Final Report

Modeling and Evaluation of Geophysical Methods for Monitoring and Tracking CO₂ Migration in the Subsurface

Reporting Period: 12/1/2009 – 11/30/2012

FOA Title: Recovery Act: Geologic Sequestration Training and Research

FOA Number: DE-FOA-0000032

NETL Award Number: DE-FE0002441

Report Issued March 26, 2013

Dr. Jeff Daniels, Principal Investigator

The Ohio State University
Office of Sponsored Programs
1960 Kenny Rd.
Columbus, OH 43210

Disclaimer: This report was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor any agency thereof, or any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or any agency thereof.

Abstract

Geological sequestration has been proposed as a viable option for mitigating the vast amount of CO₂ being released into the atmosphere daily. Test sites for CO₂ injection have been appearing across the world to ascertain the feasibility of capturing and sequestering carbon dioxide. A major concern with full scale implementation is monitoring and verifying the permanence of injected CO₂. Geophysical methods, an exploration industry standard, are non-invasive imaging techniques that can be implemented to address that concern.

Geophysical methods, seismic and electromagnetic, play a crucial role in monitoring the subsurface pre- and post-injection. Seismic techniques have been the most popular but electromagnetic methods are gaining interest. The primary goal of this project was to develop a new geophysical tool, a software program called GphysCO₂, to investigate the implementation of geophysical monitoring for detecting injected CO₂ at test sites. The GphysCO₂ software consists of interconnected programs that encompass well logging, seismic, and electromagnetic methods. The software enables users to design and execute 3D surface-to-surface (conventional surface seismic) and borehole-to-borehole (cross-hole seismic and electromagnetic methods) numerical modeling surveys. The generalized flow of the program begins with building a complex 3D subsurface geological model, assigning properties to the models that mimic a potential CO₂ injection site, numerically forward model a geophysical survey, and analyze the results.

A test site located in Warren County, Ohio was selected as the test site for the full implementation of GphysCO₂. Specific interest was placed on a potential reservoir target, the Mount Simon Sandstone, and cap rock, the Eau Claire Formation. Analysis of the test site included well log data, physical property measurements (porosity), core sample resistivity measurements, calculating electrical permittivity values, seismic data collection, and seismic interpretation. The data was input into GphysCO₂ to demonstrate a full implementation of the software capabilities. Part of the implementation investigated the limits of using geophysical methods to monitor CO₂ injection sites. The results show that cross-hole EM numerical surveys are limited to under 100 meter borehole separation. Those results were utilized in executing numerical EM surveys that contain hypothetical CO₂ injections. The outcome of the forward modeling shows that EM methods can detect the presence of CO₂.

Table of Contents

Abstract	ii
List of Figures	v
List of Tables	xi
List of Equations	xii
Chapter 1: Introduction	1
1.1 Carbon Sequestration	1
1.2 Geophysics and Carbon Sequestration.....	2
1.3 Geophysical Properties	3
1.3.1 Electromagnetic Geophysics.....	4
1.3.2 Seismic Geophysics	9
1.4 Necessity for a New Geophysical Tool	10
Chapter 2: GphysCO2 Software	12
2.1 Software Introduction	12
2.2 Seismic Software	13
2.3 EM Software	15
2.4 Well Logging Software.....	17
Chapter 3: Testing and Verification.....	18
3.1 Introduction.....	18
3.2 Regional Geology	18
3.3 Warren County Test Case	21
3.4 Geophysical Well Log Analysis	25
3.5 Porosity Data.....	27
3.6 Resistivity Data.....	29
3.6.1 Laboratory Resistivity Data	29
3.6.2 Resistivity Data Corrections	32
3.6.3 Resistivity Data Analysis	36
3.7 Electrical Permittivity Data.....	42
3.7.1 Permittivity Calculation	42
3.7.2 Permittivity Data Analysis	44
3.8 Seismic Data	45
Chapter 4: Three Dimensional Data Analysis	49

4.1 3-Dimensional Property Models	49
4.1.1 Electrical Property Model	51
4.1.2 Seismic Property Model.....	56
4.2 Seismic and EM Property Model Summary	58
Chapter 5: Numerical Simulations.....	59
5.1 Cross-hole Electromagnetic Simulations	59
5.1.1 Cross-hole EM Spatial Limitations.....	59
5.1.2 EM Detection of Injected CO ₂	64
5.1.3 Cross-hole EM Discussion.....	70
5.2 Seismic Simulation	71
Chapter 6: Conclusions	75
6.1 GphysCO2 and Carbon Sequestration	75
6.2 Software Implementation.....	76
6.3 Discussion	76
References	78
Appendix A: Seismic Software Module	83
A.1 Seismic Module Outline.....	83
A.2 Seismic Wave Equation Theory.....	88
A.3 Seismic Numerical Modeling Theory	90
Appendix B: EM Module.....	92
B.1 EM Module Outline	92
B.1.1 Three Dimensional EM Modeling.....	92
B.1.2 Two Dimensional	100
B.1.3 Three Dimensional	118
B.2 PFDTD Code.....	122

List of Figures

Figure 1.1. Typical Ranges of Resistivity Values for Earth Materials (Adapted from Palacky, 1987).	7
Figure 1.2. The permittivity consists of the vector sum of the real and imaginary parts. The tangent of the resulting angle is the loss tangent.	8
Figure 2.1. Software outline for the GphysCO2 program. The top control program interfaces between the data input, forward modeling (seismic & EM), and display/interpretation in a fully integrated network.	12
Figure 2.2. Top level program menu for GphysCO2. From this menu the EM, Seismic, and well logging modules can be accessed.	13
Figure 2.3. This software outline of the seismic module shows the interfacing between IDL, Madagascar, and OpendTect.....	14
Figure 2.4. Model sub-blocks assigned a specified size, shape, cell size, conductivity, permittivity, randomization, and magnetic permeability. Antennas placed at varying locations with an assigned broadband frequency. Block and antenna parameters output for computational calculation FDTD method. Modeling response returned to the IDL code to create images.	15
Figure 3.1. (a) Overview of Ohio's subsurface structure viewing from Southwest to Northeast with the red dot representing the Warren Co. test case and (b) a close-up of the transition from the Precambrian into the Cambrian on a West to East transect across Ohio (Adapted from Wickstrom et al. 2010 and Wickstrom 2009).	19
Figure 3.2. Stratigraphic section exhibiting Ohio's sequestration potential with reservoirs (blue) and confining units (yellow). (Adapted from Wickstrom et al. 2010).....	21
Figure 3.3. Well log suite at the Warren Co. location exhibiting the major formations as well as the Gamma Ray, Resistivity, Neutron Porosity, Bulk Density, and fraction logs.	22
Figure 3.4. A closer view at the zone of focus that includes the Middle Run Formation, the Mt. Simon Sandstone, and the Eau Claire Formation. The red dots signify core sample locations...	25
Figure 3.5. Conversion chart used for correcting porosity values based on limestone, dolomite, or sandstone matrices (http://www.wellog.com/charts/neutron_porosity.jpg).	26
Figure 3.6. Mercury Porosimeter porosity data compared to the Neutron Log porosity data.	29
Figure 3.7. Core saturation container with (a) brine reservoir, (b) vacuum chamber, and (c) a rock core inside the electrode core holder.	30
Figure 3.8. Outline of the laboratory resistivity measurement system. A LabView based software (a) controls the current source (b) and the voltmeter (c) while making measurements on the rock core (d).	31
Figure 3.9. The graphs consist of the resistivity data from the well log, the rock core resistivity measurements, and the sample locations. The right side of the figure is zoomed in to the transition from the Mt. Simon Sandstone to the Eau Claire Formation where the highest density of samples occurs.	38
Figure 3.10. Brine resistivity data calculated from the well log and laboratory data.	40
Figure 3.11. A logging chart of temperature vs. resistivity of a NaCl solution. Plotting a brine resistivity with a formation temperature provides a value for the NaCl concentration in ppm. The boxes show the range of values that were calculated from resistivity log using the rock core measurements.....	41

Figure 3.12. Plot of the permittivity data that was calculated from the well log information using CRIM.	44
Figure 3.13. This processed and migrated 2D seismic line passes through the well site from West to East (left to right). On the left is the correlated time and depth scale. The borehole, the Eau Claire Formation, and the Mt. Simon Sandstone are indicated on the seismic cross-section (adapted from Shrake et al. 1990).	46
Figure 3.14. Image of the velocity analysis that was performed on the 2D seismic line (adapted from Shrake et al. 1990). Data from the seismic line was used to calculate the velocity, a time-depth conversion, and a seismic synthetic.	47
Figure 3.15. Plot of the P-wave velocity (Vp) and S-wave velocity (Vs) data through the Eau Claire Formation and Mount Simon Sandstone. The Vp data was extracted from the plot in Figure 3.14 and the Vs data was calculated from the Vp data.	48
Figure 4.1. This figure displays plots of the resistivity, permittivity, Vp, Vs, and density data created by the Logphys module in the GphysCO2 software. The Eau Claire Formation, Mt. Simon Sandstone, and Middle Run Formation are displayed on the plots.	50
Figure 4.2. Plots of the conductivity (inverse of resistivity) and permittivity data. The data sets have been separated into distinct layers, through averaging, to simplify the model building.	52
Figure 4.3. Model block depicting electrical property well logs (conductivity in the front and permittivity behind) displayed with the property layers.	53
Figure 4.4. 3-dimensional model of the electrical property data (conductivity, permittivity) from 3100 to 3500 ft. depth range. The zone includes the transitions between the Eau Claire Formation, Mt. Simon Sandstone, and Middle Run Formation.	53
Figure 4.5. 3D model of a CO ₂ injection (designated in red) into the Mount Simon Sandstone..	55
Figure 4.6. Plots of the P-wave velocity, S-wave velocity, and density data. The data sets have been separated into distinct layers, through averaging, to simplify the model building.	56
Figure 4.7. 3-dimensional model of the seismic property data (Vp, Vs, and density) from 3100 to 3500 ft. depth range. The zone includes the transitions between the Eau Claire Formation, Mt. Simon Sandstone, and Middle Run Formation.	57
Figure 5.1. Attenuation versus frequency for conductivity values 0.0001-10 and permittivity values 1-20-50. The plot demonstrates that attenuation is effected by frequency, conductivity, and permittivity (adapted from Daniels et al. 1997).	61
Figure 5.2. Attenuation versus Frequency plot utilizing a permittivity value of 14.68 and a conductivity of 0.18 (S/m). The electrical property values were extracted from the 3D property models.	62
Figure 5.3. Plot of the peak amplitude of received signals versus distance to demonstrate the attenuation of the signals.	63
Figure 5.4. Plots of the permittivity of the top portion of the Mount Simon Sandstone pre-injection (blue) and post-injection (red) of CO ₂	65
Figure 5.5. 3D model of the cross-hole survey extracted from full 3D model. The vertical red rectangle signifies a saturation of CO ₂ . The antennas are simulated in boreholes on opposite sides of the CO ₂ (transmitter, Tx, and receiver, Rx) with the saturation object at the exact center.	66
Figure 5.6. Plot of wavelength versus frequency. The wavelength decreases at higher frequency signals.	68

Figure 5.7. Plot of the 20 m cross-hole simulation. The 'homogeneous' line represents the model results from a homogeneous model where as the 'with CO ₂ ' line is the results after CO ₂ was placed in the model.	69
Figure 5.8. Plot of the 50 m cross-hole simulation. The 'homogeneous' line represents the model results from a homogeneous model where as 'with CO ₂ ' line is the results after CO ₂ was placed in the model.....	69
Figure 5.9. Side-by-side view of the CO ₂ injection model (left) and the numerical results (right). The numerical traces displayed include the 20 meter and 50 meter experiments. The trace coloration represents high amplitude in red and negative amplitude in blue.	70
Figure 5.10. Illustration of the property model sub-block that was used for the seismic simulation.....	72
Figure 5.11. Numerical results from a cross-hole seismic survey. The survey consisted of a single source and multiple receivers in bore-holes separated by 100 meters.	73
Figure 5.12. EM and Seismic trace comparison displayed in a 3D model block. Both traces represent 100 meter model runs.....	74
Figure A.1. Opening Menu.	83
Figure A.2. Attributes Menu.....	84
Figure A.3. Creating the 3D attribute model.	85
Figure A.4. IDL Menu for submitting data to Madagascar.	85
Figure A.5. Python menu for selecting the data files.....	86
Figure A.6. Message appearing in IDL when modeling is completed.....	86
Figure A.7. IDL menu with option to start OpendTect.....	86
Figure A.8. Madagascar plug-in for OpendTect. The user can create a complete processing flow.	87
Figure A.9. 3-dimensional block view and 2D cross-section of a set of seismic lines in OpendTect.....	87
Figure B.1. Top level program menu for GphysCO2. From this menu the EM, Seismic, and well logging modules can be accessed.	92
Figure B.2. A right-hand coordinate system is used in the PFDTD modeling in such a way that the positive x-axis points to the right, the y-axis backwards, and the z-axis upwards.	93
Figure B.3. GPR Visualization window now appears with the menu options on the left for populating the Maxwell block on the right.	94
Figure B.4. Regular 3D bodies menu.....	95
Figure B.5. Sub-grid Block Boundary Menu.....	96
Figure B.6. The Regular 3D Bodies GUI (left) and the main window of IDL Workbench (right) with the GPR Visualization window in the background.....	96
Figure B.7. Window for 3D triangular column objects.	97
Figure B.8. The GUI for setting up multiple models.	98
Figure B.9. The GUI for updating the conductivity of an additional model.	98
Figure B.10. The GUI for a list file of model directories.	99
Figure B.11. The GUI of parameters for importing model output data.	100
Figure B.12. At this window you must select or create a new list file for the program to write to (e.g., C:\GPHYZ data\test.lst). Now click "Save" in the bottom right of the window.	101
Figure B.13. At this window select the file type and the numbers of files you wish to analyze.	101

Figure B.14. Double-click the data files that you would like to use in the window that appears next. The number of files that you select is based on what you specified in the previous window.	102
Figure B.15. After entering the data files the Gphysgpr window will appear on the screen. There are many options available to analyze your data.	102
Figure B.16. Select the “Decimate/Interpolate truncate samples _traces” option in the Gphysgpr window. A Decimate/Interpolate files window will appear. The options are “Apply-List” or “Apply-File”.	103
Figure B.17. A window will appear telling you that there are many overflow values, select “OK”.	103
Figure B.18. Select the “Standardize Line Lengths” option in the Gphysgpr window. A Standard Line Length window will appear. Select the “Apply-List” option.	104
Figure B.19. Select the “Trace Filter and Gain” option in the Gphysgpr window. A window will now appear asking you to select a data file. The files are the ones that have already specified when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file you would like to use.	104
Figure B.20. The results will now appear on the screen. The graph of the data along with graph options appears. The image of the data appears on the bottom right side of the screen.	105
Figure B.21. Select the “Two Dimensional Filter” option in the Gphysgpr window. The 2D Filtering window will appear with six options.	106
Figure B.22. Select the “Smooth horizontal/vertical” option from the 2D Filter window. The Smooth window appears with options to smooth the samples, the traces, or both. An option to select the number of traces or samples to average is also available. Click on the option you would like to use and then select “Apply”. If you choose “Smooth Samples” a window appears warning you that there are many overflow values. Select “OK” to this message. The other options do not have this warning.	106
Figure B.23. Select the “Average Trace Subtract” option from the 2D Filter window. The Trace Subtraction window now appears. This menu has the options of single fixed, multiple fixed and running average. You can select the number of traces for the multiple or running options. There is another option to center the trace for the single or multiple fixed options. Click on the option you would like to use and then select “Apply”. After selecting any of the options a window appears warning you that there are many overflow values. Select “OK” to this message.	107
Figure B.24. Select the “Kirkoff Migration” option from the 2D Filter window. The Kirkoff Migration of 2D files menu will appear. It contains the options “Apply-List” and “Apply-File”. There are also options to select trace spacing, velocity, number of traces for calculation, first sample for migration, and the last sample for migration.	107
Figure B.25. Select the “2D Scan Plot” option from the Gphysgpr menu. A window will now appear asking to select a data file. The files are the ones that have already designated when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file to use.	108
Figure B.26. Three windows will now appear. The window to the right is a one dimensional representation of some of the data. The window to the left has options for altering the plot once it is ready. In the small window in the middle, select “Okay” to continue with the plotting.	109

Figure B.27. The 2D scan of your data now appears in the center of the screen with the options menu still present on the left side of the screen.	110
Figure B.28. Select the “Active Interpretation” option in the Gphysgpr window. The InterActive Interpretation window will now appear. This menu has the options “trace max/min cutoffs”, “pick anomalies”, and “velocity analysis”.	110
Figure B.29. Select the “Trace Max/Min cutoffs” option from the InterActive Interpretation window. An information window will appear telling you that there are many overflow values. Select “OK” to this window. Two windows will now appear. One is the trace of your data and the other is an options window. Select “Okay” in the smaller options window.	111
Figure B.30. The next window that appears contains options for interpreting your data. Click on the option that you would like to use. The “Display 2d result” option produces a two-dimensional image of the data. The “Add a cutoff line” option brings up a new menu.	112
Figure B.31. This menu allows the user to specify the line to insert. It has options for selecting the lower sample number, upper sample number, lower sample cutoff value, and upper sample cutoff value. After selecting the values to use select the “Apply Line” option at the top of the menu to add the specified line to the data trace.	113
Figure B.32. The “delete a cutoff line” option allows the removal of any line that was added to the trace. Once selecting this option a new menu will appear. The slide rule option allows you to select the line segment number to delete. After selecting this line number click “Delete the line segment shown” to implement this action.	113
Figure B.33. Select the “Pick Anomalies” option from the InterActive Interpretation window. Two windows will now appear. One is the trace of the data and the other window is an options window. Select “Okay” in the smaller options window.	114
Figure B.34. A window will now appear and ask to select a data file. The files listed in the window are the ones that have already designated when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file to analyze. A new window will appear with an image on the right and a menu on the left.	115
Figure B.35. Select the “Velocity Analysis” option from the InterActive Interpretation window. Two windows will now appear. One is the trace of the data and the other window is an options window. Select “Okay” in the smaller options window.	116
Figure B.36. A window will now appear and ask to select a data file. The files listed in the window are the ones that have already designated when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file to analyze. The Hyperbolic Velocity Analysis window will now appear. An image of the data appears on the right and the menu is on the left.	117
Figure B.37. Select the “Single Trace Output” option from the Gphysgpr window. The “Select Trace for ASCII output” window appears on the screen. Choose between the two options, “Apply to List” or “Apply to File”. The “Apply to File” option will bring up a window asking to select a specific data file instead of working on the entire list.	117
Figure B.38. Select the “Reverse Polarity on all Traces” option from the Gphysgpr window. Another information window will appear telling the new reverse polarity is complete and to restart GPYZ to activate.	118

Figure B.39. The next window that appears is where you specify your data file type and the number of files to analyze. The file type should be GSSI and choose the number of files to analyze in the slide rule. Once selecting these two options click the “Okay” button.	118
Figure B.40. A window will appear to select your data files. Go to the location of the data using this window and select the files by double-clicking each one. Select the same number of files that were specified in the previous window.	119
Figure B.41. For the next window that appears select “Done” in the top of the window.	119
Figure B.42. Two windows will now appear. One is the trace of your data and the other window is an options window. Select “Okay” in the smaller options window.	120
Figure B.43. In the window that appears next to select or create a file for the output to be sent to. Select the file that to use and click “Save” (e.g. C:\GPHYZ data\gphys output).	121
Figure B.44. Click “Okay” in the top left of the Edit Block window for no changes to the plot.	121
Figure B.45. The results for the data now appears as a three dimensional plot in a GPR visualization window. The image can be rotated for multiple viewing angles by clicking and dragging the mouse on the image. The menu bar on the left hand side allows the user to change the images characteristics such as color, transparency, and opacity.	122
Figure B.46. Staggered-grid where electric and magnetic field vectors are located tangent to the edges and normal to the sides, respectively (modified from Yee, 1966; Holt, 2004).	123

List of Tables

Table 3.1. List of core samples from the Warren Well including depth, formation, lithology, and core size.	24
Table 3.2. Resistivity values for rock core samples located throughout the Mt. Simon Sandstone and the Eau Claire Formation.	32
Table 3.3. List of common substances with the corresponding permittivity values (Knight et al. 1987).	43
Table 4.1. Thickness, conductivity, and permittivity data for layers 1 through 6 as seen in Figure 4.3.	54
Table 4.2. P-wave velocity, S-wave velocity, and density data for layers 1 through 6 of the seismic model.	58

List of Equations

Ohms Law: (1.1)	6
Permittivity: (1.2)	7
Loss Tangent: (1.3)	7
Shale Volume from Gamma Log: (3.1)	26
Neutron Log Porosity Correction for Shale: (3.2)	27
Resistivity Calculation: (3.3)	32
Archie's Law: (3.4)	33
Formation Factor: (3.5)	33
Resistivity Index: (3.6)	33
Water Saturation: (3.7)	33
Relationship between density, porosity and water saturation: (3.8)	34
Where clays are present, the resistivity can be expressed as: (3.9)	34
Waxman-Smits: (3.10)	34
Modified Waxman-Smits: (3.11)	35
Lithostatic Pressure: (3.12)	35
Arp's Formula: (3.13)	36
Permittivity by volume: (3.14)	42
Complex Refractive Index Method (CRIM): (3.15)	42
Propagation Constant: 5.1	60
Attenuation Constant: 5.2	60
Phase Constant: 5.3	60
Wavelength: 5.4	67
1-D Scalar Wave Equation: (A.1)	88
3-D scalar wave equation: (A.2)	88
Compression Wave Phase Velocity: (A.3)	88
Shear Wave Phase Velocity: (A.4)	88
Vector Wave Equation (general form): (A.5)	88
Vector Wave Equation (component form): (A.6)	88
Wave Number: (A.7)	89
Bulk Modulus: (A.8)	89
Shear Modulus: (A.9)	89
Poisson's Ratio: (A.10)	89
Young's Modulus: (A.11)	89
Stress, strain, and Elastic modulus: (A.12)	90
Isotropy matrix: (A.13)	90
Transverse isotropy matrix: (A.14)	90
Lame's parameters: (A.15)	91
Maxwell's curl relations: (B.1)	123
Faraday's and Ampere's Law in rectangular coordinates (Holt, 2004): (B.2)	124
The central difference approximation: (B.3)	124
FDTD calculation: (B.4)	124

Isotropic medium: (B.5)	125
The second curl equation is given by: (B.6).....	125
Updated curl equation with scaled electric field: (B.7).....	126
Discretized equations: (B.8).....	126
Electric field updated with the magnetic field equation: (B.9)	126

Chapter 1: Introduction

1.1 Carbon Sequestration

Recent research has raised concerns about the role that greenhouse gas (GHG) plays in global climate change. Greenhouse gas that collects in the Earth's atmosphere can cause a greenhouse effect, warming the earth. Carbon Dioxide (CO₂) has been identified as a major contributor to the levels of GHG in the atmosphere and although CO₂ is naturally occurring humans have astronomically increased CO₂ emissions through energy production and transportation. In the now carbon conscious world, carbon sequestration methods are being developed to decrease the amount of CO₂ that is being emitted into the atmosphere. Carbon sequestration is a collective term that includes storing CO₂ in the ocean, terrestrial environments (vegetation, sediments), and in geological formations. All of the carbon sequestration methods require advancements to attain full scale implementation. This project focuses on advancing the science of geological carbon sequestration.

