, J. J. and Carrera, J. (2009). Effect of dispersion on the onset of convection during co2 sequestration. Journal of Fluid Mechanics, 640:441–452.

- Johannsen, K., Oswald, S., Held, R., and Kinzelbach, W. (2006). Numerical simulation of threedimensional saltwater-freshwater fingering instabilities observed in a porous medium. Advances in Water Resources, 29(11):1690 – 1704.
- Jougnot, D. (2020). Developing hydrogeophysics for critical zone studies, importance of heterogeneities and processes at the mesoscopic scale. PhD thesis.
- Jougnot, D., Jiménez-Martínez, J., Legendre, R., Le Borgne, T., Méheust, Y., and Linde, N. (2018). Impact of small-scale saline tracer heterogeneity on electrical resistivity monitoring in fully and partially saturated porous media: Insights from geoelectrical milli-fluidic experiments. Advances in Water Resources, 113:295–309.
- Jougnot, D. and Linde, N. (2013). Self-potentials in partially saturated media: The importance of explicit modeling of electrode effects. *Vadose Zone Journal*, 12.
- Jougnot, D., Revil, A., and Leroy, P. (2009). Diffusion of ionic tracers in the callovo-oxfordian clay-rock using the donnan equilibrium model and the formation factor. *Geochimica et Cosmochimica Acta*, 73(10):2712 – 2726.
- Langer, R. E. (1936). On the determination of earth conductivity from observed surface potentials. Bull. Amer. Math. Soc., 42(10):747–754.
- Lide, D. R. (2006). Crc handbook of chemistry and physics, 86th edition edited by david r. lide (national institute of standards and technology). crc press (an imprint of taylor and francis group): Boca raton, fl. 2005. 2544 pp. \$125.96. isbn 0-8493-0486-5. Journal of the American Chemical Society, 128(16):5585– 5585.
- Linde, N. and Pedersen, L. (2004). Evidence of electrical anisotropy in limestone formations using the rmt technique. *Geophysics*, 69.
- Müller, T. M., Gurevich, B., and Lebedev, M. (2010). Seismic wave attenuation and dispersion resulting from wave-induced flow in porous rocks a review. *GEOPHYSICS*, 75(5):75A147–75A164.
- Neufeld, J. A., Hesse, M. A., Riaz, A., Hallworth, M. A., Tchelepi, H. A., and Huppert, H. E. (2010). Convective dissolution of carbon dioxide in saline aquifers. *Geophysical Research Letters*, 37(22).
- Nolet, G. (1987). Seismic wave propagation and seismic tomography, pages 1–23. Springer Netherlands, Dordrecht.
- Rayleigh, L. (1900). Investigation of the character of the equilibrium of an incompressible heavy fluid of variable density. *Scientific papers*, pages 200–207.
- Reuss, A. (1929). Berechnung der Fließgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle. Zeitschrift Angewandte Mathematik und Mechanik, 9(1):49–58.

- Revil, A., Karaoulis, M., Johnson, T., and Kemna, A. (2012). Review: Some low-frequency electrical methods for subsurface characterization and monitoring in hydrogeology. *Hydrogeology Journal*, 20(4):617–658.
- Riaz, A. and Hesse, M. (2006). Onset of convection in a gravitationally unstable diffusive boundary layer in porous media. *Journal of Fluid Mechanics*, 548:87 – 111.
- Saffman, P. G. and Taylor, G. I. (1958). The penetration of a fluid into a porous medium or hele-shaw cell containing a more viscous liquid. Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences, 245(1242):312–329.
- Schlumberger, C. (1912). Premières expériences. Carte des courbes équipotentielles, tracées au courant continu Val-Richer (Calvados).
- Schlumberger, C. (1920). Etude sur la prospection electrique du sous-sol. Gauthier-Villars.
- Sen, P. N. and Goode, P. A. (1992). Influence of temperature on electrical conductivity on shaly sands. GEOPHYSICS, 57(1):89–96.
- Sharqawy, M. H., V, J. H. L., and Zubair, S. M. (2010). Thermophysical properties of seawater: a review of existing correlations and data. *Desalination and Water Treatment*, 16(1-3):354–380.
- Simmons, C. (2005). Variable density groundwater flow: From current challenges to future possibilities. Hydrogeology Journal, 13:116–119.
- Simmons, C. T., Fenstemaker, T. R., and Sharp Jr, J. M. (2001). Variable-density groundwater flow and solute transport in heterogeneous porous media: approaches, resolutions and future challenges. *Journal of Contaminant Hydrology*, 52(1-4):245–275.
- Taylor, G. I. (1950). The instability of liquid surfaces when accelerated in a direction perpendicular to their planes. i. Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences, 201(1065):192–196.
- Voigt, W. (1889). Ueber die beziehung zwischen den beiden elasticitätsconstanten isotroper körper. Annalen der Physik, 274(12):573–587.
- Vreme, A., NADAL, F., Pouligny, B., Jeandet, P., Liger-Belair, G., and Meunier, P. (2016). Gravitational instability due to the dissolution of carbon dioxide in a hele-shaw cell. *Physical Review Fluids*, 1.

Wiener, O. (1912). Theory of composite bodies. Abh. Saechs. Ges. Wiss, 33:507-525.