Geological sequestration is the act of injecting CO₂ into subsurface geological formations for long term storage and disposal. The primary sequestration targets are deep saline aquifers, un-mineable coal seams, and hydrocarbon reservoirs. CO₂ can be sequestered in hydrocarbon reservoirs through a process called enhanced oil recovery wherein the injected CO₂ pushes unproduced hydrocarbons to a production well. Coal seams that are located deep in the subsurface and beyond feasible mining methods can also serve as carbon storage zones. The final subsurface targets, deep saline aquifers, are un-useable as a drinking water source and provide ample storage space by replacing the saline water with CO₂.

Numerous concerns abound in the successful implementation of geological sequestration. First and foremost is the task of efficiently capturing CO₂ at the emission source (e.g. coal fired power plant). Next is the selection of an injection site that is within close proximity to the emission source and can safely contain the injected CO₂. Following that, is implementing policy and regulation for a continuous safe injection operation. Finally, monitoring the CO₂ after it has been injected is a major concern. Operators are responsible for the injection site many decades after injection and must ensure that the CO₂ does not leak into overlying formations. The upward leakage of CO₂ can adversely affect drinking water aquifers.

The necessity to monitor and account for the injected CO₂ requires an array of monitoring methods that include many branches of subsurface science. There are many proven and state of the art methods being employed for monitoring CO₂ injection projects including: monitoring the cement bonded walls of the injection well for pathways, analyzing CO₂ levels at the surface, monitoring overlying drinking water aquifers for increasing CO₂ levels, and monitoring surrounding wells for increased CO₂. All of these methods involve geochemistry but also include another proven method for analyzing changes in the subsurface, geophysics. Geophysical methods are a non-invasive means of imaging the subsurface, enabling the ability to track the movement of injected CO₂.

1.2 Geophysics and Carbon Sequestration

Geophysical methods are emerging as useful techniques in the expanding field of geological sequestration. The process of sequestering carbon dioxide in the subsurface requires vigorous site characterization and monitoring. CO₂ injection test sites have been appearing around the world and serve as great examples of how geophysical methods can be implemented as useful monitoring tools.

Geophysical methods have been used for decades in mining, petroleum, and engineering applications to investigate objects in the subsurface. The primary role of geophysical methods is to detect and image objects in the subsurface, a role that is very applicable to monitoring a CO₂ injection site. Geophysical investigations cover a wide range of methods implemented with a variety of survey techniques. The techniques are dependent upon the information sought after and the subsurface properties. The geophysical surveys can be completed from the surface, borehole, and cross-borehole configurations. The resultant geophysical data ranges from line graphs collected with borehole wireline tools to 3-dimensional images created by electromagnetic (EM) and seismic surveys.

Test sites for geological sequestration injection projects are spread across the world and each has implemented a specific geophysical monitoring method. Example injection sites include the American Electric Power (AEP) Mountaineer facility in New Haven, West Virginia, the Sleipner project located in the North Sea off the coast of Norway, and the Frio project in Dayton, Texas. Each of the pilot projects used variations of seismic and borehole geophysical methods when selecting, characterizing, and monitoring the injection site.

The Mountaineer project conducted a two line, 2-dimensional surface seismic survey to identify formation horizons and structure. A borehole was then drilled and wire-line data was collected. The logs included gamma ray, density, neutron porosity, electrical resistivity, caliper, monopole sonic, gamma ray spectroscopy for mineralogy, nuclear magnetic resonance for permeability, and electrical borehole images to identify fractures. These tests were completed to gain knowledge about geology, mechanical properties, mineralogy, permeability, saturation, salinity, and fracturing. Rock cores were taken and used for numerous experiments including porosity, permeability, density, petrography, velocity, and CO₂ tests. Reservoir testing was also conducted within the borehole to investigate transmissivity, pressure, and hydraulic response (Gupta et al. 2005).

The Sleipner project, located in a productive hydrocarbon region of the North Sea, completed a site characterization similar to the Mountaineer investigation except a 3-dimensional surface seismic survey was utilized instead of 2-dimensional lines. The characterization at the site progressed into using geophysics to monitor the injected CO₂. A baseline 3D seismic survey was acquired before the injection and was repeated three more times post-injection to create a 4D data set (addition of time). The 4D data set, otherwise known as time-lapse seismic, was the main method of monitoring and verifying the CO₂ plume. This technique allowed the operators to successfully image where the CO₂ was at the time of each survey. After seismic processing, the CO₂-saturated rocks produced bright reflections with a noticeable velocity pushdown.

Seismic waves moved through the CO₂ saturated reservoir slower than through the original aquifer. Seismic modeling, inversion modeling and forward modeling, was coupled with the 4D seismic data. The forward modeling method used history matched reservoir simulations to replicate the observed data. Inversion gave the ability to quantify the amount of CO₂ by pulling attributes from the seismic anomalies. Although this method was very successful for this project the effectiveness greatly depends on the geological system. High porosity units with small but thick plumes of CO₂ are more detectable to seismic. Detection becomes less effective if the accumulations are in low permeable units with fault leakage (Chadwick et al. 2006). An EM investigation at the Sleipner site was researched by Norman et al. (2008), who constructed a resistivity model from seismic data and Archie's law. The time-lapse responses for the 2001 and 2006 plumes at Sleipner versus the case without CO₂ indicated peak anomalies of 25% and 50% at 3 km offsets respectively.

The Frio project completed a site characterization and continued recording measurements post-injection to monitor and verify the plume of supercritical CO₂ in a brine aquifer. The geophysical methods that were utilized included time-lapse vertical seismic profiling (VSP), cross-well seismic topography, and saturation logs. The saturation logs are from a wire-line reservoir saturation tool (Schlumberger RST) that measures the change in brine saturation as it is affected by the injected CO₂. Conducting the log test numerous times during the injection effectively monitored when the CO₂ plume reached observation wells. The RST log also produced information on which units were CO₂ saturated hence the thickness of the plume at that location. Cross-well seismic surveys and vertical seismic profiling were conducted in the boreholes to attempt to monitor the plume. From these seismic methods the project members hoped to gain information about the plume geometry by recording across multiple azimuths. The comparison of pre- and post-injection measurements from the cross-well seismic showed a strong decrease in velocity. The velocity differences helped to discern where the injected CO₂ was moving. Vertical seismic profile tests were completed in surrounding wells and the results showed an increase in signal amplitude. The amplitude change meant that the VSP detected the plume but estimating the plume edge was not very accurate (Hovorka et al. 2006).

1.3 Geophysical Properties

Many methods are available for characterizing and monitoring carbon sequestration sites, as seen in the previous section. Beyond wireline methods the two most common imaging methods that can be implemented in a sequestration monitoring program are seismic and electromagnetic (induction and ground penetrating radar). Seismic and electromagnetic methods play a crucial role in imaging and monitoring the subsurface. Throughout history seismic has been the primary tool to image beyond the shallow subsurface. Although seismic techniques have been the most popular, electromagnetic methods are gaining interest.

EM methods have thus far been inhibited by the fact that they are a shallow penetration technique that ranges from less than 1 m to 100 m depending on the signal frequency and the properties of the test medium (Reitz, et al. 1992). The advancement of borehole technology has allowed deep formations to now be imaged with EM surveys. EM is also becoming more

popular because of how electrical methods image the subsurface. The seismic technique utilizes an active noise source to send compression and shear waves through the medium where changes in the elastic and density properties of the rock reflect the waves back to the receiver. EM methods send electromagnetic waves that are more sensitive to the pore fluids than the actual rock, at low frequencies, because the fluids are more electrically conductive. Therefore, the replacement of pore fluids with CO₂ can create a noticeable electrical anomaly over time. Both EM and seismic methods provide a direct pseudo image of the subsurface (e.g., travel time based measurements). The images provide cross sectional images that can be combined into a 3D block view of the subsurface.

1.3.1 Electromagnetic Geophysics

Electromagnetic geophysical methods encompass a large variety of techniques that are each tailored to a specific survey goal (e.g. imaging or plotting). The techniques are also dependent upon the survey environment (e.g. ice, soil, rock formations). Electrical geophysics can be separated into three types, each based on the transmission source (frequency); electrical conduction, electromagnetic induction, and electromagnetic wave propagation. All of these types have been employed to study the fluid properties of rock formations.

Electrical conduction techniques utilize sources in the range from DC to low frequency and are based on the conduction of electrons through a medium. The primary property measured is the resistivity (the inverse of conductivity) and is detailed in the proceeding section. Specific techniques include surface resistivity, wire-line resistivity, and Electrical Resistivity Tomography (ERT).

The other important EM property, the electrical permittivity becomes crucial when considering the third type of electrical geophysics, electromagnetic wave propagation imaging. EM wave propagation is attained by increasing the signal frequency (above the frequency ranges of conduction and induction techniques) through specialized antennas. As the frequency of the electrical signal increases, the primary electrical property switches from conduction (resistivity) to the permittivity. At higher frequencies the signal becomes an electromagnetic wave that is primarily influenced by the dielectric properties of the medium. The permittivity and dielectric terms are both used in this discussion. The terms are used interchangeably in numerous research papers because the dielectric constant equals the relative permittivity and the permittivity parameter refers to the dielectric properties of a material. Permittivity will be the primary term utilized because it is used most commonly used when discussing EM wave propagation. Ground Penetrating Radar (GPR) is an example of an EM wave propagation technique.

GPR is a noninvasive geophysical method that utilizes electromagnetic waves to image the subsurface. Electromagnetic imaging includes broadband propagation in the upper GPR frequency range and extends to frequencies as low as 1 MHz. GPR has primarily been used to image the shallow subsurface (~10m) for a variety of buried object applications (e.g. archeology). One of the primary objectives of this project is applying the GPR technique to a borehole environment for CO₂ monitoring. The key concerns with this application are the

penetration distance, the ability to detect changes that occur as CO₂ is injected, and the availability of electrical permittivity data. Data availability is an issue because minimal research has been undertaken to research how the dielectric properties change with differing reservoir conditions. The majority of EM studies have been focused on monitoring geological sequestration with resistivity techniques (Christensen et al. 2006 and Hagrey 2010) wherein dielectric properties are not a major contributing factor.

In summary, more research has been conducted on resistivity than electrical permittivity mainly due to the shallow penetration distance of EM imaging. A high frequency signal produces a high resolution image that is very dependent on the dielectric properties of the medium but results in small penetration distance. A low frequency signal becomes more sensitive to the resistivity of the medium with superior penetration but produces a lower resolution image. Section 1.3.1.1 discusses the details of resistivity. As stated above, resistivity is the inverse of conductivity. Both properties are utilized in this project because well log data is based on resistivity measurements, rock core measurements utilize resistivity techniques, and EM wave propagation modeling uses conductivity data. Section 1.3.1.2 details the electrical permittivity (dielectric) property.

1.3.1.1 Resistivity

Resistivity is a geophysical property that is measured with borehole tools, surface surveys, and rock core measurements. The measurement method depends on the scale and environment one is investigating. The information that can be gained from resistivity measurements includes details about pore fluid, porosity, saturation, and lithology. G.E. Archie pioneered the relationship between resistivity measurements and rock properties by developing Archie's Law (Equation Archie's Law: (3.4), but understanding Archie's law requires an overview of how resistivity is measured.

As discussed previously, there are numerous techniques for measuring resistivity but this research utilizes resistivity measurements from rock core and resistivity well logs so this discussion will be focused on those techniques. The laboratory and bore-hole measurements are used in conjunction because core sample measurements conducted in a laboratory, with known parameters, can be applied to the associated resistivity well log enabling more information to be extracted from the well log data. Resistivity measurement techniques vary in apparatus type, scale, and electrical source but all are similar in the fact that they require the passing of electricity through a medium and measuring the electrical changes over a specific area. This discussion will begin with an overview of laboratory measurements and will be followed by the application of the laboratory data to the well log data.

The two most common laboratory methods for measuring rock core resistivity are the 2- and 4-electrode techniques. The 2-electrode technique involves attaching two ring or pad electrodes to the sample, passing a current through the electrodes, and then measuring the voltage drop between the electrodes. After the voltage difference is recorded, the sourced current and Ohm's Law (Equation Ohm's Law: (1.1) is used to calculate the resistance of the medium. To find the resistivity, the resistance must be multiplied by a geometric factor that is dependent upon the

sample size and shape, as well as the electrode spacing. Although 2- and 4-electrode techniques measure the same value the later has some benefits. The outer two electrodes source current and the inner two electrodes measure the voltage (Figure 3.8.d), whereas the 2-electrode method sources current and measures the voltage on the same electrodes. Utilizing 4 electrodes eliminates the lead and contact resistance that occurs when using only two electrodes.

Ohms Law:

(1.1)

$$V = \frac{I}{R}$$

V = voltage

I = current

R = resistance

Resistivity is a useful geophysical property for investigating rock formations based on how electricity interacts with the rock. The fundamental understanding of electricity is that it will take the path of least resistance. In metallic materials the flow of electricity is, in actuality, the flow of electrons within the material. When considering a rock, the path of least electrical resistance is through the contained fluids and not the actual rock matrix. Therefore, current flows through the fluid due to the flow of ions. In brine saturated rocks the ions are mostly sodium (Na^+) and chloride (Cl^-). This means that when electricity is induced on a non-metallic rock, the current will flow through the pore fluid and provide information about the pore fluid and porosity. Therefore, a simplified relationship is as follows: an unsaturated minimally porous rock will produce a very high resistivity while a very porous saturated rock produces a very low resistivity. Resistivity values for Earth materials can vary over several orders of magnitudes due to factors that include fluid properties, porosity, pore structure, mineral content, clay content, and cementation (Figure 1.1). This investigation exclusively deals with rocks found in Ohio's subsurface so the focus will be on sedimentary rocks and the factors associated with those rocks that affect resistivity.

Figure 1.1. Typical Ranges of Resistivity Values for Earth Materials (Adapted from Palacky, 1987).

1.3.1.2 Electrical Permittivity

Permittivity is the other major electrical property that represents how a material will interact with an electric field. As discussed previously, the resistivity is dependent upon the flow of ions through a medium. The permittivity (Equation Permittivity: (1.2) depends upon the polarization of the medium, essentially how the charges within a material can be polarized by an electric field. This real part of the parameter is a measure of the amount of electrical energy stored in the material from an external field and the imaginary part is the loss factor (a measure of how lossy a material is when subjected to an external electric field). The loss factor is influenced by dielectric loss and the conductivity (inverse of the resistivity). The loss tangent describes the relative “lossiness” of a material.

Permittivity: (1.2)

$$\epsilon_r^* = \frac{\epsilon^*}{\epsilon_0} = \epsilon_r' - j\epsilon_r'' = \left(\frac{\epsilon'}{\epsilon_0} \right) - j \left(\frac{\epsilon''}{\epsilon_0} \right)$$

ϵ_r^* = Complex relative permittivity

ϵ^* = Permittivity

ϵ_0 = Permittivity of free space

Loss Tangent: (1.3)

$$\tan(\delta) = \frac{\epsilon_r''}{\epsilon_r'}$$

Figure 1.2. The permittivity consists of the vector sum of the real and imaginary parts. The tangent of the resulting angle is the loss tangent.

Obtaining the permittivity of a porous rock presents multiple difficulties. In the electrical engineering world a dielectric media is usually assumed to be uniform throughout but subsurface rock formations are rarely uniform. Even clean sandstone has a varied mineralogical make-up, porosity throughout the matrix, and the complexities that arise when analyzing a clay rich rock. There are two techniques for obtaining the permittivity of rock, a laboratory approach and a numerical approach (both methods are discussed next).

Measuring the dielectric of a material in the laboratory is a complex procedure that adapts techniques that were originally designed for testing electrical components. The most common method that has been adapted to measuring the dielectric of rock samples is the Time-Domain Reflectometry (TDR) technique described by Nguyen et al. (1999). A TDR device that is adapted for measuring the dielectric of a rock sample consists of a signal generator, a sampler, and an oscilloscope. The signal generator launches the EM wave into the cable, the sampler contains the rock sample, and the oscilloscope monitors the transmitted wave.

The basic principle of the TDR technique is based on the behavior of an EM wave that is launched through a coaxial cable. Essentially, any change in the electrical and dielectric properties along the cable will cause a partial or total reflection of the wave. The electrical property change that may occur within the cable causes a change in the impedance. The properties of the impedance change are directly related to the dielectric change that occurred along the cable. The sampler portion of the coaxial transmission line enables the rock sample to be part of the coaxial line. Therefore, the transmitted EM wave is influenced by the change in the impedance that the rock causes and the dielectric of the rock can be measured.

The laboratory technique for measuring the dielectric of rock samples is a topic worthy of its own research project. Measurements require specialty equipment and experience that were not feasible for this project. Therefore, the research in this work utilizes a numerical approach based

on The Complex Refractive Index Method (CRIM). The CRIM method is discussed in detail in section 3.7.1.

1.3.2 Seismic Geophysics

Seismic methods are extremely useful tools that dominate subsurface imaging in the exploration industry. Seismic is the industry standard for subsurface exploration and, as exhibited in the previous discussion of geophysical applications in carbon sequestration, has become a standard in geological sequestration projects. This project focuses heavily on EM monitoring but, as stated, seismic is the premier method against which experimental techniques should be compared.

The basis for seismic geophysical methods is the propagation of mechanical waves through the subsurface. The seismic waves are emitted utilizing detonation or vibration sources. Once the wave enters the subsurface, the rock formations have specific properties that determine how the seismic wave will propagate through it. In a general sense, materials have mechanical (elasticity, stress, strain) and geophysical (velocity, density) properties. The geophysical properties are measurable properties whose magnitude and directional variation is determined by the mechanical properties of the rock. Appendix A.2 discusses the relationships between the fundamental mechanical properties of the rocks and the geophysical properties (velocity and density).

The first step of the seismic process is propagating the wave through the subsurface and the second step is recording the seismic wave after it has interacted with the subsurface utilizing an array of sensors (geophones). Seismic wave propagation occurs in the subsurface as body waves. Body waves include Primary waves (P-waves) that propagate in a compression longitudinal motion and Secondary waves (S-waves) that propagate in a shearing transverse motion. The other differences between the two waves are P-waves travel at a faster velocity and S-waves cannot travel through fluid. The waves that are received by the geophones include direct (wave travel directly from the source to the receiver), reflection (wave reflects off of subsurface targets), and refraction (waves strike a plane at a critical angle, causing the wave to travel along that plane for a certain distance before continuing to the receiver) waves. The geophones record these waveforms and information pertaining to the properties of the subsurface can be gained from the collected data.

Seismic surveys can be conducted from the borehole (cross-hole tomography, single-hole vertical seismic profiling) and surface (terrestrial, marine). Borehole surveys provide a 2-dimensional cross-sectional image of the subsurface by sending waves between wells (cross-hole) and between the surface and borehole (VSP). Surface surveys place geophones along the surface and transmit waves from multiple locations to create images of the subsurface. Depending on the geophone arrays, data can be collected as 2-dimensional lines (surface distance in a single direction versus time), 3-dimensional (surface distance in x direction and y direction versus time), and 4-dimensional (multiple 3D surveys are completed over a period of time).

1.4 Necessity for a New Geophysical Tool

Technology is a crucial part of monitoring, verifying, and accounting (MVA) of CO₂ sequestered in the subsurface, specifically technology applied to geophysical methods. Geophysical methods, originally developed for other functions, need to be adapted and specialized to monitor the effects of CO₂ injection. The value and impact is that geophysical methods are the only means to evaluate the site geology and hydrology, non-invasively away from drill holes. Geophysics may be able to monitor and detect potential changes caused by the injection of CO₂, including the structural integrity of the reservoir, the structural integrity of the confining caprock, and the migration of the injected CO₂.

Seismic methods, as discussed previously, have wide-spread implementation in the hydrocarbon industry and are proving adequate in the role of a carbon monitoring method. The application of EM imaging methods to monitoring CO₂ injection is at a very early stage and is still mostly at the laboratory phase. The sole application of EM methods lacks the superior penetration distance that seismic methods provide but does contribute the benefits of using the electrical properties. A combination EM-seismic imaging survey technique may prove to be an ideal method that utilizes the mechanical and electrical properties of an injection site to image the movement of injected CO₂. The seismic method is sensitive to the rock matrix where as the EM method is more sensitive to the pore fluid (brine and CO₂).

Adapting geophysical methods for geological carbon sequestration monitoring while in the field can be a costly and time intensive endeavor. Trial and error may yield results but to the detriment of time and finances. An alternative that can decrease the time and cost is to numerically calculate a geophysical forward model for a potential injection site before full-scale field implementation. Executing a forward model pre-injection enables the user to test numerous methods and obtain the best geophysical technique for a specific geological system.

The modeling process requires a software program that can input geophysical data sets, create 3D property models, and realistically forward model geophysical surveys (EM and Seismic). There are multiple software suites available commercially that contain programs for geophysical data interpretation and modeling. Some of the major software packages include LandMark Promax® (<http://www.halliburton.com/ps/>), Petrel® (<http://www.slb.com/services/software/geo/petrel.aspx>), and SMT Kingdom Suite® (<http://www.seismicmicro.com/>). These programs are extremely useful but each has issues when applying them to a geological sequestration task. The major downside is the lack of an EM imaging module in each of the major software suites. The other issues with the software packages is that they were all designed for the oil exploration industry with a heavy focus on seismic methods, reservoir modeling, and risk assessment among many other oil specific applications.

Commercially available software programs do not adequately fulfill all of the requirements for analyzing and modeling a CO₂ injection site. A new software program is needed to fill the void between commercial software and the software that is needed for carbon sequestration. The focus of this project is the development and implementation of a software program (GphysCO2)

that can be effectively utilized for studying geological sequestration sites. GphysCO2 is a suite of programs that encompass well logging, seismic, and electromagnetic methods (Figure 2.1). The primary objective of the program was to develop a graphical user interface to enable users to design and execute 3D surface-to-surface (conventional surface seismic) and borehole-to-borehole (cross-hole seismic and EM) modes of imaging. GphysCO2 is designed for the implementation of a numerical, physical, and geophysical property investigation approach that ascertains the suitability of geophysical surveying at potential carbon sequestration injection sites.

Chapter 2: GphysCO2 Software

2.1 Software Introduction

The GphysCO2 software consists of interconnected programs that encompass well logging, seismic, and electromagnetic methods. The software enables users to design and execute 3D surface-to-surface (conventional surface seismic) and borehole-to-borehole (cross-hole seismic and electromagnetic methods) surveys through numerical models. The generalized flow of the program (Figure 2.1) begins with building a complex 3D subsurface geological model, assigning properties to the models to mimic a potential site that has been affected by a CO₂ injection, numerically forward model a geophysical survey, and analyze the results.

Figure 2.1. Software outline for the GphysCO2 program. The top control program interfaces between the data input, forward modeling (seismic & EM), and display/interpretation in a fully integrated network.

GphysCO2 was developed in the Interactive Data Language (IDL version 8.2, Exelis Visual Information Solutions, Boulder, Colorado, www.exelisvis.com/idl/) environment. The IDL graphical user interface (GUI) serves as the main infrastructure and interfaces with other programs (written in the C++ and Python languages). The top level IDL program acts as the interface to the other components of the GphysCO2 program. Figure 2.2 is an image of the opening software menu with options to enter the well logging, seismic, and EM modules.

Figure 2.2. Top level program menu for GphysCO2. From this menu the EM, Seismic, and well logging modules can be accessed.

The primary objective that shaped the development of the GphysCO2 software was to provide a robust and flexible tool for modeling, imaging, and analyzing geophysical data. The secondary objectives included:

- The determination of detection limits of geophysical imaging techniques at a CO₂ injection well on a site-by-site basis through numerical forward modeling.
- The utilization of numerical modeling as a means for determining the optimum number and spatial distribution of boreholes for tracking injected CO₂.
- Exploring the possibility of implementing EM imaging as an effective imaging method for monitoring injected CO₂.
- Combining EM and seismic imaging techniques to gain more information than a single method could provide.

2.2 Seismic Software

The seismic component of the GphysCO2 software consists of data input, the building of property models, forward modeling, processing, imaging, and interpretation. The seismic module code was developed with an interface written in the IDL language that links multiple external open-source programs with in-house code (Figure 2.3). The three major components of the module are the IDL GUI, Madagascar (Madagascar software, version 1.4, <http://www.ahay.org/>), and OpendTect (OpendTect software version 4.1, dGB Earth Sciences, <http://www.opendtect.org/>). The IDL GUI builds the attribute models, the Madagascar suite is an external program that executes numerical models, and OpendTect is an external program that provides the processing, imaging, and interpretation capabilities. A brief description of the seismic program follows but a step-by-step look at the module starting with the IDL Interface and culminating with the OpendTect program is located in Appendix A.1.

Figure 2.3. This software outline of the seismic module shows the interfacing between IDL, Madagascar, and OpendTect.

The IDL GUI has the capability to build completely customizable 3D seismic attribute models. Velocity (P- & S-wave) and density values can be assigned to various layers and objects (cylinders, ellipsoids, pyramids, and spheres). The block size, grid cell size, modeling time, source/receiver locations, and source frequency is also chosen. The module automatically submits the attribute model to Madagascar for numerical calculations. Madagascar is a software package designed for data processing and numerical experiments consisting of over 300 programs written in C and C++. The final component of the module inputs the simulated seismic data from the numerical code into OpendTect, an open-source processing, imaging, interpretation, and analysis program.

A large portion of the Madagascar programs were developed for seismic geophysics. Seismic tools include model building, forward modeling, and processing. A unique aspect of Madagascar is its ability to interface with other programs. Script files written in the Python programming language execute a preordained series of programs. Available conversion tools allow data from IDL codes to be input into Madagascar codes. The package is an open-source program that is continuously reviewed and improved by a very active community. Many prominent research groups such as the Stanford Exploration Project, Jackson School of Geosciences, and Center for Wave Phenomena utilize Madagascar for research.

The numerical modeling component utilizes the Madagascar modeling code 'ewefd3d' (Dr. Paul Sava, Colorado School of Mines, Madagascar Development Team, <http://www.reproducibility.org/RSF/sfewefd3d.html>). The code uses an elastic finite difference time-domain (FDTD) forward modeling method. The robust code accepts the attribute model created with the IDL interface as input and outputs a seismogram in 2- or 3-dimensions. The

seismogram output is calculated with the seismic wave equation applied to elastic anisotropy. A discussion of the theory implemented in the numerical code is located in Appendix A.3.

The seismogram data that is output from the Madagascar numerical calculation is raw 3-component data that needs to be processed and imaged. This step is accomplished with the OpendText component of the seismic module. OpendText is an open-source seismic program that is very beneficial, not only because it is open-source but it also contains a plug-in for the implemented Madagascar suite. The plug-in allows the user to utilize Madagascar's pre- and post-stack processing routines through a GUI. After the processing is completed, OpendText has the capability to display the segy files for interpretation.

2.3 EM Software

The EM module utilizes an IDL GUI as the command program. This interface includes the ability to build attribute models, submit attribute models for numerical forward modeling, process data, display data, and interpret data. The program flow is outlined in Figure 2.4. A basic overview of the EM module follows but a more detailed discussion of the module's components is located in Appendix B: EM Module.1.

Figure 2.4. Model sub-blocks assigned a specified size, shape, cell size, conductivity, permittivity, randomization, and magnetic permeability. Antennas placed at varying locations

with an assigned broadband frequency. Block and antenna parameters output for computational calculation FDTD method. Modeling response returned to the IDL code to create images.

The IDL interface provides the user with numerous options for creating a realistic 3D model of the subsurface and associated antennas. This part of the modeling is shown in the first two steps of Figure 2.4. The following is an outline of steps involved in creating a completely customizable 3D electromagnetic attribute model:

- Assign electrical properties (conductivity, permittivity, and magnetic permeability) to various layers and objects (cylinders, ellipsoids, pyramids, and spheres).
- Assign block size, grid cell size, and modeling time.
- Designate source and receiver locations.
- Design antenna properties (phase and frequency).

The above sequence defines the overall model block but sub-blocks are an important part of the model. By creating numerous sub-blocks with differing properties a complex subsurface environment and antenna system can be modeled. Random noise consisting of a varying standard deviation to a mean is implemented to more accurately represent a heterogeneous subsurface. Another available feature is the ability to submit multiple runs, varying different parameters for each run (e.g. assigning different background property values). This capability easily enables the comparison of the model response for a block with varying physical and antenna properties. The same structure can be retained while parameters are altered to define the limits of the designed antenna.

Once the model is fully defined in terms of the background properties, antenna, and targets (sub-blocks) the parameter files are output for numerical modeling. The numerical modeling code utilized in this software module was designed at The Ohio State University Electrical Science Laboratory. The finite difference time domain (FDTD) method was implemented through single- and multi-processor systems leading to the name, parallel finite difference time domain (PFDTD). The FDTD method is a robust computational technique useful for modeling electromagnetic processes. A detailed review of the modeling theory utilized in the PFDTD code is located in Appendix B: EM Module.2.

The user can implement sub-gridding into certain parts of the model allowing increased detail for modeling antenna designs and subsurface targets without the computationally intensive approach of fine-gridding the entire model. The PFDTD code is able to model antennas with input pulses from 500 kHz to 2GHz. The attribute model parameters include a wide range of conductivity (0.001-10) and permittivity (1-80) values. The models can also introduce random stochastic heterogeneity background noise to represent realistic subsurface environments.

After the PFDTD code completes the modeling computation the output is then returned to the IDL interface for the final step of visualization and interpretation. The IDL program can display the outputted model data as plots, 2D scans, and 3D images. The interface is unique because

model data and field data can be input into the same program. This feature is very useful for the comparison between real and modeled data. The interactive software contains a suite of processing tools as well as display options. The data can be processed through filtering, with the ultimate goal of inversion. The display options are also paramount in interpreting both model data and raw field data. Analyzing 3D data involves 4-C (3 spatial dimensions and color) interpretation.

2.4 Well Logging Software

The logging module, LOGphys, integrates geophysical, geochemical, and geologic well logs into the software package. Well logs gathered from wire-line borehole surveys are a critical component to any geophysical survey and were a necessity for the GphysCO2 software. Well logs provide a wealth of information including; formation identification, formation depths, physical properties (e.g. porosity, density), and geophysical properties (e.g. resistivity, sonic velocity). The primary purpose for the logging module is to provide field data input for designing the geophysical models.

The components of the logging system include:

- Log input in LAS standard format.
- Log plotting of geophysical well log traces.
- Multi-log and multi trace input and handling.
- Plotting logs within the 3D model blocks to improve the design of Seismic and EM forward models.

Chapter 3: Testing and Verification

3.1 Introduction

GphysCO₂, as with any newly developed software program, requires a large amount of testing before it is considered a validated tool. A potential CO₂ injection site was required in order to validate all of the GphysCO₂ modules. A robust implementation of the entire software suite was completed by utilizing data collected from a potential injection site and experimenting with geophysical modeling. Selecting a potential site was largely dependent upon the available data sets that were provided by the Ohio Department of Natural Resources Division of Geological Survey. The data sets, including well logs, seismic data, geological interpretations, and core samples, were collected from various locations across Ohio. The test site, located in Warren County, Ohio, was selected for this research based on the quality and quantity of data, as well as the location.

The following list describes the primary objectives that designed to ensure a complete implementation of the software:

- 1) Test a software technique that utilizes well logs, laboratory measurements, field data, and forward modeling for determining the effectiveness of a geophysical survey at a test site.
- 2) Conduct a geological and geophysical analysis of well log information (lithology interpretation, formation identification, well log calculations, well log corrections).
- 3) Conduct physical property measurements (porosity) on rock core samples.
- 4) Make resistivity measurements on rock core samples.
- 5) Calculate permittivity values for the core samples.
- 6) Collect and input seismic data.
- 7) Utilize the GphysCO₂ software by inputting the available data, executing EM forward models, executing seismic forward models, processing the data outputs, and producing images.
- 8) Analyze the modeling results to determine the effectiveness and limits of a geophysical survey at the test location.
- 9) Validate the GphysCO₂ software.

3.2 Regional Geology

Ohio's deep formations are currently being investigated for potential geological carbon sequestration. Ohio has a long history in the petroleum industry as well as waste injection. Numerous deep saline formations that have been used for production and injection before are now being considered for CO₂ injection. The Mountaineer power plant, a CO₂ capture and injection pilot site discussed in section 1.2, investigated the possibility of a successful injection into these formations.

A successful carbon sequestration industry in Ohio depends on numerous factors including capture, transport, policy, regulation, site selection, and monitoring. This research focuses on two topics; (1) potential reservoirs and confining units must be studied for their injection and

sealing potential and (2) efficient methods for post-injection monitoring must be developed.

There are multiple factors to consider when selecting a site for geological sequestration. Among those factors are the proximity to a CO₂ source (e.g. coal-fired power plant), transportation (e.g. pipeline, trucking), land availability (injection requires mineral rights across a large acreage), and possibly the most crucial component, the geological suitability. Ascertaining the geological suitability of a potential site for injection requires a complete geological characterization. The primary goal of that investigation is to identify possible injection reservoirs with overlying confining layers (cap-rocks) that prohibit upward migration.

The geological characterization process begins at a regional scale (the state of Ohio) and narrows down to the micro scale (pore space and mineralogy). At the regional scale Ohio's subsurface structure is shaped by structural arches and basins. The western half of the state consists of two major structural arches; the Cincinnati Arch in the South and the Findlay Arch in the North. The northern flank of the Findlay Arch dips into the Michigan Basin and the eastern flanks of both arches dip into the Appalachian basin (Figure 3.1.a). The Precambrian crystalline basement rock includes the Greenville Complex to the East and a Granite-Rhyolite Complex overlain by the Middle Run Formation in the western section of Ohio. The basement structure dominates the structure of the overlying sedimentary rocks that thicken towards the basins (Figure 3.1.b).

Figure 3.1. (a) Overview of Ohio's subsurface structure viewing from Southwest to Northeast with the red dot representing the Warren Co. test case and (b) a close-up of the transition from the Precambrian into the Cambrian on a West to East transect across Ohio (Adapted from Wickstrom et al. 2010 and Wickstrom 2009).

A survey was completed by the Midwest Regional Carbon Sequestration Partnership (MRCSP) to characterize potential formations for geologic sequestration. The MRCSP covers an interstate region that includes Michigan, Indiana, Ohio, Pennsylvania, West Virginia, and Kentucky. The investigation into Ohio's subsurface revealed that the stratigraphy and structure across Ohio

provides numerous sequestration reservoir targets as well as confining units (Figure 3.2). The optimal sequestration targets differ across the state due to the underlying basement structure. The general trend exhibits units thickening and deepening toward the Appalachian (east) and Michigan (north) basins. In the eastern part of the state, the Upper Cambrian Rose Run Sandstone and the Lower Silurian Lockport Dolomite hold the most sequestration potential. The Mount Simon Sandstone, Cambrian basal sand, has been identified as a key target in the western part of Ohio (Wickstrom et al. 2010). The Mt. Simon is not a target in the eastern region because it pinches out and becomes more sporadic (Figure 3.1.b). The heterogeneity of the sedimentary units at a regional scale requires the need for site specific investigations. In this research project a test case located in Warren County (southwest corner of the state) was chosen. The following section discusses the numerous reasons and benefits of choosing the test case location.

economical potential (mineral and hydrocarbon) in western Ohio (Shrake et al. 1990). Well 2627 has a full wire-line suite that includes Gamma Ray, Resistivity, Neutron Porosity, Bulk Density, and Lithologic Fraction logs as well as full rock core. This site was chosen as the test case because of the availability of the wire-line data and the core samples as well as the western Ohio location. Another benefit of well 2627 is that it penetrates the key formations for potential sequestration in that part of the state, the Mt. Simon Sandstone (reservoir) and the Eau Claire Formation (confining) (Figure 3.3).

Figure 3.3. Well log suite at the Warren Co. location exhibiting the major formations as well as the Gamma Ray, Resistivity, Neutron Porosity, Bulk Density, and fraction logs.

The major formations found at this well location begin with the Precambrian Middle Run Formation (3455' - > 5170') overlain by the Mt. Simon Sandstone (3235' - 3455'), the Eau Claire Formation (2685' - 3235'), the Knox Dolomite (1605' - 2685'), the Wells Creek Formation (1550' - 1605'), the Black River Group (1090' - 1550'), the Lexington Limestone (925' - 1090'), the Utica/Point Pleasant Formation (820' - 925'), and finally the Kope Formation

(520' - 820'). From a geological sequestration point of view, the Middle Run Formation, the Mount Simon Sandstone, and the Eau Claire formation are the primary focus.

The Mt. Simon Sandstone is approximately 220 feet thick at the well location and based on the well logs appears to be very clean quartz sandstone. A lithologic description of the Mount Simon Sandstone based on the rock core was completed by the ODNR (Shrake et al. 1990). The description defines the unit as a fine- to coarse-grained, sub-rounded to rounded, well-sorted sandstone. The unit is dominated by quartz, partially feldspathic, and glauconitic near the top. The bottom 10 feet contains hematitic cement whereas the remaining top portion is dominated by siliceous cement.

The overlying Eau Claire Formation is approximately 550 feet thick. The lithologic description from Shrake et al. (1990) describes this unit as a large mix of various lithologies. The unit consists of fine layers of interbedded sandstone, siltstone, shale, and mudstones.

Based on the depth (greater than 2,600'), thickness, and lithology the Mount Simon Sandstone and the Eau Claire Formation appear to form an ideal confined reservoir for CO₂ injection. A detailed investigation of the Mount Simon Sandstone and the Eau Claire Formation located at the test case was conducted utilizing borehole and core sample data (physical and geophysical).

As discussed previously, the Warren County well provided geophysical well log data and access to core samples throughout the majority of the depth of the well. Core samples were collected throughout the zone that includes the Middle Run Formation, Mount Simon Sandstone, and Eau Claire Formation. The samples were hand selected to investigate the reservoir capacity of the Mount Simon Sandstone and the sealing potential of the Eau Claire Formation.

Table 3.1 provides a complete list of core samples that were collected from this well. Quarter core sample sizes represent the majority of the samples but 9 full diameter core samples were selected. The quarter cores were scattered throughout the zone of interest where as the full core was concentrated at the top of the Mount Simon Sandstone, at the transition into and through the Eau Claire Formation. Figure 3.4 shows the core sample locations imposed on the well logs.

Sample ID	Depth	Formation	Lithology	Core Size
wa110	859.5	Utica	black shale	Small Pcs.
wa203	2710.1	Eau Claire	mudstone	Quarter
WA9	2710.1	Eau Claire	mudstone	Full 1.5"
WA8	2845.75	Eau Claire	siltstone	Full 1.5"
wa204	2846	Eau Claire	mudstone	Quarter
WA3-1	2903.4	Eau Claire	siltstone	Quarter
WA3-2	2962.8	Eau Claire	siltstone	Quarter
WA3-3	3004.5	Eau Claire	shale	Quarter
WA3-4	3075.8	Eau Claire	siltstone	Quarter
WA7	3100.7	Eau Claire	Siltstone	Full 1.5"
wa205	3102.8	Eau Claire	sandstone	Quarter
wa206	3107.7	Eau Claire	sandstone	Quarter
WA6	3107.7	Eau Claire	Sandstone	Full 1.5"
wa207	3195.9	Eau Claire	sandstone	Quarter
WA5	3196.2	Eau Claire	Sandstone	Full 1.5"
wa208	3215.5	Eau Claire	sandstone	Quarter
WA4	3221.95	Eau Claire	mudstone	Full 1.5"
wa209	3222.8	Eau Claire	mudstone	Quarter
wa210	3235.4	Eau Claire	fine sand/mud	Quarter
WA3	3235.8	Eau Claire	siltstone	Full 1.5"
WA2	3257.4	Mt. Simon	Sandstone	Full 1.5"
wa211	3257.65	Mt. Simon	sandstone	Quarter
WA3-5	3262	Mt. Simon	sandstone	Quarter
WA1	3269.45	Mt. Simon	Sandstone	Full 1.5"
wa212	3269.75	Mt. Simon	sandstone	Quarter
WA3-6	3287.3	Mt. Simon	sandstone	Quarter
WA3-7	3319	Mt. Simon	sandstone	Quarter
WA3-8	3366	Mt. Simon	sandstone	Quarter
WA3-9	3398	Mt. Simon	sandstone	Quarter
wa109	3426.35	Mt. Simon	sandstone	Quarter
wa108	3430.4	Mt. Simon	sandstone	Quarter
wa107	3435.8	Mt. Simon	sandstone	Quarter
wa106	3447.4	Mt. Simon	sandstone	Quarter
wa105	3457.8	Middle Run	gran. congl./sandstone	Quarter
wa104	3462.5	Middle Run	gran. congl./mudstone	Quarter
wa103	3463.6	Middle Run	gran. congl.	Quarter
wa102	3474.2	Middle Run	sandstone	Quarter
wa101	3567.8	Middle Run	sandstone	Quarter

Table 3.1. List of core samples from the Warren Well including depth, formation, lithology, and core size.

Figure 3.4. A closer view at the zone of focus that includes the Middle Run Formation, the Mt. Simon Sandstone, and the Eau Claire Formation. The red dots signify core sample locations.

Having access to core samples is extremely useful when conducting a geological and geophysical investigation for several reasons. One major reason immediately becomes apparent when analyzing the geophysical well logs. Well logs are a very good investigative tool but require a large amount of interpretation and corrections. Also, multiple logs must be used in a decision matrix style of analysis since the dependence on a single log can lead to inaccuracies in interpretation.

3.4 Geophysical Well Log Analysis

The Warren County well log suite included a neutron porosity log. A neutron porosity log is measured with a neutron logging tool that operates by emitting neutrons into the borehole wall and measuring the amount of neutrons that are sent back. Essentially, the emitted neutrons are interacting with the hydrogen ions in the rock formations and sent back to the borehole tool. The most common source of hydrogen ions in the subsurface is found in water molecules; therefore the tool is sensitive to the amount of water found within the rock. The data that is first collected from this tool is a plot of neutron counts. The neutron counts are then used to calculate the percent porosity at each measurement location. The porosity calculation is based on rock standards and assumes a specific rock matrix. The most common matrix utilized is the limestone matrix. Since the entire Warren County porosity well log was based on a Limestone matrix it

was corrected to a sandstone matrix (the predominant lithology in the zone). The Mount Simon Sandstone is accurately represented by a sandstone matrix and the Eau Claire Formation is more similar to sandstone than limestone. The presence of shale in the Eau Claire Formation is accounted for in another correction.

Figure 3.5. Conversion chart used for correcting porosity values based on limestone, dolomite, or sandstone matrices (http://www.wellog.com/charts/neutron_porosity.jpg).

As mentioned previously, the neutron tool measures all of the hydrogen found in the rock and assumes that all of the hydrogen ions are in the pore water. In actuality water is found in the pore fluid and in bound water, water that does not represent actual pore space rather it is absorbed into the clay minerals matrix. The result of this assumption is an over-estimation of porosity. To correct for this assumption, one must take into account the amount of clay that is present. An estimate of clay volume can be found from a calculation on the Gamma Ray (GR) Log. The GR tool measures the gamma ray counts emitted by different radioactive minerals including potassium, a major component found in clay. This means that the GR log is a good indicator of clay content and is used as the primary means to discern between high clay lithologies (shale) and low clay lithologies (sandstone & limestone). Equation Shale Volume from Gamma Log: (3.1 provides an estimate of clay volume based on the GR values of clean sandstone and shale formations.

Shale Volume from Gamma Log:

$$V_{sh} = \frac{(GR - GR_{cs})}{(GR_{sh} - GR_{cs})}$$

(3.1)

Where:

V_{sh} = Shale Volume

GR = Gamma log reading at point of interest

GR_{CS} = Gamma log reading in clean sand

GR_{sh} = Gamma log reading in shale

Neutron Log Porosity Correction for Shale:

(3.2)

$$\Phi_C = \Phi_N - (V_{sh} * \Phi_{Nsh})$$

Where:

Φ_C = Corrected Log Porosity

Φ_N = Neutron Log Porosity

V_{sh} = Shale Fraction (from GR log)

Φ_{Nsh} = Neutron Log Porosity in Shale

The corrected neutron log provides porosity data for the entire zone of interest but there is approximately a 5 foot difference between the recorded core sample depths and the well log depths due to the collection process. Therefore, porosity values specific to the rock samples is crucial for electrical property measurements. To satisfy this necessity, porosity measurements for each rock core sample were completed in the laboratory.

3.5 Porosity Data

The primary goal of geologically characterizing an injection site is to identify and analyze potential reservoir and confining layers. The analysis of formations involves investigating the porosity, permeability, and mineralogy. Due to lab restrictions and the focus of this research, porosity of the potential units was the only property that was investigated.

Rock core porosity measurements were measured with a Mercury Porosimeter. The porosimeter accepts a small rock sample placed in a glass penetrometer. The sample properties are input into the computer software and then the penetrometer is inserted into the machine. The sample is then evacuated with a vacuum pump. At this point liquid mercury is injected into the penetrometer, as well as the sample, with pressures incrementally increasing up to 60,000 psi. The computer takes continuous measurements throughout the pressurization to obtain a pore size distribution as well as an overall porosity.

The Mercury Porosimeter porosity measurements from the rock core provide information specific to each sample where as the data from the well logs (section 3.4) provide a continuous look at how the porosity changes throughout the Mount Simon Sandstone and the Eau Claire Formation. The results of the porosity analysis are shown in Figure 3.6, wherein the corrected neutron log data is overlain by the Mercury Porosimeter data. There appears to be a close correlation between the data sets. The discrepancies that do appear could be caused by various factors. There is a difference between the core sample depth and the log depth due to the rock

core extraction process. There is also a fundamental difference between how the methods produce a porosity value. The log porosity is calculated and corrected from the neutron log that measures total water content, not simply the water found in the pore space. The Mercury Porosimeter only measures the pore volume that is accessible to the mercury. Finally, the discrepancies may be caused by the state of the core. The core was extracted from the borehole over 20 years ago. The extraction process causes a large pressure decrease to atmospheric pressure that may cause fracturing, increasing the porosity. During the core drilling and extraction the samples come into contact with and are contaminated by the drilling mud. Also, since the time of extraction, the core has been sitting in warehouse storage. The fluids that were once present have now evaporated, desiccating the clay matrices and leaving behind residue (usually in the form of salt).

Figure 3.6. Mercury Porosimeter porosity data compared to the Neutron Log porosity data.

3.6 Resistivity Data

3.6.1 Laboratory Resistivity Data

Resistivity measurements were conducted with a system that was designed and built for this project. The system saturates the rock sample with brine and measures the resistivity on full

diameter rock core (Figure 3.7). The experimental setup included a saturation container, a current source, a voltmeter, and an electrode core holder (Figure 3.8). The core samples, originally collected at the Warren County well in 1989, were chosen from the Ohio core repository. 28 rock cores were collected but only 9 of the samples were full diameter core conducive to resistivity measurements. Each core was cleaned by saturating the pores with de-ionized water and then allowed to dry multiple times.

Figure 3.7. Core saturation container with (a) brine reservoir, (b) vacuum chamber, and (c) a rock core inside the electrode core holder.

A brine solution was created specifically to saturate the core for the resistivity measurements. The brine creation process was based on the Society of Core Analysts (SCA) guidelines (Worthington et al. 1990). The brine was a pure NaCl solution with a concentration of approximately 30,800 ppm, a value that closely represents the brine found in Ohio's deep saline aquifers. The SCA guideline calculations were applied to the brine, resulting in a resistivity value of $0.2 \text{ } \Omega \cdot \text{m}$. Knowing the resistivity of the brine is critical when utilizing Archie's Equation because it removes an unknown parameter from the calculations. This topic is discussed in more detail in section 3.6.2.

The electrode core holder is a Teflon sleeve that is attached to the rock core. The sleeve has 4 platinum wire electrodes rings embedded within the sleeve. The ring electrodes are at regularly spaced intervals of 0.5 centimeters. The outer two rings serve as the current electrodes and the inner two rings are the voltage differential electrodes. A Keithley 6221 was utilized as the current source. This particular model is very useful for resistivity measurements because it produces a constant current source signal and can be remotely operated from a computer. The ideal signal was chosen by experimenting with various signals, amplitudes, and frequencies. A 1

kHz square wave signal at 90mAmps proved to be the best current source signal. A voltmeter was required to measure the voltage differential on the inner electrodes as current was passed through the sample. A National Instruments PCI-6289 card coupled with a SCB-68 box served as the voltmeter and was operated through the computer.

Figure 3.8. Outline of the laboratory resistivity measurement system. A LabView based software (a) controls the current source (b) and the voltmeter (c) while making measurements on the rock core (d).

A LabView® software application was developed to interface between the computer, the current source, and the voltmeter (Figure 3.8). The measurement process began by selecting the current source parameters: wave type, amplitude, and frequency. When the source signal was initiated the software automatically recorded the voltage differential. When the run was completed the voltage signal was processed to obtain a representative voltage value at the constant current value. As discussed in section 1.3.1.1, Ohm's Law utilizes the voltage difference and the induced current to calculate the resistance of the rock core. At that point the software completes a resistivity calculation based on the resistance and a geometric parameter (Equation Resistivity Calculation: (3.3)). The geometric factor takes into account the cross-sectional area of the medium under measurement. In this case, the core is a cylinder with a cross-sectional area of πr^2 multiplied by the radius squared. The other geometric parameter is l , the electrode spacing. The resistance is measured in ohms (Ω) and after multiplying the resistance by the geometric factor the resistivity units are measured in ohm meters ($\Omega \cdot m$).

Resistivity Calculation:

(3.3)

$$R = \frac{V}{I} \frac{\pi r^2}{l}$$

R = resistivity

V = voltage difference

I = current

r = radius

l = distance between electrodes

The resistivity measurement process that was just outlined was applied to the 9 full core samples. The samples are located throughout the Mt. Simon Sandstone and the Eau Claire Formation (Table 3.1). The resistivity values represent the total resistivity of the sample while saturated with NaCl brine with a resistivity of 0.2 Ω m. The data in Table 3.2 is essentially raw data without any corrections applied. The sandstone samples are the cleanest lithologies, with respect to clay content, and are the easiest to saturate. The low resistivity values for the sandstones reflect that relationship. The mudstones, on the other hand, show higher resistivity values reflecting the lower porosity and higher clay content. The next section, 3.6.2, discusses in detail the corrections that must be applied to the data as well as the information that can be extracted from this data set.

Sample	Depth	Unit	Lithology	Resistivity (Ω m)
WA9	2710.1	Eau Claire	Mudstone	21.96712
WA8	2845.75	Eau Claire	Siltstone	23.7652
WA7	3100.7	Eau Claire	Siltstone	23.5019
WA6	3107.7	Eau Claire	Sandstone	9.99092
WA5	3196.2	Eau Claire	Sandstone	5.91664
WA4	3221.95	Eau Claire	Mudstone	21.8261
WA3	3235.8	Eau Claire	Siltstone	10.9336
WA2	3257.4	Mt. Simon	Sandstone	11.45666
WA1	3269.45	Mt. Simon	Sandstone	12.31294

Table 3.2. Resistivity values for rock core samples located throughout the Mt. Simon Sandstone and the Eau Claire Formation.

3.6.2 Resistivity Data Corrections

The goal of laboratory resistivity measurements is to apply the core sample measurements to the resistivity well log and produce information that is not available from using the well log data

alone. The resulting information includes the grain resistivity, the water resistivity, porosity, and the formation saturation. Archie's Equations (Equation Archie's Law: (3.4) provide the capability to calculate that valuable information but numerous factors must be taken into consideration first. The equations are empirical, make several assumptions, and corrections must be made in order to apply Archie's Equations to the measured resistivity data. There are three primary corrections that must be completed before the data can be analyzed; (1) the Waxman-Smits Equation accounts for clay content, (2) a porosity compaction correction and (3) a temperature correction because the measurements were conducted at room temperature and pressure. A brief description of Archie's Equations and the corrections follow.

3.6.2.1 Archie's Equations

As discussed above, resistivity is influenced by various properties of the rock, pore fluid, and subsurface environment. What makes resistivity data useful is the ability to extract other rock properties from that data. G.E. Archie pioneered the use of resistivity relationships to find rock properties by relating well log resistivity measurements with rock core resistivity measurement made in the laboratory. Archie's Law (Equation Archie's Law: (3.4) quantifies the relationship between total resistivity, fluid resistivity, water saturation and other rock properties. The other parameters and relationships associated with Archie's law are the formation factor (Equation Formation Factor: (3.5), the resistivity index (Equation Resistivity Index: (3.6), and the water saturation (Equation Water Saturation: (3.7).

Archie's Law: (3.4)

$$R_t = \frac{a}{\Phi^m} \frac{R_w}{S_w^n}$$

Formation Factor: (3.5)

$$F = \frac{R_o}{R_w} = \frac{a}{\Phi^m}$$

Resistivity Index: (3.6)

$$I = \frac{R_t}{R_o} = \frac{1}{S_w^n}$$

Water Saturation: (3.7)

$$S_w = \left(\frac{1}{I}\right)^{-n} = \left(F \frac{R_w}{R_t}\right)^{-n}$$

Parameters:

R_t = fluid saturated rock resistivity

R_w = brine resistivity

R_o = water saturated rock resistivity ($S_w=1$)

= porosity

S_w = water saturation

a = experimental tortuosity factor

m = experimental cementation factor

n = saturation exponent

Relationship between density, porosity and water saturation: (3.8)

$$d_t = \Phi d_w S_w + (1 - \Phi) d_g$$

d_t = total (true) density of the sample

d_w = water density

d_g = rock grain density

= porosity

The parameters used in Archie's Equation are found through analyzing core samples. The tortuosity factor (a) represents the interstitial structure of the rock where as the cementation factor (m) deals with the amount of cementation between the grains of the rock. Both of these parameters relate to porosity and permeability. The cementation and tortuosity factors are measured by saturating the core sample with brine of a known resistivity and then completing a resistivity measurement. The saturated rock resistivity is divided by the resistivity of the brine to produce the formation resistivity factor (Equation Resistivity Index: (3.6). Finally, a log-log plot of the formation resistivity factor vs. porosity is plotted where the slope and intercept are the tortuosity and cementation factors respectively.

The saturation exponent, n , is related to the presence of fluid in the pores and the wettability of the rock. Different fluids saturate the pores differently with droplets or continuous films which will affect the resistivity. Finding the saturation exponent requires making resistivity measurements on the rock core at multiple saturations. Therefore, the core starts as fully water saturated and then a fluid saturation is incrementally increased while making resistivity measurements. These measurements are then plotted on a log-log plot of the resistivity index (Equation Resistivity Index: (3.6), ratio of fluid saturated rock to water saturated, vs. the fluid saturation, where the slope is the n parameter.

3.6.2.2 Waxman-Smits Equation

Archie's Equations assume that the sample is a sandstone matrix, an assumption that does not apply to the shale rich samples that are present throughout the Eau Claire Formation. The reason that the equations assume a pure sandstone matrix is due to the electrical properties of clay minerals. In clean sandstone the current flow strictly depends on ions in the pore fluid and not the rock matrix. When clays are present they act as a cation exchange, creating another current path, negating Archie's assumption. The Waxman-Smits (Equation Waxman-Smits: (3.10) and the Modified Waxman-Smits (Equation Modified Waxman-Smits: (3.11) Equations attempt to address this issue.

Where clays are present, the resistivity can be expressed as: (3.9)

$$R_0 = \frac{1}{\frac{K}{R_w * F} + X}$$

Waxman-Smits: (3.10)

$$S_{wt}^{n1} = \frac{F_1 * R_w}{R_t * \left[1 + \frac{R_w * B * Q_v}{S_w}\right]}$$

$$F_1 = \frac{a_1}{\Phi_t^{m1}}$$

Modified Waxman-Smiths: (3.11)

$$X = \frac{V_{cl} * (R_{wb} - R_w)}{2 * R_{wb}}$$

$$S_{wt} = \left(\frac{X^2 + F * R_w}{R_t} \right)^{1/n} + X$$

Where:

- K = interactive clay function
 - X = additional resistivity from clay
 - Q_v = cation concentration per unit volume of fluid in the pore space (equivalents per liter)
 - S_{wt} = total water saturation
 - B = Salinity and temperature dependent (Juhasz, 1981)
- $$= \frac{(-1.28 + 0.225 * T - 0.0004059 * T^2)}{(1.0 + (R_w * 0.045 * T) - 0.27)}$$

3.6.2.3 Porosity Compaction Correction

The laboratory resistivity measurements were conducted at ambient pressure. Pressure has been shown to greatly influence the resistivity (Brace et al., 1965). This large influence is attributed to the decrease in pore space from the overburden pressure. Essentially, less pore space means less conductive water available for current flow. Less water within the rock produces a higher resistivity value than the same rock would have under ambient pressure.

Overburden pressure, also called lithostatic pressure, is the pressure imposed by the weight of overlying material. The overburden pressure at a depth z is given by Equation (Lithostatic Pressure): (3.12).

Lithostatic Pressure: (3.12)

$$p(z) = p_0 + g \int_0^z \rho(z) dz$$

$\rho(z)$ = density of the overlying rock

z = depth

g = acceleration due to gravity

p_0 = datum pressure (pressure at the surface)

3.6.2.4 Temperature Correction

The temperature also plays a crucial role in the resistivity. The resistivity measurements made at room temperature can be corrected to formation temperature either by use of a chart or by Arp's empirical formula (Equation Arp's Formula: (3.13)).

Arp's Formula: (3.13)

Fahrenheit:

$$R_2 = R_1 \left(\frac{T_1 + 6.77}{T_2 + 6.77} \right)$$

Centigrade:

$$R_2 = R_1 \left(\frac{T_1 + 21.5}{T_2 + 21.5} \right)$$

Parameters:

$R_{1,2}$ = Resistivity at temperatures T_1 and T_2

3.6.3 Resistivity Data Analysis

Resistivity analysis of log and laboratory data is most commonly utilized for two purposes: (1) for calculating the porosity based on the log data and (2) for finding hydrocarbons. The research already has porosity data from the neutron log and from core measurements so the porosity calculation was not undertaken. There are no hydrocarbon shows in the formations being investigated for carbon sequestration but the process of using resistivity data to find and quantify the presence of hydrocarbons is still very useful.

Hydrocarbons are more resistive than brine so electrical methods are very important in a borehole environment. The primary goal of the process is to find the amount of hydrocarbons present in the pore space based on the resistivity. Archie's law, as described in section 3.6.2.1, will yield a water saturation percentage where remaining porosity percentage is assumed to be hydrocarbon based on the resistivity values from the well log and laboratory measurements. The usefulness of Archie's Equation for analyzing the water saturation and hydrocarbon content also applies to Carbon Sequestration injection. Instead of considering the non-water saturated pore space to be hydrocarbon it is considered to be CO₂, also more resistive than brine.

Figure 3.9 displays the culmination of the resistivity data analysis. The graph contains the well log resistivity data as well as the laboratory resistivity measurements with symbols placed at the core sample locations. The corrections described in section 3.6.2 (shale content, compaction, and temperature) were applied to both the core sample data and the well log data. The left side of the figure shows the log interval that corresponded to the core sample locations. The right side is zoomed in to the transition from the Mount Simon Sandstone to the Eau Claire Formation where the primary focus of this study was placed.

Large discrepancies can be seen between the log data and the laboratory data in Figure 3.9. The discrepancies can be attributed to two major factors, (1) the laboratory measurement method and (2) the core extraction process. The laboratory measurement technique, discussed in section 3.6.1, utilized saturating brine with a resistivity of 0.2 $\Omega\cdot\text{m}$. The laboratory brine was chosen because it aided in conducting accurate measurements but does not match the resistivity of the in situ fluids that saturated the formations during the well log measurements. The discrepancy in electrical properties of the fluid creates a noticeable difference in the resistivity values. The second factor, as discussed previously, is related to the core sample depths not directly corresponding to the log depths (by as much as 5 ft.) due to the margin of error associated with extracting the samples from the subsurface at an accurate depth. With these factors in mind, the trends of the two plots are generally in agreement.

Figure 3.9. The graphs consist of the resistivity data from the well log, the rock core resistivity measurements, and the sample locations. The right side of the figure is zoomed in to the transition from the Mt. Simon Sandstone to the Eau Claire Formation where the highest density of samples occurs.

A benefit of acquiring well log resistivity and laboratory resistivity data is the ability to extract information about the pore fluid by applying Archie's Equation. This is accomplished by calculating the formation factor from the rock core measurements and obtaining the total resistivity from the well log. The result is the resistivity of the formation water. Figure 3.11 is a chart that is used to convert the resistivity of the fluid to a concentration (ppm). Applying

Archie's Equation to this data set allowed the calculation of the NaCl concentration of the brine that saturated the formations during the original well log measurements.

The process includes the following steps:

1. Calculate the formation factor of the core sample by dividing the laboratory measured resistivity by the brine resistivity.
2. The division of the calculated formation factor by the well log resistivity produces the resistivity of the brine (Figure 3.10).
3. Utilize the formation temperatures from the well log data and the calculated brine resistivity in the chart shown in Figure 3.11.
4. Use the chart to find the concentration of NaCl in the brine in ppm.

Figure 3.10. Brine resistivity data calculated from the well log and laboratory data.

Figure 3.11. A logging chart of temperature vs. resistivity of a NaCl solution. Plotting a brine resistivity with a formation temperature provides a value for the NaCl concentration in ppm. The boxes show the range of values that were calculated from resistivity log using the rock core measurements.

The boxes overlaying the chart in Figure 3.11 represent the range of values that were produced in the brine resistivity analysis (Figure 3.10). The data used in the calculation was concentrated within the Mount Simon Sandstone near the transition into the Eau Claire. This zone was

utilized because it had the highest density of core samples in a small depth range (4 samples in 50 ft.). The analysis on the Mount Simon Sandstone data resulted in a range of brine resistivity values from 0.01 to 0.07 $\Omega\cdot\text{m}$, leading to the calculation of an approximate NaCl concentration of 160,000 ppm. This value is within the range exhibited in this formation in this area of the state. Brine data is very important because the well data for the chosen test site did not include any information about the saturating fluid. The brine data is also very useful because it improves the accuracy in the calculation of the permittivity (discussed in greater detail in section 3.7.1).

3.7 Electrical Permittivity Data

3.7.1 Permittivity Calculation

Measuring the permittivity in the laboratory is more accurate than calculating the value from other data but, as discussed in section 1.3.1.2, is a very complex process that was beyond the scope of this project. Calculating the dielectric of a material instead of directly measuring the value involves assumptions and serves as a dielectric estimation. Dielectric calculations are considered estimations because of the heterogeneous nature of rock samples. The equation must take into account the dielectric properties of all the mineralogical components and the pore fluids. The most accepted approach is to calculate the overall permittivity of a medium (Knight et. al, 1991) by multiplying the permittivity's of each component by its fractional volume of the whole and summing the components (Equation Permittivity by volume: (3.14). The Complex Refractive Index Method (CRIM) expands the summation approach by breaking it into three dielectric components: the rock matrix, pore water, and other substances in the pores, usually hydrocarbons (Complex Refractive Index Method (CRIM): (3.15).

Permittivity by volume: (3.14)

$$\sqrt{K^*} = \sum_i V_i \sqrt{K_i^*}$$

V_i = Volume of the i^{th} component
 K_i^* = Permittivity of the i^{th} component

Complex Refractive Index Method (CRIM): (3.15)

$$\sqrt{K^*} = (1 - \Phi)\sqrt{K_s^*} + \Phi S_w \sqrt{K_w^*} + \Phi(1 - S_w)\sqrt{K_a^*}$$

Assuming S_w is 1, the equation becomes:

$$\sqrt{K^*} = (1 - \Phi)\sqrt{K_s^*} + \Phi\sqrt{K_w^*}$$

Where:

- K_s^* = Permittivity of the rock matrix
- K_w^* = Permittivity of the pore water
- K_a^* = Permittivity of pore space not water saturated (hydrocarbons, air)

The well log data and the resistivity analysis provided the primary values that CRIM required, the permittivity of the pore fluid and the rock matrix. The acquisition of the pore fluid data will be discussed first, followed by a description of the rock matrix data. Section 3.6.3 detailed how the concentration of the in situ brine was calculated. That brine data provided the information needed to calculate the dielectric of the pore fluid.

Included in the suite of well logs was a lithologic fractions log. The lithologic log shows an estimate of the percentage of certain rock types that are present in the formation, including sandstone, limestone, dolomite, and shale. The lithologic percentages were created based on the primary mineralogical component of each lithology, quartz for sandstone, calcite for limestone, magnesium for dolomite, and clay for shale. This data greatly improves the estimation of the rock matrix dielectric by breaking the formation down into mineral percentages with known dielectric values.

Substance	Permittivity
Quartz	4.5-4.7
Calcite	7-8
Dolomite	8
Shale	13-15
Clay	10
Sandstone	4.5
Water	81
Sea Water	88

Table 3.3. List of common substances with the corresponding permittivity values (Knight et al. 1987).

Equations Permittivity by volume: (3.14 and Complex Refractive Index Method (CRIM):
 (3.15 were implemented by inputting the calculated brine and rock matrix dielectric data as well as the porosity data from the well log analysis. The mineralogical percentages were each assigned the corresponding dielectric value and input into Equation Permittivity by volume: (3.14 to produce a dielectric value for the rock matrix. The rock matrix data was then

combined with the brine and the porosity data for input into Equation Complex Refractive Index Method (CRIM): (3.15). The results from this analysis are discussed in the next section.

3.7.2 Permittivity Data Analysis

At this point in the analysis, the well log data (porosity, lithologic fraction) and the brine data (resistivity analysis) are input into the CRIM equations to calculate the permittivity of the Mount Simon Sandstone and the Eau Claire Formation. The results of the calculations are shown in Figure 3.12.

Figure 3.12. Plot of the permittivity data that was calculated from the well log information using CRIM.

The permittivity ranges in values from 3 to 45 with an outlier at 72. Focusing on the Mount Simon Sandstone, wherein the most accurate brine data was calculated, the values range from 10 to 26. Knight et al. (1987) conducted research analyzing the dielectric of brine saturated sandstone through laboratory and calculation methods. Knight's study posted values in the range from 10 to 30, a range that overlaps well with the values calculated in this study. CRIM is an

estimation technique; therefore it is only designed to provide useful constraint values for this study. CRIM does provide data in an acceptable range based on the primary goals of this project; the implementation and validation of the GphysCO2 software suite.

3.8 Seismic Data

The seismic data collection component of this project differs greatly from the electrical property data collection. The available seismic data is based on a single source, the report completed for the original investigation at the Warren Co. drill site. Ohio Division of Natural Resources (ODNR) published a report, Shrake et al. (1990), detailing the following:

- Reasoning and goals for drilling well 2627.
- Lithologic descriptions of the extracted rock core.
- Details on a 2D seismic line that passed over the well location.
- Seismic velocity and synthetic analysis.

The information gathered from the seismic line (Figure 3.13) and the seismic velocity analysis (Figure 3.14) was utilized in this project. The seismic data was not available in digital format; therefore an image of the data was pulled from the report for a qualitative investigation. The seismic line provided details about the subsurface structure, specifically the zones of interest, the Eau Claire Formation and the Mount Simon Sandstone. The cross-section shows minimal structural features over its nearly 6 mile length. If the digital data was available a detailed analysis of the structure (e.g. faulting) and seismic properties (e.g. amplitude analysis) could have been completed.

Figure 3.13. This processed and migrated 2D seismic line passes through the well site from West to East (left to right). On the left is the correlated time and depth scale. The borehole, the Eau Claire Formation, and the Mt. Simon Sandstone are indicated on the seismic cross-section (adapted from Shrake et al. 1990).

The goal of the velocity analysis shown in Figure 3.14 was to correlate the well logs with the seismic cross-section, thus utilizing the well log data to identify the rock formations on the seismic line. The velocity analysis is crucial because well logs are based on a depth scale, where as the seismic line is based on a time scale (time between wave transmission and reception). Data from the seismic line and a nearby well (that provided a sonic log) was used to calculate the velocity, complete a time-depth conversion, and create a seismic synthetic. The sonic log provided P-wave velocity (V_p) values that form a velocity depth profile. This profile was utilized to create a time-depth conversion, a correlation between the time required by the seismic wave to traverse the subsurface and the depth. The synthetic, created by calculating amplitude values from the velocity data, was utilized in matching the wavelets of the synthetic to the seismic line. The time-depth correlation and the synthetic were then used to match the well log data to the seismic cross-section. Figure 3.13 shows the culmination of this process with the identification of the Eau Claire Formation and the Mount Simon Sandstone horizons on the seismic cross-section.

Figure 3.14. Image of the velocity analysis that was performed on the 2D seismic line (adapted from Shrake et al. 1990). Data from the seismic line was used to calculate the velocity, a time-depth conversion, and a seismic synthetic.

The major goals for this seismic data investigation was to discover the structure of the primary formations (Eau Claire Formation and Mt. Simon Sandstone) and the seismic velocities (V_p , V_s) of the subsurface at the test site to aid in creating digital seismic data models. The overall structure of the formations, as stated previously, was provided by the seismic cross-section. The other goal was collecting seismic velocity data for input into the GphysCO2 model. The velocity analysis shown in Figure 3.14 provided V_p data but did not include V_s values. To overcome this obstacle, an estimation of V_s data from the V_p data was conducted. The ratio of V_p to V_s (V_p/V_s) provided the means for estimating V_s . Well log studies, summarized by Potter et al. (1997), indicate a correlation between V_p/V_s values and lithology. The well log studies led to the creation of established V_p/V_s values from core measurements. The velocity ratios include; 1.9 for limestone, 1.8 for dolomite, and 1.6 to 1.75 for clean to calcareous sandstones. The velocity ratios for the listed lithologies combined with the general rule that V_s is approximately 60% of V_p led to the estimation of the S-wave velocities shown in Figure 3.15.

Figure 3.15. Plot of the P-wave velocity (V_p) and S-wave velocity (V_s) data through the Eau Claire Formation and Mount Simon Sandstone. The V_p data was extracted from the plot in Figure 3.14 and the V_s data was calculated from the V_p data.

The seismic velocity data (V_p , V_s) presented in Figure 3.15 provided a low resolution representation of the wave velocities through the Eau Claire Formation and the Mt. Simon Sandstone. The data is low resolution because, as with the seismic cross-section, the data was extracted from an image (digital data was not available), with a sampling interval of 50 ft. Although the resultant data set is of poor quality, it does satisfactorily provide enough data to build a digital seismic model.

Chapter 4: Three Dimensional Data Analysis

Chapter 3: described the establishment of a geophysical data set that included well log, porosity, seismic, and EM data for the Warren County test site. This chapter illustrates the utilization of that geophysical data set within the GphysCO2 software. The data set was input into the software and was utilized in creating 3-dimensional digital model representations of the subsurface at the test site.

4.1 3-Dimensional Property Models

The first step in creating the 3D property model was inputting the electrical and seismic properties. Figure 4.1 displays the plots of the resistivity, permittivity, P-wave velocity, S-wave velocity, and density values created by the Logphys component of GphysCO2. This data, combined with the structural data from the seismic cross-section, provided the information needed to construct a 3D EM model and a 3D seismic model that represented the test site.

The data set was confined to a zone that included the Mt. Simon Sandstone (injection reservoir target) and the Eau Claire Formation (confining unit) in the depth range from 2,700 to 3,600 feet. The investigation was restricted to this 900 ft. zone for the following reasons:

- The injection target and confining layer are present in this zone.
- The full core samples that were utilized in the resistivity measurements are all found within this depth range.
- The constricted area decreased the model block size, thus decreasing computational times for the subsequent numerical modeling.
- This project deals exclusively with cross-hole surveys conducted within the zone of interest, thus eliminating the need to create models of the overlying formations.

Figure 4.1. This figure displays plots of the resistivity, permittivity, Vp, Vs, and density data created by the Logphys module in the GphysCO2 software. The Eau Claire Formation, Mt. Simon Sandstone, and Middle Run Formation are displayed on the plots.

The plots found in Figure 4.1, with the exception of the seismic velocity data, have a sampling interval of 0.5 feet. The plots reveal the geological heterogeneity that is found in the subsurface, even though the data sets are restricted to 3 formations in a 900 ft. zone. Creating 3-dimensional models from the data in that state would result in an extremely accurate representation of the site but the capabilities of the software restricts this process. The model building component of GphysCO2 requires the user to manually assign geophysical property values to geometric shapes placed in the model block. In short, this means that the user would be required to place a new geometric shape (e.g. a layer) in the model block for each differing value. Simplifying the data entry process requires a simplification of the data sets.

The first step in utilizing the well logs to create 3D models was separating the electrical data (resistivity, permittivity) from the seismic data (Vp, Vs, density). As discussed earlier, the electrical properties that determine the action of an EM wave are very different than the mechanical properties that influence a seismic wave. For example, a rock layer that has consistent electrical properties throughout may be separated into multiple layers based on the seismic properties. The next step was to analyze each data set for major trends. The trends were used to separate the data set into multiple layers that each consisted of similar properties. The data values in each layer were then averaged, resulting in a simplified plot that clearly displayed

the major property layers. The final step was utilizing the simplified data to create 3D property models.

The next two sections describe how the electrical and seismic data sets were simplified and utilized in creating 3D geophysical models of the subsurface.

4.1.1 Electrical Property Model

The analysis of the resistivity and permittivity data resulted in the creation of the plots shown in Figure 4.2. As previously stated, the resistivity term was utilized when discussing the field and laboratory measurements. In this portion of the project the data is being applied to EM wave propagation, a technique that primarily uses conductivity data. For that reason the inverse of the resistivity data was completed resulting in conductivity values in Siemens per meter (S/m).

The conductivity and permittivity data were separated into 6 distinct layers; 3 layers within the Eau Claire Formation, 2 layers in the Mount Simon Sandstone, and 1 representing the top of the Middle Run Formation. The selection of the layers was based on an interpretation of the trends in the permittivity data. The focus was on the permittivity data because at the EM imaging frequencies the wave action is more dependent upon the dielectric of the medium. At lower frequencies the dependence transfers to the conductivity properties. The creation of the 6 layers improved the transition into the next step of creating 3D property models from the line data.

Figure 4.2. Plots of the conductivity (inverse of resistivity) and permittivity data. The data sets have been separated into distinct layers, through averaging, to simplify the model building.

The creation of the 3D electrical property model (Figure 4.4) was completed with the EM module. The model block is 300'x300'x400' (x,y,z) and is centered around the Warren Co. well site in the 3100' to 3500' depth range. The electrical property data that corresponds with the numbered layers in the figure are listed in Table 4.1. The accuracy in the creation of the 3D layers was vastly improved by plotting the electrical property logs in the 3D model block (Figure 4.3). The individual layers in the model are horizontal based on the interpretation of the seismic cross-section. The cross-section displayed minimal dip across a 5 mile range; therefore a 300 ft. cube around the site would not exhibit any discernible dip or structure.

Figure 4.3. Model block depicting electrical property well logs (conductivity in the front and permittivity behind) displayed with the property layers.

Figure 4.4. 3-dimensional model of the electrical property data (conductivity, permittivity) from 3100 to 3500 ft. depth range. The zone includes the transitions between the Eau Claire Formation, Mt. Simon Sandstone, and Middle Run Formation.

Layer	Thickness (ft.)	Conductivity (S/M)	Permittivity
1	30	0.1866	23.97
2	20	0.0832	16.69
3	100	0.5066	28.66
4	150	0.1803	14.65
5	50	0.1682	18.44
6	50	0.0713	16.42

Table 4.1. Thickness, conductivity, and permittivity data for layers 1 through 6 as seen in Figure 4.4.

4.1.1.1 Effects of CO₂ on Electrical Properties

The creation of the 3D electrical property model laid the foundation for numerically investigating the geophysical effects caused by injecting supercritical CO₂. The conductivity and permittivity data for the layers displayed in Figure 4.4 were utilized as the base values in calculating the changes that result when CO₂ is injected into the formation. Different approaches were employed when investigating the changes in the conductivity and permittivity values. The alteration to the conductivity values was investigated through a literature review, where as CRIM was implemented in the study of the changes to the permittivity values.

There have been multiple studies focused on the effects that injected CO₂ has on the resistivity of a saline formation. Newmark et al. (2001) investigated the resistivity change in a study centered on utilizing Electrical Resistance Tomography (ERT) to monitor a CO₂ injection. The results of Newmark's numerical study resulted in an increase in resistivity in the range from 0.2 to 10 times that of the initial value. The numerical study was coupled with an investigation at the Maljamar pilot site in New Mexico. Induction logs were completed at the site before, during, and after a CO₂ flood. The resistivity of the injection layers exhibited an increase in resistivity by a factor of 5 (approximate increase of 400%) during the CO₂ flood. Another important study was conducted by Myer (et al. 2001) wherein a laboratory investigation into the effects of CO₂ on geophysical properties was completed. The study looked at the change in resistivity as CO₂ was injected into brine saturated sandstone at increasing pressures in the laboratory. The research was conducted with a 3.5 -m brine and 1.1 -m brine on one sample, reporting a 114% and 218% increase in resistivity respectively. Supercritical CO₂ is more resistive than brine, thus the overall resistivity increases as the CO₂ replaces the brine in the pore space. The two studies mentioned above discussed the increase in resistivity due to the presence of CO₂ but not the actual resistivity of the supercritical CO₂ itself. Therefore, the effect of a partial and full CO₂ saturation was inferred from the results reported by the studies.

The effects of injected CO₂ on the permittivity of the rock formations can be found with CRIM. CRIM, described in Section 3.7.1, is utilized in calculating the permittivity of a material based on the dielectric values of the individual components. Therefore, the original calculation of the permittivity values that were input into the 3D models was based on the percentage of the mineral components as well as the brine saturating the formation. The rocks were assumed to have 100% brine saturation of the pore space. The presence of injected CO₂ would result in CO₂ and brine filling the pore space. Based on a combined CO₂ and brine saturation, the portion of the porosity designated as brine saturated in the original CRIM calculation will decrease. The new calculation will utilize a permittivity value of 1.3 (Holmes et al. 2005) to represent supercritical CO₂. The permittivity value of CO₂ is much lower than the value of the brine (permittivity of 90) located at the test site; therefore, the injection of CO₂ results in a decrease in the overall permittivity of the formation.

4.1.1.2 CO₂ Injection Models

The introduction of CO₂ into the pore space results in an increase in resistivity (decrease in conductivity) and a decrease in the permittivity. The degree of the change in the electrical properties is dependent upon the fraction of the previously brine saturated pore space that has been replaced by supercritical CO₂. To simulate an injection at the test site, the 3D base models were altered to represent supercritical CO₂ saturating the Mount Simon Sandstone (Figure 4.5).

Figure 4.5. 3D model of a CO₂ injection (designated in red) into the Mount Simon Sandstone.

The 3-dimensional injection model depicts a generalized CO₂ saturation geometry after injection. The creation of a more accurate representation of a CO₂ would most likely be more spherical in shape and require a detailed analysis of the area surrounding the injection well. Examples of that information would be permeability trends, porosity trends, reservoir pressures, and detailed

information on fluid flow. Reservoir flow modeling would provide the ideal information to build an accurate CO₂ injection saturation but the primary objective of this project is to display the software capabilities and provide the foundation for further investigation, therefore the generalized geometry depicted above was selected.

The hypothetical supercritical CO₂ was injected at the base of the Mount Simon Sandstone. CO₂ is more buoyant than the brine that it replaced leading to an upward flow through the sandstone in widening horizontal layers. The upward flow of the CO₂ saturation was halted at the confining Eau Claire Formation. The 3D injection model served as a base plate for the numerical forward modeling that consists of more detailed cross-hole models. Therefore, the specifics of the CO₂ saturations and the resulting changes in the electrical property values are discussed later.

4.1.2 Seismic Property Model

The density, P-wave velocity, and S-wave velocity data were utilized in creating the 3D seismic model. As with the electrical data, the data sets were analyzed with the intention of simplifying the model. The interpretation of the seismic data set was restricted due to the poor sample spacing (25 ft.) of the velocity data. Therefore, the layers were primarily based on the density data in corroboration with the velocity data. The trends in the density data led to the creation of 6 distinct layers (Figure 4.6).

Figure 4.6. Plots of the P-wave velocity, S-wave velocity, and density data. The data sets have been separated into distinct layers, through averaging, to simplify the model building.

The 3D model that was created based on the seismic data (Figure 4.7) is similar to the electrical property model but does differ slightly in the Mount Simon Sandstone zone. The 2 layers in the Mount Simon Sandstone area of the seismic model consist of a 75 ft. layer overlying a 125 ft. layer. The electrical property model (Figure 4.4) of the Mount Simon Sandstone consists of a 150 ft. layer overlying a 50 ft. layer. The dimensions and depth range are the same in both property models. The horizontal structure of the layers also corresponds with the electrical model. The specific data values for each layer in the seismic model are listed in Table 4.2.

Figure 4.7. 3-dimensional model of the seismic property data (V_p , V_s , and density) from 3100 to 3500 ft. depth range. The zone includes the transitions between the Eau Claire Formation, Mt. Simon Sandstone, and Middle Run Formation.

Layer	Thickness (ft.)	Vp (m/s)	Vs (m/s)	Density (g/cc)
1	30	1560	936	2.485
2	20	1520	912	2.585
3	100	1353	811.8	2.442
4	75	1372	823.2	2.5
5	125	1417	850.2	2.53
6	50	1536	921.6	2.611

Table 4.2. P-wave velocity, S-wave velocity, and density data for layers 1 through 6 of the seismic model.

4.2 Seismic and EM Property Model Summary

The Seismic and EM property models supply the spatial limits of the primary zone of interest at the test site. They represent the culmination of the data collection, site characterization, and interpretation of the Warren County test site. Additionally, the models provided the modeling base for the seismic and EM numerical simulations. All of the simulations consisted of sub-blocks of these property model blocks. The simulations are cross-hole surveys that include more detail than the 3D property models.

Chapter 5: Numerical Simulations

The final stage of the project was the implementation of the numerical simulation components, EM and seismic, in the GphysCO2 software. The forward modeling simulations utilized the 3D EM and Seismic property models that were described in Chapter 4:. The simulations were conducted in 3-dimensional sub-blocks of the full scale property models. The simulated geophysical surveys consisted of cross-hole arrays that were designed to investigate the following primary goals:

- Demonstrate an implementation of the numerical modeling component of the software (EM and Seismic).
- Determine the spatial limits of cross-hole EM surveys.
- Investigate the geophysical effects and detection of injected CO₂.
- Conduct a seismic cross-hole survey for comparison with the EM simulations.

5.1 Cross-hole Electromagnetic Simulations

The EM simulations were focused on experimenting with multiple variables (frequency, antenna separation distance, CO₂ saturation) to test the software and investigate EM imaging at the Warren County test site. The numerical simulations were conducted as cross-hole EM surveys within the Mount Simon Sandstone layer of the established 3D property model.

5.1.1 Cross-hole EM Spatial Limitations

High frequency EM imaging provides excellent images of the subsurface with the specific advantage of being highly sensitive to changes in the pore fluid. The method appears to be ideal for monitoring the injection of CO₂ into the subsurface. The largest obstacle that needed to be addressed before implementing cross-hole EM monitoring is the restrictions caused by the depth of penetration. The investigation into the spatial limits of EM monitoring must be prefaced with a brief discussion of GPR penetration factors.

GPR antennas typically operate in the Very High Frequency (VHF) to Ultra High Frequency (UHF) range of the electromagnetic spectrum (Dolphin et al. 1997). As previously stated, the lowest possible frequency is desirable because low frequencies give better penetration depths into the earth. The shortcoming with utilizing low frequency is that the radar wavelength becomes so large that detection and resolution of small objects becomes impossible. The implemented frequency range varies depending on the goals of the survey. Common cart mounted radars, used in surface surveying, have a typical center frequency of 150 MHz; however frequencies up to 500 MHz can be used for shallow, high-resolution probing. 20 MHz signals, at the lower end of the GPR spectrum, are utilized for locating deep caves or tunnels (Dolphin et al. 1997).

Analyzing the depth of penetration of an EM wave starts with a look at the factors that determine the propagation. Conductivity and the permittivity affect how a wave will travel through a material but a variable called the propagation constant aides in the understanding of how a wave attenuates as it scatters through the subsurface. The propagation constant (

Propagation Constant: 5.1) defines how the electromagnetic wave-field interacts with the electrical properties of a material. The two variables in the propagation constant equation are the attenuation constant (α) and the phase constant (β). These terms define how the permittivity (ϵ), conductivity (σ), angular frequency (ω), and magnetic permeability (μ) effect how the wave travels.

Propagation Constant: 5.1

$$\gamma = \alpha + i\beta$$

Attenuation Constant: 5.2

$$\alpha = \omega \left\{ \frac{\mu\epsilon}{2} \left[\left(1 + \frac{\sigma^2}{\epsilon^2\omega^2} \right)^{1/2} - 1 \right] \right\}^{1/2}$$

Phase Constant: 5.3

$$\beta = \omega \left\{ \frac{\mu\epsilon}{2} \left[\left(1 + \frac{\sigma^2}{\epsilon^2\omega^2} \right)^{1/2} + 1 \right] \right\}^{1/2}$$

The attenuation of the EM signal was of the most concern when determining the spatial limitations of EM monitoring at the Warren County site. The attenuation constant represents the loss in EM wave intensity as the wave is scattered by properties of the material. Figure 5.1 depicts the effects that the conductivity, the permittivity, and the frequency have on the attenuation of a wave. The conductivity and the frequency are the primary attenuating factors for the signal as compared to the relatively minor influence of the permittivity. This appears counter intuitive considering importance of the permittivity compared to the conductivity in high frequency wave imaging. The difference between the two cases is that a large change in permittivity will produce a strong reflection where as a large change in conductivity will attenuate the signal without the accompanying reflection.

Figure 5.1. Attenuation versus frequency for conductivity values 0.0001-10 and permittivity values 1-20-50. The plot demonstrates that attenuation is effected by frequency, conductivity, and permittivity (adapted from Daniels et al. 1997).

The numerical code, PFDTD, utilized in the EM module of GphysCO2 was implemented to experiment with the spatial limits of an EM monitoring survey at the Warren County test site. The first task was determining frequency ranges to input into the numerical simulation. To accomplish the task, the attenuation constant was calculated based on electrical properties in the Mount Simon Sandstone. A permittivity value of 14.68 and a conductivity value of 0.18 (S/m) were input based on the 3D property models that were detailed in Chapter 4:. Figure 5.2 depicts the attenuation of an EM signal over a frequency range from 1 MHz to 1.0E+10 Hz, utilizing the electrical properties of the Mount Simon Sandstone layer that was created within the 3D property model.

Figure 5.2. Attenuation versus Frequency plot utilizing a permittivity value of 14.68 and a conductivity of 0.18 (S/m). The electrical property values were extracted from the 3D property models.

Based on the attenuation plot three frequencies were chosen; 2 MHz, 20 MHz, and 300 MHz. The 2 MHz frequency was chosen because it is at the lowest end of EM imaging frequencies where as the 20 MHz signal was chosen because it is a common frequency for surface GPR antennas. Finally, the 300 MHz signal was selected because it is a frequency implemented for high resolution surveys at the surface. The frequency selections are corroborated by the plot in Figure 5.2. Frequencies in the hundreds of MHz range and above have an exponentially increasing amount of attenuation. The attenuation flattens out in the hundreds of GHz range but imaging at that frequency is not practical.

Numerical simulations were executed for the above mentioned frequency ranges for a homogeneous sub-block of the Mount Simon Sandstone model. The electrical properties were kept constant with a permittivity value of 14.68 and a conductivity value of 0.18 (S/m). Besides varying the frequency the distance between the transmit antenna and the receiver antenna were also varied from 4 meters to 100 meters. The results of the numerical simulations are depicted in Figure 5.3. The plot displays the peak amplitude of the three different signals (2 MHz, 20 MHz, and 300 MHz) over multiple antenna separation distances (4, 14, 20, 30, 40, 50, 60, 70, 100 meters). The waveform that was utilized was a Gaussian pulse with a 6.4 delay factor.

Figure 5.3. Plot of the peak amplitude of received signals versus distance to demonstrate the attenuation of the signals.

The plots displayed in Figure 5.3 illustrate the degree of attenuation that the different frequency signals exhibit. The plot mimics the attenuation constant calculations shown in Figures Figure 5.1 and Figure 5.2. The attenuation has the greatest effect on the 300 MHz frequency signal and the least effect on the 2 MHz signal. The attenuation was so great at 300 MHz that the only discernible signal that could be received was at a separation distance of 4 meters. The 2 MHz signal exhibited the most promising results based on the fact that a signal was received at a distance of 100m.

Based on the numerical simulations, 100 meters (~300 ft.) would be the best case scenario for cross-hole EM imaging. The 100 m distance is considered optimistic because the numerical simulations were completed within a homogeneous representation of the Mount Simon Sandstone. The actual environment is full of electrical property heterogeneities in the electrical properties that would most likely result in a diminished signal. Possible examples of the diminishing factors include high conductivity zones (e.g. increased porosity or higher brine concentration) that would cause an increase in the attenuation and large changes in permittivity that would cause increased scattering of the signal. The effects caused by electrical property heterogeneities were investigated in more detail in the next section. The model that was used for the spatial limitations was altered by placing a saturation of CO₂ inside the model. The addition of CO₂ provides useful information for determining possible signal changes caused by heterogeneity within the model.

5.1.2 EM Detection of Injected CO₂

The next stage in the implementation of the GphysCO₂ software was experimenting with numerical simulations of cross-hole surveys with the goal of detecting injected CO₂. The primary tasks included:

- Creating 3D models that represented a CO₂ injection within the 3D property models of the Warren County test site.
- Completing numerical simulations at multiple frequencies and antenna separation distances.
- Analyzing the results to deduce EM detection limits of CO₂.

The first step in the experimentation was defining a sub-block of the 3D property model to numerically model a cross-hole monitoring survey. The Mount Simon Sandstone zone of the model (layer 4 in property model above) was chosen as the injection layer and the layer that would contain the cross-hole survey. The next step was adjusting the electrical properties of a zone within the sandstone layer to accurately represent a volume of CO₂ saturation. The electrical properties of the CO₂ saturation were calculated based on the electrical property effects that were discussed in section 4.1.1.

The electrical properties were calculated with the assumption that injected CO₂ replaced 90% of the brine, leaving a residual amount of brine in the pore space. The permittivity for the Mount Simon Sandstone layer saturated with CO₂ was calculated with CRIM. The overall effect on the permittivity values of the Mount Simon Sandstone is displayed in Figure 5.4. The replacement of most of the brine with supercritical CO₂ greatly reduced the permittivity value of the sandstone. The calculation and subsequent averaging resulted in a permittivity value of 3.63 for the Mount Simon Sandstone layer.

Figure 5.4. Plots of the permittivity of the top portion of the Mount Simon Sandstone pre-injection (blue) and post-injection (red) of CO₂.

The conductivity value was deduced from the results posted by Myer et al. (2001); wherein a 100% to 200% increase in resistivity was reported with residual brine remaining in the pore space. Based on those results a resistivity increase of 150% was utilized in the model. The percentage increase in resistivity caused by the CO₂ was estimated due to the lack of available research data. Unlike the CRIM method, there is not a simple calculation that can be completed without laboratory experimentation. Therefore, the 150% increase was chosen based on the only readily available laboratory results produced by Myer's (et al. 2001) research.

The increase in resistivity caused by the CO₂ resulted in a conductivity value of 0.072 (S/m) for the Mount Simon Sandstone layer. The geometry of the cross-hole surveys is displayed in Figure 5.5. A portion of the full 3D property model was extracted wherein the antennas and CO₂ saturation were placed. The transmitter and receiver antennas are placed on opposite sides of the CO₂ saturation (red rectangle). The simulations had various distances between the antennas but the saturation zone remained at the center of the model, exactly half way between the antennas. As discussed previously, the geometry that was chosen to represent a saturation of CO₂ is most likely not what actually occurs in an injection zone. The model was created to represent a small pocket of CO₂ that is on the outskirts of the main saturation zone (e.g. a highly porous and permeable zone that allowed increased flow). The primary goal is not to investigate the intricacies of fluid flow but how geophysical surveys would change with the addition of CO₂.

Figure 5.5. 3D model of the cross-hole survey extracted from full 3D model. The vertical red rectangle signifies a saturation of CO₂. The antennas are simulated in boreholes on opposite sides of the CO₂ (transmitter, Tx, and receiver, Rx) with the saturation object at the exact center.

The saturation model in Figure 5.5. 3D model of the cross-hole survey extracted from full 3D model. The vertical red rectangle signifies a saturation of CO₂. The antennas are simulated in boreholes on opposite sides of the CO₂ (transmitter, Tx, and receiver, Rx) with the saturation object at the exact center. Figure 5.5 served as the boilerplate for the numerical simulations. The numerically simulated cross-hole surveys consisted of the following:

- 8 meter thick zone of CO₂ saturation located in the center of the model.
- Transmitter and receiver antennas placed equidistantly from the saturation zone with antenna separation distances of 20, 50, and 100 meters.
- Execute time-lapse surveys (execute a cross-hole survey before and after CO₂ injection and compare the difference).
- A single Gaussian pulse signal with a delay factor of 6.4 with a frequency of 2 MHz.

The 2 MHz signal was chosen based on the attenuation investigation that was performed in section 5.1.1. EM frequencies in the MHz range are not commonly used because of decrease in resolution that accompanies low frequencies. The primary reason for the loss in image resolution is the change that occurs in wavelength of the EM signal. Figure 5.6 displays how the wavelength becomes larger as the frequency is decreased and is based on Equation Wavelength:

5.4 Wavelength: 5.4. In traditional surface surveys this is a major concern because a large wavelength limits the size of the object that can be imaged. Surface surveys have the receiver and transmitter antennas in close proximity and is dependent upon reflection scattering back to the surface. Essentially, a large wavelength is only sensitive to large anomalies and small anomalies do not produce a significant reflection.

Wavelength becomes less of a factor when utilizing cross-hole monitoring surveys. The main reasons for the decreased dependence on wavelength is that the cross-hole surveys utilize two antennas (transmitter and receiver) located in separate boreholes. The separation of the transmitter and receiver is crucial because the method no longer solely relies on reflection back to the source. The wave-field signal in a cross-hole survey depends upon propagation through the subsurface from the transmitter to the receiving antenna a certain distance away. Scattering still influences the signal but the major point is; the received signal does not depend upon a strong reflection from anomalies to provide valuable information about the subsurface properties.

Another aspect to the 2 MHz signal choice is that EM surveys that implement frequencies below the MHz range may experience a change in the primary EM mechanism. At lower frequencies EM wave propagation becomes EM induction. Induction is a useful technique that measures changes in the magnetic field that is induced by an electric field. The downfall of utilizing induction is the survey is no longer a wave-field imaging technique.

Wavelength:

$$\lambda = \frac{2\pi}{\beta}$$

5.4

Figure 5.6. Plot of wavelength versus frequency. The wavelength decreases at higher frequency signals.

The results of the numerical simulations are depicted in Figure 5.7 and Figure 5.8. The former displays the numerical results for the 20 meter spaced cross-hole survey and the later shows the results of the 50 meter survey. A 100 meter survey was executed but the signal attenuation was very large and a discernible signal was not received. This model run is discussed in more detail in the proceeding section. As stated previously, the models were executed with a 2 MHz frequency.

The time-lapse methodology was utilized in the forward modeling experiments. The major goal of time-lapse surveys is to conduct multiple surveys over a time span to detect changes that occur in the subsurface. The Sleipner project (described in the introduction) utilized time lapse seismic surveys to highlight the changes that were occurring as injected CO₂ replace the pore fluids. A similar technique was implemented in these numerical models. In both plots the ‘homogeneous’ line represents the numerical results of a homogeneous model (before injection). The ‘with CO₂’ line illustrates the model that included the zone of CO₂ saturation that represents a hypothetical period of injection that occurred in the time between the two surveys.

Figure 5.7. Plot of the 20 m cross-hole simulation. The 'homogeneous' line represents the model results from a homogeneous model where as the 'with CO₂' line is the results after CO₂ was placed in the model.

Figure 5.8. Plot of the 50 m cross-hole simulation. The 'homogeneous' line represents the model results from a homogeneous model where as 'with CO₂' line is the results after CO₂ was placed in the model.

The numerical data is plotted directly as it was collected at the numerical receiving antenna. The plot is displayed as the signal amplitude (eV) versus the number of computation time steps. The data was kept in this format because the primary goal of the model experiments was to discover if cross-hole EM propagation could detect the presence of CO₂. Essentially, this is the first step that must be established before more advanced techniques can be implemented.

The trace plots above are useful for data analysis but one of the major benefits of GphyzCO2 is the capability to model and plot in 3D. Although 3D surveys were not completed for this project the numerical model traces can be displayed in the 3D model blocks for real time comparison to the initial property model. Figure 5.9 displays the original CO₂ property model and the associated numerical results. The ability to plot the traces within the same block clearly illustrates the difference between the 20 meter and 50 meter cases. The true advantage would come to fruition when designing cross-hole surveys in a heterogeneous environment. The numerical results could be directly compared to the property model and changes could be made on the fly to improve the survey design.

Figure 5.9. Side-by-side view of the CO₂ injection model (left) and the numerical results (right). The numerical traces displayed include the 20 meter and 50 meter experiments. The trace coloration represents high amplitude in red and negative amplitude in blue.

5.1.3 Cross-hole EM Discussion

The largest hindrance to full scale field implementation of cross-hole EM surveys is the penetration distance. The maximum achieved distance utilizing the EM numerical modeling in GphyzCO2 was 100 meters and provided the upper spatial limit of a cross-hole EM monitoring

survey. The caveat is that the 100 meter numerical calculation was executed on a homogeneous model. The numerical simulation that was conducted for the CO₂ injection experiments provided insight into how introducing heterogeneity into the system can influence the signal penetration distance. The cross-hole spatial limitation model runs produced a discernible signal at 100 meters but the introduction of a CO₂ saturation zone (8 meters wide) attenuated the signal to the level that discernible results could not be collected. This numerical result agrees with the theory that 100 meters is the absolute maximum distance for EM monitoring at the Warren County site. Therefore, in realistic heterogeneous subsurface conditions, the spatial range would most likely be between 50 and 100 meters.

The CO₂ saturation models did provide evidence that CO₂ can be detected with time-lapse cross-hole surveys. The numerical results for the CO₂ saturation models revealed that the 20 and 50 meter separation model runs produced a noticeable change between the homogeneous and heterogeneous (presence of CO₂) numerical results. A direct comparison between the homogeneous and CO₂ received signals clearly shows signal attenuation with a decrease in amplitude and a longer travel time. The implication of that observation is that a time-lapse cross-hole EM survey implemented in the field, with sufficiently close boreholes, would detect the change caused by the replacement of brine with CO₂ between the wells.

The results of the cross-hole EM investigation are preliminary but are a necessity for the advancement of the technology. The simulations were focused on the foundation of the problem; can cross-hole EM be implemented in a cross-hole environment and detect injected CO₂. The cross-hole time lapse numerical surveys that were implemented in this study were designed to assess the feasibility of cross-hole EM for CO₂ detection. The numerical simulations did provide evidence that EM can be successfully implemented in an injection monitoring role.

Detection limits are a crucial step towards considering the next stage of the research; imaging CO₂ saturations in the subsurface. Cross-hole EM imaging requires advanced antenna geometries. Instead of a single source and receiver, multiple sources and receivers would be utilized to gain multiple angles of propagation through the zone between boreholes. Advanced antenna geometries require full tomographic analysis for each cross-section. The cross-sectional images would then be conducted over time as CO₂ is injected into the subsurface. The final product would be a 2D cross-section that highlights the anomalies (changes) that occur over time as CO₂ is injected. Tomographic image analysis is a critical stage in the advancement of EM methods for monitoring CO₂. Image analysis is beyond the scope of this project because a tomographic analysis algorithm would have needed to be written for the software and the main goals of this project were to provide an implementation of the software as well as lay a foundation for EM imaging in a cross-hole environment.

5.2 Seismic Simulation

The seismic method, unlike the EM method, is an industry standard for subsurface imaging. Seismic surveys commonly include surface, hole-surface, and cross-hole arrays. The spatial limits of seismic methods, as well as the property effects of a CO₂ injection have received

intense research (e.g. Sleipner project discussed in the introduction) and are well understood. Therefore the numerical simulations that were completed with the seismic module of GphysCO2 were focused on displaying the capabilities of the software and not an investigation.

The simulations were implemented on the Mount Simon Sandstone zone (layer 5) of the 3D property model (Figure 5.10). A 100 meter long sub-block was extracted from the sandstone layer for executing the numerical simulation. The numerical survey was designed with a single source in one bore-hole and a string of receivers in another bore-hole. Seismic methods commonly utilize multiple receivers whereas EM methods employ a single source with a single receiver. The bore-holes were placed 100 m apart and the source signal was a 45 MHz Ricker wavelet. The numerical result of the cross-hole simulation is displayed as a 2D scan in Figure 5.11. The data resembles a 'v' with the point representing the receiver directly across from the source. The 'arms' of the 'v' depict the time delay caused by traveling the farther distance.

Figure 5.10. Illustration of the property model sub-block that was used for the seismic simulation.

Figure 5.11. Numerical results from a cross-hole seismic survey. The survey consisted of a single source and multiple receivers in bore-holes separated by 100 meters.

The seismic numerical results were input back into GphysCO2 and displayed in a 3D block to complete the implementation of the seismic module. A single trace was extracted from the data set and plotted in the block displayed in Figure 5.12. To further demonstrate the flexibility of the software the 100 meter EM numerical simulation was plotted in the same block as the seismic trace. Although the amplitudes of the signals do not represent the same thing the traces can be compared in a qualitative manner. The main difference between the traces is that the seismic trace displays the signal earlier in the trace than the EM trace. Essentially the seismic signal has a higher velocity than the EM signal.

Figure 5.12. EM and Seismic trace comparison displayed in a 3D model block. Both traces represent 100 meter model runs.

The EM and seismic data display provides insight into the benefits and difficulties associated with a combined data set. A major benefit is combining the strength of both methods into a single monitoring method. The seismic component provides superior signal penetration and the EM part provides a higher sensitivity to changes in the pore fluid. The difficulties associated with the combined technique focus on how to compare two different types of data into a single image. The amplitudes do not represent the same values and, as discussed above, the velocities of the signals are very different.

A unique benefit of GphysCO2 is the open source flexible environment. The software provides a foundation that will allow a way to overcome the obstacles. The first step would be to move beyond the single trace method that was implemented in this project. Time-lapse tomographic images would have to be created for both geophysical methods. This method would produce cross-sectional images that highlight anomalous changes that occurred. The images could then be converted from a time to depth scale, utilizing velocity information. At that point the images could be overlaid to produce a true combined image.

Chapter 6: Conclusions

6.1 GphysCO2 and Carbon Sequestration

The growing interest in reducing the vast amount of CO₂ that is being released into the atmosphere on a daily basis has led a focus on carbon sequestration, specifically geological sequestration. The primary concern with geological sequestration is monitoring the CO₂ after injection. Numerous techniques that include hydrogeology, geochemistry, and geophysics have been proposed. Geophysical methods are the only technique that can non-destructively monitor the subsurface from the surface or between bore-holes. Although geophysical methods have been utilized for decades, the monitoring of injected CO₂ was a new application that required further research and advancement.

Adapting geophysical methods for geological carbon sequestration monitoring while in the field can be a costly and time intensive endeavor. A geological and geophysical investigation that utilizes numerical modeling can greatly reduce error and improve the monitoring method for a potential injection site before a full-scale field implementation. Executing a forward model pre-injection enables the user to test numerous methods and obtain the best geophysical technique for a specific geological system.

The modeling process requires a software program that can input geophysical data sets, create 3D property models, and realistically forward model geophysical surveys (EM and Seismic). There are multiple software suites commercially available but each has issues when applying them to a geological sequestration task. The major downside is the lack of an EM imaging module. Other issues arise because the commercial software is designed for the oil exploration industry with a heavy focus on seismic methods, reservoir modeling, and risk assessment among many other oil specific applications. Commercially available software programs do not adequately fulfill all of the requirements that a CO₂ injection site necessitates. The GphysCO2 software was designed to provide the capabilities and flexibility to perform a geophysical investigation of a potential injection site.

The GphysCO2 software is a suite of programs that encompass well logging, seismic, and electromagnetic methods. The software enables users to design and execute 3D surface-to-surface and cross-hole (seismic and electromagnetic methods) surveys. The generalized flow of the program (Figure 2.1) begins with building a complex 3D subsurface geological model, assigning properties to the models that mimic a potential site that has injected CO₂, numerically forward model a geophysical survey, and analyze the results.

The primary objective that shaped the development of the GphysCO2 software was to provide a robust and flexible tool for modeling, imaging, and analyzing geophysical data. The secondary objectives include:

- The determination of detection limits of geophysical imaging techniques at a CO₂ injection well on a site-by-site basis through numerical forward modeling.
- The utilization of numerical modeling as a means for determining the optimum number and spatial distribution of boreholes for tracking injected CO₂.

- Exploring the possibility of implementing EM imaging as an effective imaging method for monitoring injected CO₂.
- Combining EM and seismic imaging techniques to gain more information than a single method could provide.

6.2 Software Implementation

A potential CO₂ injection site, located in Warren County, Ohio, was selected in order to validate all of the GphysCO2 modules. A robust implementation of the entire software suite was completed by utilizing data collected from a potential injection site and experimenting with geophysical modeling. The data sets, including well logs, seismic data, geological interpretations, and core samples were all collected for analysis.

The following list describes the primary steps that ensured a complete implementation of the software:

- 1) Test a software technique that utilizes well logs, laboratory measurements, field data, and forward modeling for determining the effectiveness of a geophysical survey at a test site.
- 2) Conduct a geological and geophysical analysis of well log information (lithology interpretation, formation identification, well log calculations, well log corrections).
- 3) Conduct physical property measurements (porosity) on rock core samples.
- 4) Make resistivity measurements on rock core samples.
- 5) Calculate permittivity values for the core samples.
- 6) Collect and input seismic data.
- 7) Utilize the GphysCO2 software by inputting the available data, executing EM forward models, executing seismic forward models, processing the data outputs, and producing images.
- 8) Analyze the modeling results to determine the effectiveness and limits of a geophysical survey at the test location.

6.3 Discussion

The implementation of GphysCO2, utilizing the Warren County well as a test site, demonstrated a new technique for investigating a potential carbon injection site. Physical, geophysical, and geological data sets were collected, measured, interpreted, calculated, and analyzed to produce a complete data base that represented the test site. That data base was input into the well-logging, EM, and seismic modules for a numerical investigation of the injection site.

The numerical simulations of the CO₂ saturation models did provide evidence that CO₂ can be detected with time-lapse cross-hole EM surveys. The largest hurdle to full scale field implementation of cross-hole EM surveys is the penetration distance. 100 meters appeared to be the upper spatial limit of a cross-hole EM monitoring survey. The numerical results for the shorter distance surveys revealed that a noticeable change in the EM wave could be seen. The waves were clearly attenuated with a decrease in amplitude and a longer travel time. The implication of that observation is that a time-lapse cross-hole EM survey implemented in the

field, with sufficiently close boreholes, would detect the change that occurs when CO₂ replaces brine between the wells. The results of the cross-hole EM investigation are preliminary but are a necessity for the advancement of the technology. The first step in implementing full-scale EM monitoring arrays is the proof that EM surveys can detect injected CO₂.

This investigation and the GphysCO2 software have laid the foundation for developing state-of-the-art geophysical monitoring techniques for geological injection sites. The next stage is to fully realize a combined EM and seismic tomographic technique. Tomography alone will reveal more subsurface detail and provide the location of CO₂ saturation zones. The geophysical method combination will supply the superior penetration of seismic methods with the sensitivity to pore fluid that the EM method grants.

References

- Agilent, Solutions for Measuring Permittivity and Permeability with LCR Meters and Impedance Analyzers, Application Note 1369-1
- Archie, G. E., Electrical Resistivity an Aid in Core-Analysis Interpretation, Bulletin of the American Association of Petroleum Geologists, Vol. 31, No. 2, pp. 350-366, February, 1947.
- Archie, G. E., The Electrical Resistivity Log as an Aid in Determining Some Reservoir Characteristics, Petroleum Technology, T.P. 1422, January 1942.
- Archie, G. E., Introduction to Petrophysics of Reservoir Rocks, Bulletin of the American Association of Petroleum Geologists, Vol. 34, No. 5, pp. 943-961, May, 1950.
- Arps, J. J., The Effect of Temperature on the Density and Electrical Resistivity of Sodium Chloride Solutions, *Journal of Petroleum Technology*, Technical Note 195, p. 17-20, 1953.
- Bergmann, T., J.O. Blanch, J.O.A. Robertsons, and K. Holliger, 1999, A Simplified Lax-Wendroff Correction for Staggered-grid FDTD Modeling of Electromagnetic Wave Propagation in Frequency-Dependent Media, *Geophysics*, 64, no. 5, pg. 1369-1377 Holt, J. J., 2004, Finite difference time domain modeling of dispersion from heterogeneous ground properties in ground penetrating radar, PhD Thesis, Department of Geological Sciences, The Ohio State University.
- Bahr, A., A. Lauer, and I. Wolff, 1995, Application of the PML absorbing boundary condition to the FDTD analysis of microwave circuits, *IEEE MTT-S Int. Microwave Symp. Dig.*, pp. 27-30.
- Berenger, J.P., 1994, A perfectly matched layer for the absorption of electromagnetic waves, *Journal of Computational Physics*, vol. 114, pp. 185-200.
- Bergmann, T., J.O. Blanch, J.O.A. Robertsons, K. Holliger, 1999, A Simplified Lax-Wendroff Correction for Staggered-grid FDTD Modeling of Electromagnetic Wave Propagation in Frequency-Dependent Media, *Geophysics*, 64, no. 5, pg. 1369-1377.
- Brace, W. F., A. S. Orange, and T. R. Madden, 1965, The Effect of Pressure on the Electrical Resistivity of Water-Saturated Crystalline Rocks, *Journal of Geophysical Research*, Vol. 70, No. 22, pp. 5669.
- Chadwick, R.A., R. Arts, O. Eiken, P. Williamson, and G. Williams, [2006a] Geophysical monitoring of the CO₂ plume at Sleipner, North Sea: an outline review. *In: Lombardi, S., Altunia, L.K., and Beaubien, S.E. (Eds.) Advances in the Geological Storage of Carbon*

- Dioxide*. Springer, Dordrecht, NATO Science, IV Earth and Environmental Sciences Vol. 65, 303-314.
- Chew, W.C., and W.H. Weedon, 1994, A 3-D perfectly matched medium from modified Maxwell's equations with stretched coordinates, *Microwave Opt. Technol. Lett*, pp. 599-604, September.
- Collett, T.S. and J. Ladd, Detection of Gas Hydrate with Downhole Logs and Assessment of Gas Hydrate Concentrations (Saturation) and Gas Volumes of the Blake Ridge with Electrical Resistivity Log Data, *Proceedings of the Ocean Drilling Program*, Vol. 164, Ch. 19, May, 2000.
- Daniels, J.J., R. Roberts, B. Schilling, and R. Erickson, 1992, "GPR measurements for locating underground mine workings at an active open-pit mine": *Trans. Of the Fourth International Conference on Ground Penetrating Radar*, June 8-13, 1992, Rovaniemi, Finland.
- Daniels, J.J., D. Grumman, and M. Vendl, 1997, Coincident Antenna Three Dimensional GPR: *Jour. Env. Eng. Geoph.*, V. 2, No. 1, p. 1-9.
- Dolphin, L., *Ground Penetrating Radar (GPR) Usage and Limitations*, <http://ldolphin.org/GPRLimits.html>, November, 1997.
- Eyuboglu, S., 2005, Applications of ground penetrating radar for environmental and geotechnical problems, *PhD Dissertation*, Department of Applied Sciences, University of Arkansas at Little Rock.
- Gedney, S.D., 1996, An anisotropic perfectly matched layer – absorbing medium for the truncation of FDTD lattices, *IEEE Trans. Ant. Prop.*, vol. 44, no. 12.
- Gupta, N., P. Jagucki, J. Sminchak, D. Meggyesy, F. Spane, T.S. Ramkrishnan, and A. Boyd, 2005, Determining Carbon Sequestration Injection Potential at a site-specific location within the Ohio River Valley Region, in: *Proceedings of the 7th International Conference on Greenhouse Gas Control Technologies*, 5–9 September, 2004, Vancouver, Canada, D.W. Keith, et al.(Eds.), Elsevier, New York. p. 511–520.
- Gurel, L., and U. Oguz, 2000, Three-dimensional FDTD modeling of a ground-penetrating radar, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 38, no. 4, pp. 1513-1521.
- Holmes, A.B., 2005, Solubilities of 4-Phenyltoluene, Phenylboric Acid, Biphenyl, and Iodobenzene in Carbon Dioxide from Measurements of the Relative Permittivity. *J.Chem.Eng.Data*, Vol. 50, pp. 1370-1374.

- Holt, J. J., 2004, Finite difference time domain modeling of dispersion from heterogeneous ground properties in ground penetrating radar, PhD Thesis, Department of Geological Sciences, The Ohio State University.
- Hovorka, S.D., S.M. Benson, C. Doughty, B. M. Freifeld, S. Sakurai, T.M. Daley, Y.K. Kharaka, M.H. Holtz, R.C. Trautz, H.S. Nance, L.R. Myer, and K.G. Knauss. Measuring Permanence of CO₂ Storage in Saline Formations: the Frio Experiment. *Environmental Geosciences*; June 2006; v. 13; no. 2; p. 105-121.
- Juhasz, I., 1979, "The Central Role of Q_v and Formation Water Salinity in the evaluation of Shaly Formations", *The Log Analyst*, Jul-Aug.
- Katz, D.S., E. T. Thiele, and A. Taflove, 1992, Validation and extension to three dimensions of the Berenger PML absorbing boundary condition for FDTD meshes, *IEEE Microwave Guided Wave Letter*, vol. 4, pp.268-270.
- Knight, R. and A. Endres, 1991, A New Concept in Modeling the Dielectric Response of Sandstones: Defining a Wetted Rock Bulk Water System, *Geophysics*, Vol. 55, No. 5 (May).
- Knight, R., A. Nur, 1987, The Dielectric Constant of Sandstones 60kHz to 4 MHz, *Geophysics*, Vol. 52, No. 5 (May).
- Myer, L. R., 2001, Laboratory Measurement of Geophysical Properties for Monitoring of CO₂ Sequestration, Lawrence Livermore National Laboratory Report.
- Newmark, R. L., A. L. Ramirez, W. D. Daily, 2001, Monitoring Carbon Dioxide Sequestration Using Electrical Resistance Tomography (ERT): Sensitivity Studies, Lawrence Livermore National Laboratory Report.
- Palacky, G.J., 1987, Resistivity Characteristics of Geologic Targets, M. Nabighian (Ed) *Electromagnetic Methods in Applied Geophysics – Theory*. Society of Economic Geology, Tulsa, Oklahoma, pp 53–129.
- Potter, C.C. and D.S. Foltinek, 1997, Formation Elastic Parameters by Deriving S-wave Velocity Logs, CREWES Research Report, Vol. 9.
- Pyke, K., Daniels, J.J., Vendl, M., and Eyuboglu, S., 2006, Controlled Experiment to Determine GPR Water Table Response and FDTD modeling. In Review, *Journal of Environmental and Engineering Geophysics*.
- Rao, R K., K-H. Lee, C-C. Chen, and R. Lee, 2001, Application of full-polarimetric ground penetrating radar for buried UXO classification, Lecture notes, ElectroScience Laboratory, Department of Electrical Engineering, The Ohio State University.

- Reitz, J., F. Milford, R. Christy, 1992, Foundations of Electromagnetic Theory (4th ed.). Addison Wesley.
- Reuter, C.E., R.M. Joseph, E.T. Thiele, D.S. Katz, and A. Taflove, 1994, Ultrawideband absorbing boundary condition for termination of waveguiding structures in FDTD simulations, IEEE Microwave Guided Wave Letter, vol. 4, pp.344-346, October.
- Roberts, R.L., J.J. Daniels, and L. Peters, 1992, Improved GPR interpretation from analysis of buried target polarization properties: Proceedings of SAGEEP, April 26-29, 1992, Oakbrook, Il, p.597-611.
- Roberts, R.L., and J.J. Daniels, 1993, Analysis of the effectiveness of velocity-depth inversion using bistatic data collected over targets of different sizes, shapes, and orientations: Proceedings on Advanced Ground Penetrating Radar, Second Govt. Workshop on GPR, The Ohio State University Columbus, OH, Oct.26-28.
- Roberts, R. L., 1994, Analysis and Theoretical Modeling of GPR Polarization Data, PhD Thesis, The Ohio State University.
- Roberts, R.L., and J.J. Daniels, 1997, Modeling Near Field GPR in three dimensions using the FDTD Method: Geophysics, Vol. 62, No. 4, p. 1114-1126.
- Sacks, Z. S., D.M. Kingsland, R. Lee, and J.F. Lee, 1995, A perfectly matched anisotropic absorber for use as an absorbing boundary condition, IEEE Transactions on Antennas and Propagation, vol. 43, pp. 1460-1463.
- Nguyen, B., A.M. Geels, J. Bruining, and E.C. Slob, 1999, Calibration Measurements of Dielectric Properties of Porous Media, SPE Journal 4, December.
- Thomsen, L., 1986, Weak Elastic Anisotropy, Geophysics, vol. 51 no. 10, pp. 1954-1966.
- Wickstrom, L., et al. 2010, Characterization of Geological Sequestration Opportunities in the MRCSP Region, Task Report.
- Wickstrom, L., 2009, Geologic Challenges for Carbon Sequestration in the Midwest, Advancing the Science of Geologic Carbon Sequestration Conference at OSU March.
- Wang, T., and G.W. Hohmann, 1993, A finite difference time domain solution for three dimensional electromagnetic modeling, Geophysics, Vol. 58, pp. 797-809.
- Wang, G.L., W.C. Chew, T.J. Cui, A.A. Aydinler, D.L. Wright, and D.V. Smith, 2004, 3D near-to-surface conductivity reconstruction by inversion of VETEM data using the distorted

Born iterative method: Inverse Problems, (Special Section on Electromagnetic Characterization of Buried Obstacles) Vol 20, No. 6, p. S195- S216.

Worthington, A. E., J.H. Hedges, and N. Pallatt, 1990, SCA Guidelines for Sample Preparation and Porosity Measurement of Electrical Resistivity Samples Part I -Guidelines for Preparation of brine and Determination of Brine Resistivity for Use in Electrical Resistivity Measurements, The Log Analyst, Jan.-Feb.

Unalmiser, S. and J.J. Funk, 1998, "Engineering Core Analysis," paper SPE 36780, April.

Yee, K. S., 1966, Numerical Solutions of Initial Boundary Value Problems Involving Maxwell's Equation in Isotropic Material, IEEE Trans. Anten. Propa., vol. AP-14, no. 3, pg. 302-307.

Appendix A: Seismic Software Module

A.1 Seismic Module Outline

The following is a step-by-step look at the seismic module beginning with creating a model and culminating with the OpendTect program:

The opening menu provides the user with the option to build a model or input data for Madagascar or OpendTect.

Figure A.1. Opening Menu.

The next menu is for assigning block size, grid cell size, modeling time, source/receiver locations, and source frequency to a 3D block.

Create FDMENU items

0.00200000	cell size (m)
2.00000	P-wave velocity of background (km/s)
1.00000	S-wave velocity of background (km/s)
2.00000	density of background (units)
info 601	number of time steps
0.302000	Dimension in x-dir (km)
0.302000	Dimension in y-dir (km)
0.302000	Dimension in z-dir (km)
45.0000	Freq in MHz
transmit antenna center x location (m)	
0.150000	
transmit antenna center y location (m)	
0.150000	
transmit antenna center z location (m)	
0.150000	
receiver antenna center x location (m)	
0.150000	
receiver antenna center y location (m)	

Figure 0.2. Attributes Menu.

Now the user can assign layers and objects (cylinders, ellipsoids, pyramids, and spheres) of differing seismic parameters (P-wave velocity, S-wave velocity, and density) to the model.

Figure 0.3. Creating the 3D attribute model.

IDL outputs the data after the model is created. The user can now choose if they want to submit the model data to Madagascar. If they choose to submit, IDL calls Madagascar to numerically calculate the seismic response. When the numerical modeling is completed a message appears in IDL alerting the user that the results are ready. The data is output as a segy file (the universal standard for seismic software). The sequence is shown below.

Figure 0.4. IDL Menu for submitting data to Madagascar.

Figure 0.5. Python menu for selecting the data files.

Figure 0.6. Message appearing in IDL when modeling is completed.

A new window appears giving the user the option to start OpendTect analysis. At this point the user can use OpendTect to build a new project from the data for processing, imaging, and interpretation.

Figure 0.7. IDL menu with option to start OpendTect.

Figure 0.8. Madagascar plug-in for OpenTect. The user can create a complete processing flow.

Figure 0.9. 3-dimensional block view and 2D cross-section of a set of seismic lines in OpenTect.

A.2 Seismic Wave Equation Theory

The wave equation simulates the propagation of elastic waves in a medium. The theory begins with the scalar wave equation (1-D Scalar Wave Equation: (A0.1 & 3-D scalar wave equation: (A.2) representing a wave propagating through a medium.

1-D Scalar Wave Equation: (A0.1)

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2}$$

$$u(x, t) = f(x \pm ct)$$

3-D scalar wave equation: (A.2)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2}$$

Where:

u = wave-field
C = phase velocity
x, y, z = spatial variables
t = time variable.

While the scalar version accounts for the propagation of a wave through an isotropic medium it does not account for different types of waves. The two main body wave types are compression (P-) and shear (S-) waves. The phase velocities for compression and the shear wave type are listed in Equations Compression Wave Phase Velocity: (A.3 and Shear Wave Phase Velocity: (A.4 respectively. As the wave moves through a medium it undergoes mode conversions from P- to S-wave or vice versa. To account for this mode conversion the vector form of the equation must be utilized (Equations Vector Wave Equation (general form): (A.5 & Vector Wave Equation (component form): (A.6).

Compression Wave Phase Velocity: (A.3)

$$v_p = \sqrt{\frac{K + \frac{4}{3}\mu}{\rho}}$$

Shear Wave Phase Velocity: (A.4)

$$v_s = \sqrt{\frac{\mu}{\rho}}$$

Vector Wave Equation (general form): (A.5)

$$(2\mu + \lambda)\nabla(\nabla \cdot u) - \mu\nabla \times (\nabla \times u) = \frac{\partial^2 u}{\partial t^2}$$

89

Vector Wave Equation (component form): (A.6)

$$\mu \nabla^2 u_x + (\mu + \lambda) \left(\frac{\partial}{\partial x} \right) \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) = \frac{\partial^2 u}{\partial t^2}$$

Rocks and other material have specific properties that determine how a seismic wave will propagate through it. In a general sense, materials have mechanical (elasticity, stress, strain) and geophysical (velocity, density) properties. The geophysical properties are measurable properties whose magnitude and directional variation is determined by the mechanical properties of rocks and other materials. Equations Wave Number: (A.7 -

Young's Modulus: (A.11 provide the relationships that relate the fundamental mechanical properties of the rocks to the geophysical properties (velocity and density).

Wave Number: (A.7)

$$k = 2\pi/\lambda = \omega/c$$

Bulk Modulus: (A.8)

$$K = \frac{2\mu(1 + \nu)}{3(1 - 2\nu)}$$

Shear Modulus: (A.9)

$$\mu = \frac{3KE}{9K - E}$$

Poisson's Ratio: (A.10)

$$\nu = \frac{E}{2\mu} - 1 = \frac{3K - 2\mu}{2(3K + \mu)}$$

Young's Modulus: (A.11)

$$E = 2\mu(1 + \nu) = 3K(1 - 2\nu)$$

Where:

= wavelength

= angular frequency

c = speed of light

Stress and strain are crucial when considering how

A.3 Seismic Numerical Modeling Theory

The numerical modeling component in Madagascar is the modeling code ewefd3d, developed by Dr. Paul Sava (Colorado School of Mines). The code uses an elastic finite difference time-domain (FDTD) forward modeling method to calculate seismograms. The seismogram output is calculated with the seismic wave equation applied to elastic anisotropy. Elastic anisotropy is the anomaly where waves travel at different velocities in different directions. Basically, the velocity of the material is not isotropic. The theory is based upon the relationship that each component of stress (σ_{ij}) is linearly dependent upon every component of strain (ϵ_{kl}) (Thomsen, 1986). The 3 directional components (x, y, z) can have the value 1, 2, or 3. This relationship creates 9 instances where each instance has a component of stress and 9 components of strain. This relationship is collapsed down to Equation ($\sigma_{ij} = \sum_{k=1}^3 \sum_{l=1}^3 C_{ijkl} \epsilon_{kl}$, $i, j = 1, 2, 3$), where the elastic modulus tensor (C_{ijkl}) completely describes the elasticity of the medium.

Stress, strain, and Elastic modulus: (A.12)

$$\sigma_{ij} = \sum_{k=1}^3 \sum_{l=1}^3 C_{ijkl} \epsilon_{kl}, \quad i, j = 1, 2, 3$$

The tensor can be represented as C ($=ij$ and $=kl$) in a 6x6 matrix. The matrix can be altered to represent an isotropic media with the isotropy matrix (Isotropy matrix: (A.13) or an anisotropic media with the transverse isotropy matrix (Transverse isotropy matrix: (A.14) where only the non-zero components are shown.

Isotropy matrix: (A.13)

$$C_{\alpha\beta} = \begin{bmatrix} C_{33} & (C_{33} - 2C_{44}) & (C_{33} - 2C_{44}) & & & \\ & C_{33} & (C_{33} - 2C_{44}) & & & \\ & & C_{33} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{bmatrix}$$

Transverse isotropy matrix: (A.14)

$$C_{\alpha\beta} = \begin{bmatrix} C_{11} & (C_{11} - 2C_{66}) & C_{13} & & & \\ & C_{11} & C_{13} & & & \\ & & C_{33} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{bmatrix}$$

$\sigma_{ij} = k = 13l = 13C_{ijkl} \epsilon_{kl}$, $i, j = 1, 2, 3$. The calculation utilizes the bulk modulus (K) and Lamé's parameters (λ and μ) to create the stiffness matrix from geophysical parameters (Equation Lamé's parameters: (A.15).

Lamé's parameters: (A.15)

$$\begin{aligned} \lambda &= \rho * (v_p^2 - 2v_s^2) \\ \mu &= \rho * v_s^2 \\ C_{33} &= \lambda + 2\mu = K + \frac{4}{3}\mu \\ C_{44} &= \mu \end{aligned}$$

The stiffness matrix is a crucial component when modeling the propagation of seismic waves. A model consisting of velocity and density parameters is converted to a model consisting of stiffness matrices. The matrices determine how the simulated wave propagates through the model. This sequence exhibits how geophysical properties are converted into physical properties in the numerical code.

Raw seismic data is output from the numerical modeling code in a SEG-Y format back to the IDL interface. At this point another external program, OpendTect is called. OpendTect is an open-source seismic processing, imaging, and interpretation software package. The unique advantage of using OpendTect is that Madagascar has a plug-in for OpendTect that allows the user to create and execute a complete processing flow utilizing Madagascar programs. Some of the routines include automatic gain control, band-pass filtering, deconvolution, wavelet estimation, de-noising, DMO/AMO/Offset continuation, and velocity analysis. Madagascar also has a suite of migration routines for pre- and post-stack data utilizing Kirchhoff and least-squares techniques. Once the data set has been processed OpendTect provides all of the tools necessary for imaging and interpretation.

Appendix B: EM Module

B.1 EM Module Outline

The top level menu (Figure B.1) for the GphysCO2 software contains four options for entering the EM module: (1) Three Dimensional EM Modeling, (2) Import a line of model data, (3) Two Dimensional GPR, and (4) Three Dimensional GPR. The following sections outline each of these options in detail.

Figure B.1. Top level program menu for GphysCO2. From this menu the EM, Seismic, and well logging modules can be accessed.

B.1.1 Three Dimensional EM Modeling

The purpose of this IDL session mode is to set up data files that are to be fed to the PFDTD modeling software for GPR antenna simulation. The 3-dimensional domain of a PFDTD model of the electromagnetic (EM) wave propagation is called the Maxwell domain or Maxwell region. In the PFDTD modeling, the Maxwell domain is terminated or encapsulated by an absorbing boundary layer called the Perfectly Matched Layer (PML) which has a finite thickness. Basically the dimension, grid cell size, and EM properties, for each sub-block of the Maxwell domain and the PML region are interactively set up in this IDL session. The information for the source and receivers is also defined.

Figure B.2. A right-hand coordinate system is used in the PFDTD modeling in such a way that the positive x-axis points to the right, the y-axis backwards, and the z-axis upwards.

B.1.1.1 Model Parameters

When the dialog Select means to Input appears, the user can choose either to start from the default values of modeling parameters or to get a copy of them from an existing .par file. In the former case, click the Use fdmenu defaults button. The Create FDMENU Items window appears with modeling parameters initialized with default values. If a .par fdmenu file already exists:

1. Click the Start from existing fdmenu file button. The box Pick an existing fdmenu.par file appears.
2. If needed, navigate to a directory in which an earlier saved .par will now be used. Click that .par fdmenu file in the Files box and click OK. The Create FDMENU Items window appears with the modeling parameters initialized with values from the picked .par file.

The model parameters that can be defined in the Create FDMENU Items window are the grid cell size of the Maxwell domain, model dimension, maximum number of time steps, the EM constitutive parameters of the background medium, and the frequency band parameters of excitation source. To set up multiple models of various sets of parameter values, the number of additional variations can be set for some parameters. In the lower part of the window under the title ANTENNA PROPERTIES, locations of transmitter and receiver pairs for traces along multiple lines in the x-direction can be set up. To finish:

1. Click the CONTINUE to Next Step button on the top of the window. If the Use fdmenu defaults button was clicked to get here, save the new parameter data in a .par file whose path and name can be specified when the enter name of NEW fdmenu.par file dialog appears.
2. A Message box displays the new default path information which may have been updated according to the path of existing or new .par fdmenu file.
3. Click OK. The Geophysical Data Analysis dialog appears.

B.1.1.2 Maxwell Block Properties

Figure B.3. GPR Visualization window now appears with the menu options on the left for populating the Maxwell block on the right.

To define every component block of the Maxwell domain:

1. Click Work from Blanks. The GPR Visualization window appears. At the top-left-back corner of the Maxwell block in the graphics view, where the origin of the coordinate system is located, the three navy-blue Cartesian axes are indicated. Note, unlike the coordinate system of the PFDTD simulation software, the one defined and used in this section is a rotated right-hand coordinate frame in such a way that the positive z-axis points down and the positive y-axis points front. However, the positive x-axis direction remains from left to right. Thus the z-coordinate of the top face of the Maxwell domain is zero and the z-coordinate here can be regarded as the depth from the ground surface.
2. Click Add Regular 3D Bodies. The ENTER # of Layers dialog appears. After entering a positive number of layers, press Done. The Regular 3D Bodies window appears. Starting from layer #1 (top layer), thickness and physical properties of each layer can be entered and the input parameters are stored by clicking the ADD a Layer to block bar. For the last layer, thickness field is disabled for input. After the final layer is added, the ADD a Layer to block bar is disabled and the button of Sub-grid size list is enabled. The physical properties of internal grid cells have been initialized with the data of the free space and the corresponding grid cells are not updated for them unless each data input field of the layers is clicked or changed.

Figure B.4. Regular 3D bodies menu.

3. Select a sub-grid size ratio in the drop down list if more objects need to be added to the model. Otherwise, click End + Store Results button in the Regular 3D Bodies window and skip to step. The Sub-grid Block Boundary dialog appears when a sub-grid size ratio is selected. The top line # of Sub-cells/ Base cell (1-D) displays the reciprocal of the sub-grid size ratio selected. To make sure the successful progress, it is advised to monitor the Console view in the main window of IDL Workbench throughout the IDL session.
4. To define the extent of the sub-grid rectangular block, enter the 3-D coordinates (upper fields in meters and lower in cell index numbers) of left-back-top corner (labeled Min. X Y Z in m.) and right-front-bottom corner (Max. X Y Z in m.). After specifying two corners of the sub-grid block, you can replace the physical property data prefilled to the block. The grid cells in the sub-grid block inherit the data of the base grid cells at the corresponding location. If needed, update data fields of the constitutive EM parameters under the line SET OR CHANGE BLOCK PHYSICAL PROPERTIES. Also you can randomize the EM parameter data for the block by entering positive values to fields under the title line NOISE STD. DEV. of PHYSICAL PROPERTIES. To finish the sub-grid block, click the button Done. The Sub-grid Block Boundary dialog disappears.

Figure B.5. Sub-grid Block Boundary Menu

Figure B.6. The Regular 3D Bodies GUI (left) and the main window of IDL Workbench (right) with the GPR Visualization window in the background.

5. The frame edges of the sub-grid block are highlighted in red in the graphics view of the GPR Visualization window after clicking Done in the Sub-grid Block Boundary window. Also a separate viewing window of Sub-grid block appears to display the 3D volume data of the sub-grid block whose values can be defined later. In addition, the drop down list button Shape of 3D shapes in the Regular 3D Bodies window is enabled to start adding any number of the 3D objects to the sub-grid block.
6. For example, the widow of Triangular Columns appears if the Triangular column is selected in the drop down list. Update the location, shape, and the constitutive EM parameters of the 3D shape object in the sub-grid block. Click Apply Property and then click Okay to go back to the window Regular 3DBodies. To add more 3D regular bodies, go back to the drop down list button Shape. The edges of just added object are highlighted in cyan in both viewing windows of GPR Visualization and Sub-grid block.
7. Click End + Store Results button in the Regular 3DBodies dialog when all objects are defined. The window Setup output of multiple files for sequential PFDTD runs appears if any multiple models with additional set(s) of parameter values were chosen. Otherwise, the box enter the LIST file name of PFDTD work directories appears to proceed just for a single model that has been defined already.

Triangular Columns (on node09.viowk)

Okay # of Sub-cells/ Base cell (1-D) = 4,00000

Vertex A: X Y Z in m.
 2,00000 2,00000 5,00000
 8 8 20
 A: in cell index

Vertex B: X Y Z in m.
 2,00000 2,00000 5,00000
 8 8 20
 B: in cell index

Vertex C: X Y Z in m.
 2,00000 2,00000 5,00000
 8 8 20
 C: in cell index

height in m. 0,250000 height in cell index 1

SET OR CHANGE SUBBLOCK PHYSICAL PROPERTIES

Permeability 1,00000 Conductivity 0,00100000 Dielectric 2,00000

NOISE STD. DEV. of PHYSICAL PROPERTIES

Permeability 0,00000 Conductivity 0,00000 Dielectric 0,00000

Apply Property

Figure B.7. Window for 3D triangular column objects.

Figure B.8. The GUI for setting up multiple models.

8. The example shows a simple case wherein more values of the conductivity parameter is being defined. If an additional number of the permittivity variations were selected in the Create FDMENU Items window, there would be a button corresponding to the permittivity in this Setup output of multiple files for sequential PFDTD runs box. Click SETUP MULTI CONDUCTIVITY RUNS to enter the conductivity values of additional models using the box Enter New Conductivity for next run.

Figure B.9. The GUI for updating the conductivity of an additional model.

After the input step of any additional models is finished, you create a list file that contains the directory path names of all the models. To specify the list file name of the current modeling directories, the enter the LIST file name of PFDTD work directories window appears. You must enter the name in Selection box after navigating to its parent directory. It may exist already. If it doesn't exist, it is created.

For each PFDTD model, a directory is produced. The directory name of each model that starts with the name of the list file is appended with the model's parameter values.

First, in the base model's directory, three input data files of the PFDTD simulation software are produced: block.data, antenna.data, and geo.dat.013. Data file block.data keeps the main parameters of the PFDTD computation, such as, grid cell size of the base Maxwell blocks, number of grid cells, number of time steps, frequency band of the excitation source, etc. Data file antenna.data contains the location data of pairs of transmitter and receiver which do not vary with models. Data file geo.dat.013 contains for each grid cell the constitutive EM parameter data which can change from cell to cell. A message "output to geo.dat.013 DONE" is displayed in the Console view of the IDL Workbench main window when its output is done. In addition to these three data files, file subgrid00 is produced also by the IDL software for a model that has a sub-grid block with the sub-grid size ratio different from 1. Subsequently, in the directory of each of

other model(s), three or four PFDTD data files are produced replacing the base model parameters.

If the IDL program multi_runs.pro is properly set, the simulation software PFDTD is run automatically right after its input data files are produced in each model directory. However, normally this option of automatic run of PFDTD is turned off as the modeling computation for each model can take substantially long time. After each model processing is done, a message “PFDTD done” is displayed following “PFDTD running. Pls wait..” in the Console view of the IDL Workbench main window. A message “All data output DONE” is displayed in the Console view of the main menu window when the IDL session is all done. To end the IDL software after a PFDTD modeling session is done, click File ? Exit on the main menu.

Figure B.10. The GUI for a list file of model directories.

B.1.1.3 Importing PFDTD Model Output Data

- The data files that are output from the PFDTD simulation must be imported before entering the Gphyz processing and imaging modules.
- Click Import a line of model data. After model parameters are updated in the Create FDMENU Items dialog, a Question box appears asking if anomaly data, that is, difference of two input data files are needed.
- If anomaly data are going to be produced during the import process, two data files of model output are to be selected as input data files for import: one with a target modeled

and another from a model without the target. Otherwise, only one input data file needs to be selected.

- Pick an existing or name a new output file of model data to be imported. The file name convention of this software requires the name of this output file ends with a .mod extension.
- There is a single line of header in model output data files Ex1.dat, Ey1.dat, and Ez1.dat. To skip this line during the data import, enter 1 in the box Number of input header lines to skip. The samples/trace count is the parameter ‘number of time steps’ used by the PFDTD simulation software. Click Done and the imported data file is produced.
- Click DONE in the Geophysical Data Analysis dialog and then click File? Exit on the main menu to close the IDL session.

Figure B.11. The GUI of parameters for importing model output data.

B.1.2 Two Dimensional

After selecting the two dimensional option, a window asking to “Enter the list of file names to read, or hit cancel for a new file” appears. Select “Cancel” in this window.

Figure B.12. At this window you must select or create a new list file for the program to write to (e.g., C:\GPHYZ data\test.lst). Now click “Save” in the bottom right of the window.

Figure B.13. At this window select the file type and the numbers of files you wish to analyze.

Figure B.14. Double-click the data files that you would like to use in the window that appears next. The number of files that you select is based on what you specified in the previous window.

Figure B.15. After entering the data files the Gphysgpr window will appear on the screen. There are many options available to analyze your data.

B.1.2.1 Decimate/Interpolate truncate samples_traces

Figure B.16. Select the “Decimate/Interpolate truncate samples _traces” option in the Gphysgpr window. A Decimate/Interpolate files window will appear. The options are “Apply-List” or “Apply-File”.

- The “Apply-List” option will bring up an information window telling you that there are many overflow values, select “OK”. Another window will appear telling that “new decimated files now active”, select “OK”.
- The “Apply-File” option brings up another window that contains the data files that you selected when opening “Two Dimensional gpr.” Select the data file to use, then click “OK”.

Figure B.17. A window will appear telling you that there are many overflow values, select “OK”.

B.1.2.2 Standardize Line Lengths

Figure B.18. Select the “Standardize Line Lengths” option in the Gphysgpr window. A Standard Line Length window will appear. Select the “Apply-List” option.

B.1.2.3 Trace Filter and Gain

Figure B.19. Select the “Trace Filter and Gain” option in the Gphysgpr window. A window will now appear asking you to select a data file. The files are the ones that have already specified when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file you would like to use.

Figure B.21. Select the “Two Dimensional Filter” option in the Gphysgpr window. The 2D Filtering window will appear with six options.

Figure B.22. Select the “Smooth horizontal/vertical” option from the 2D Filter window. The Smooth window appears with options to smooth the samples, the traces, or both. An option to select the number of traces or samples to average is also available. Click on the option you would like to use and then select “Apply”. If you choose “Smooth Samples” a window appears warning you that there are many overflow values. Select “OK” to this message. The other options do not have this warning.

Figure B.23. Select the “Average Trace Subtract” option from the 2D Filter window. The Trace Subtraction window now appears. This menu has the options of single fixed, multiple fixed and running average. You can select the number of traces for the multiple or running options. There is another option to center the trace for the single or multiple fixed options. Click on the option you would like to use and then select “Apply”. After selecting any of the options a window appears warning you that there are many overflow values. Select “OK” to this message.

Figure B.24. Select the “Kirkoff Migration” option from the 2D Filter window. The Kirkoff Migration of 2D files menu will appear. It contains the options “Apply-List” and “Apply-File”. There are also options to select trace spacing, velocity, number of traces for calculation, first sample for migration, and the last sample for migration.

- The “Apply-List” option will bring up an information window telling that there are many overflow values, select “OK”. Another window will appear telling that “new Kirkoff files now active”, select “OK”.
- The “Apply-File” option will open a window asking to select a file. The files in this window are the files that you have already specified when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file to use. The data will be analyzed and the migrated value will be printed in the IDL log window in the lower part of the screen.

Figure B.25. Select the “2D Scan Plot” option from the Gphyzgpr menu. A window will now appear asking to select a data file. The files are the ones that have already designated when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file to use.

Figure B.26. Three windows will now appear. The window to the right is a one dimensional representation of some of the data. The window to the left has options for altering the plot once it is ready. In the small window in the middle, select “Okay” to continue with the plotting.

Figure B.27. The 2D scan of your data now appears in the center of the screen with the options menu still present on the left side of the screen.

Figure B.28. Select the “Active Interpretation” option in the Gphyszgr window. The InterActive Interpretation window will now appear. This menu has the options “trace max/min cutoffs”, “pick anomalies”, and “velocity analysis”.

Figure B.30. The next window that appears contains options for interpreting your data. Click on the option that you would like to use. The “Display 2d result” option produces a two-dimensional image of the data. The “Add a cutoff line” option brings up a new menu.

Figure B.31. This menu allows the user to specify the line to insert. It has options for selecting the lower sample number, upper sample number, lower sample cutoff value, and upper sample cutoff value. After selecting the values to use select the “Apply Line” option at the top of the menu to add the specified line to the data trace.

Figure B.32. The “delete a cutoff line” option allows the removal of any line that was added to the trace. Once selecting this option a new menu will appear. The slide rule option allows you to select the line segment number to delete. After selecting this line number click “Delete the line segment shown” to implement this action.

Figure B.34. A window will now appear and ask to select a data file. The files listed in the window are the ones that have already designated when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file to analyze. A new window will appear with an image on the right and a menu on the left.

Figure B.35. Select the “Velocity Analysis” option from the InterActive Interpretation window. Two windows will now appear. One is the trace of the data and the other window is an options window. Select “Okay” in the smaller options window.

Figure B.36. A window will now appear and ask to select a data file. The files listed in the window are the ones that have already designated when opening “Two Dimensional gpr”. Click the “OK” button after highlighting the data file to analyze. The Hyperbolic Velocity Analysis window will now appear. An image of the data appears on the right and the menu is on the left.

Figure B.37. Select the “Single Trace Output” option from the Gphyzgpr window. The “Select Trace for ASCII output” window appears on the screen. Choose between the two options, “Apply to List” or “Apply to File”. The “Apply to File” option will bring up a window asking to select a specific data file instead of working on the entire list.

Figure B.38. Select the “Reverse Polarity on all Traces” option from the Gphysgpr window. Another information window will appear telling the new reverse polarity is complete and to restart GPYZ to activate.

B.1.3 Three Dimensional

Select the “Three Dimensional Plot” option in the Geophysical Data Analysis window. After selecting this option a window asking you to select a block file, or “Cancel”, or create new will appear. Select “Cancel” in this window. Select “Cancel” to the next window to get to a new file. A third and final window will appear after selecting “Cancel” to the previous two windows. There needs to be a block file (~.blk) for the program to write to. An example is to use “test.blk” located at C:\GPHYZ data\test.blk. Click “Save” once the appropriate block file has been selected.

Figure B.39. The next window that appears is where you specify your data file type and the number of files to analyze. The file type should be GSSI and choose the number of files to analyze in the slide rule. Once selecting these two options click the “Okay” button.

Figure B.40. A window will appear to select your data files. Go to the location of the data using this window and select the files by double-clicking each one. Select the same number of files that were specified in the previous window.

Figure B.41. For the next window that appears select “Done” in the top of the window.

Figure B.42. Two windows will now appear. One is the trace of your data and the other window is an options window. Select “Okay” in the smaller options window.

The software will now run through all of the selected data. Click “OK” for the two information windows that appear one after the other. The first is telling that the block is finished and the second is telling that an output file needs to be created next.

Figure B.43. In the window that appears next to select or create a file for the output to be sent to. Select the file that to use and click “Save” (e.g. C:\GPHYZ data\gphysz output).

Figure B.44. Click “Okay” in the top left of the Edit Block window for no changes to the plot.

Figure B.45. The results for the data now appears as a three dimensional plot in a GPR visualization window. The image can be rotated for multiple viewing angles by clicking and dragging the mouse on the image. The menu bar on the left hand side allows the user to change the images characteristics such as color, transparency, and opacity.

B.2 PFDTD Code

The PFDTD Code was designed at The Ohio State University Department of Electrical and Computer Engineering in conjunction with the School of Earth Sciences. The finite difference time domain (FDTD) method was implemented through single- and multi-processor systems leading to the name parallel finite difference time domain (PFDTD). The numerical modeling PFDTD code calculates the EM simulation data based on electrical parameter models. The modeling block consists of two types of sub-blocks, Maxwell Blocks and boundary blocks. The Maxwell blocks contain the actual area of modeling interest (e.g. objects and antenna information). The boundary blocks are a perfectly matched layer (PML) (Sacks et al. 1995).

The FDTD method is a robust computational technique useful for modeling electromagnetic processes. It has been used in induction EM (Hohmann, 1988) and in GPR (Roberts, 1994) studies. Yee described a method (Yee, 1966) for EM induction and GPR that uses a staggered-

grid approximation of Maxwell's curl relations (Holt, 2004) seen in Equation Maxwell's curl relations: (B.1.

Maxwell's curl relations:

(B.1)

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t}$$

$$\nabla \times \mathbf{H} = \mathbf{j} + \frac{\epsilon \partial \mathbf{E}}{\partial t}$$

$\mathbf{E}$ = electric field intensity (V/m)

$\mathbf{H}$ = magnetic field intensity (A/m)

ϵ = permittivity (F/m)

μ = magnetic permeability (H/m)

$\mathbf{j}$ = current density (a/m²)

t = time (s)

Figure B.46. Staggered-grid where electric and magnetic field vectors are located tangent to the edges and normal to the sides, respectively (modified from Yee, 1966; Holt, 2004).

The staggered grid (Figure B.46) used in this method is represented by a perfect square. The electric field ($\mathbf{E}$) values are obtained from the center point of each of the edges and the magnetic field ($\mathbf{H}$) values are taken from the center of each of cube faces. The electric and magnetic field

vectors are offset by one-half of a time step, therefore updating either the electric or magnetic fields requires only previously calculated values (Holt, 2004; Eyuboglu, 2005).

Faraday's and Ampere's Law in rectangular coordinates (Holt, 2004): (B.2)

$$\epsilon \frac{\partial}{\partial t} E_x = \frac{\partial}{\partial y} H_z - \frac{\partial}{\partial z} H_y - \sigma E_x$$

$$\epsilon \frac{\partial}{\partial t} E_y = \frac{\partial}{\partial z} H_x - \frac{\partial}{\partial x} H_z - \sigma E_y$$

$$\epsilon \frac{\partial}{\partial t} E_z = \frac{\partial}{\partial x} H_y - \frac{\partial}{\partial y} H_x - \sigma E_z$$

$$\mu \frac{\partial}{\partial t} H_x = \frac{\partial}{\partial z} E_y - \frac{\partial}{\partial y} E_z$$

$$\mu \frac{\partial}{\partial t} H_y = \frac{\partial}{\partial x} E_z - \frac{\partial}{\partial z} E_x$$

$$\mu \frac{\partial}{\partial t} H_z = \frac{\partial}{\partial y} E_x - \frac{\partial}{\partial x} E_y$$

= conductivity at a specific point in the grid (S/m)

The central difference approximation: (B.3)

$$\frac{\partial}{\partial x} f(x) \approx \frac{f(x + \Delta x / 2) - f(x - \Delta x / 2)}{\Delta x}$$

$$f(i \Delta x, j \Delta y, k \Delta z, n \Delta t) = f^n(i, j, k).$$

Equation FDTD calculation: (B.4 shows an example of the finite difference calculation yielding an approximation of E_x at the location $(i+1/2, j, k)$ at time step $(n+1)$ and H_y at the location $(i+1/2, j, k+1/2)$ at time step $(n+1/2)$ (Roberts, 1994).

FDTD calculation: (B.4)

$$E_x^{n+1}(i + \frac{1}{2}, j, k) =$$

$$\frac{2\epsilon(i+\frac{1}{2}, j, k) - \sigma(i+\frac{1}{2}, j, k)\Delta t}{2\epsilon(i+\frac{1}{2}, j, k) + \sigma(i+\frac{1}{2}, j, k)\Delta t} E_x^n(i + \frac{1}{2}, j, k) + \frac{2\Delta t}{2\epsilon(i+\frac{1}{2}, j, k) + \sigma(i+\frac{1}{2}, j, k)\Delta t} \left[\frac{H_y^{n+\frac{1}{2}}(i+\frac{1}{2}, j+\frac{1}{2}, k) - H_y^{n+\frac{1}{2}}(i+\frac{1}{2}, j-\frac{1}{2}, k)}{\Delta y} - \right.$$

$$\left. H_{yn+1/2, i+1/2, j, k+1/2} - H_{yn+1/2, i+1/2, j, k-1/2} \Delta z \right]$$

$$H_y^{n+\frac{1}{2}}\left(i+\frac{1}{2}, j, k+\frac{1}{2}\right) = H_y^{n-\frac{1}{2}}\left(i+\frac{1}{2}, j, k+\frac{1}{2}\right) - \frac{\Delta t}{\mu\left(i+\frac{1}{2}, j, k+\frac{1}{2}\right)} \left[\frac{E_x^n\left(i+\frac{1}{2}, j, k+1\right) - E_x^n\left(i+\frac{1}{2}, j, k+\frac{1}{2}\right)}{\Delta x} - \frac{E_{i+12, j, k+1} - E_{i+12, j, k} \Delta z}{\Delta z} \right]$$

The PML forms the boundary around the computation block (Gurel and Oguz, 2000). PML is a reflection less adsorption boundary for EM fields. The original work by Berenger (1994) soon became a popular research area (Chew and Weedon, 1994; Katz et al. 1994; Reuter et al. 1994; and Bahr et al. 1995). Sacks et al. (1995) also studied the use of PML but applied it toward a lossy anisotropic media. Gedney (1996) showed that a lossy uni-axial medium can be perfectly matched to an isotropic space by implementing PML with appropriate parameters. Gedney's PML formulation can be applied to the FDTD methods based on generalized grids or the finite element methods to yield a more computationally efficient process. Rao et al. (2001) further investigated the use of PML (Equation Isotropic medium: (B.5) based on the importance of terminating the isotropic lossy media in the computational area.

Isotropic medium: (B.5)

$$\begin{aligned} \nabla \cdot \mathbf{E} &= -jS \mu [\Lambda] \mathbf{H} \\ \nabla \cdot \mathbf{H} &= jS v_{eff} [\Lambda] \mathbf{E} \end{aligned}$$

Where:

$$[\Lambda] = \begin{pmatrix} \frac{s_y s_z}{s_x} & 0 & 0 \\ 0 & \frac{s_x s_z}{s_y} & 0 \\ 0 & 0 & \frac{s_y s_x}{s_z} \end{pmatrix}, \quad s_p = 1 + \frac{\sigma_p}{j\omega \epsilon_0}$$

When considering a lossy media the permittivity formulation becomes $v_{eff} = v + \frac{\sigma}{j\omega \epsilon_0}$ and the original equation needs to be modified (Rao et al. 2001).

The second curl equation is given by: (B.6)

$$\left(1 + \frac{\sigma_p}{j\omega \epsilon_0}\right) (\nabla \times \vec{H})_p = jS \left(v + \frac{\sigma}{j\omega \epsilon_0}\right) \left(1 + \frac{\sigma_q}{j\omega \epsilon_0}\right) \left(1 + \frac{\sigma_r}{j\omega \epsilon_0}\right) E_p$$

$p, q, r = \text{coordinate directions}$

This equation also has $\frac{1}{(j\tilde{S})^2}$ dependence and is solved by introducing a scaled electric field $\vec{D}$ (Rao et al. 2001).

Updated curl equation with scaled electric field: (B.7)

$$\left(1 + \frac{\dagger_p}{j\tilde{S}}\right) (\nabla_x \vec{H})_p = j\tilde{S} \left(1 + \frac{\dagger_q}{j\tilde{S}}\right) \left(1 + \frac{\dagger_r}{j\tilde{S}}\right) D_p$$

$$D_p = \left(v + \frac{\dagger}{j\tilde{S}}\right) E_p$$

Discretized equations: (B.8)

$$D_p^{n+1} = \left[\frac{2 - (\dagger_q + \dagger_r)\Delta t}{2 + (\dagger_q + \dagger_r)\Delta t} \right] D_p^n - \left[\frac{2\dagger_q \dagger_r (\Delta t)^2}{2 + (\dagger_q + \dagger_r)\Delta t} \right] \sum_{m=0}^n D_p^m + \left[\frac{(2 + \dagger_p \Delta t)\Delta t}{2 + (\dagger_q + \dagger_r)\Delta t} \right] (\nabla_x \vec{H})_p^{n+\frac{1}{2}} +$$

$$\left[\frac{2\dagger_q (\Delta t)^2}{2 + (\dagger_q + \dagger_r)\Delta t} \right] \sum_{m=0}^{n-1} (\nabla_x \vec{H})_p^{m+\frac{1}{2}}$$

$$E_p^{n+1} = \frac{2}{2v + \dagger \Delta t} \left(D_p^{n+1} - \dagger \Delta t \sum_{m=0}^n E_p^m \right)$$

Electric field updated with the magnetic field equation: (B.9)

$$H_p^{n+1} = \left[\frac{2 - (\dagger_q + \dagger_r)\Delta t}{2 + (\dagger_q + \dagger_r)\Delta t} \right] H_p^n - \left[\frac{2\dagger_q \dagger_r (\Delta t)^2}{2 + (\dagger_q + \dagger_r)\Delta t} \right] \sum_{m=0}^n H_p^m - \left[\frac{(2 + \dagger_p \Delta t)\Delta t}{2 + (\dagger_q + \dagger_r)\Delta t} \right] (\nabla_x \vec{E})_p^{n+\frac{1}{2}} -$$

$$\left[\frac{2\dagger_q (\Delta t)^2}{2 + (\dagger_q + \dagger_r)\Delta t} \right] \sum_{m=0}^{n-1} (\nabla_x \vec{E})_p^{m+\frac{1}{2}}$$

In review, an anisotropic PML is used to prevent reflections from the truncated boundary of the model. The conductivity of the PML is chosen to establish a quadratic profile in the outward direction along which the attenuation is preferred (Rao et al. 2001). The PML layers are 20 cells thick on all sides. The permittivity and conductivity of the PML layer are matched to the adjacent Maxwell region for impedance continuity.