Determining the degree of saturation and porosity from the velocity fields of elastic and electromagnetic waves - Application in an area contaminated by hydrocarbon derivatives

Manuelle Santos Góis, Georadar Levantamentos Geofísicos S.A.
E-mail: manuelle.sis@georadar.com.br or manu_usp@msn.com

This paper was prepared for presentation during the 14th International Congress of the Brazilian Geophysical Society held in Rio de Janeiro, Brazil, August 3-6, 2015.

Abstract

Starting from petrophysical models, we have formulated an inverse problem in order to estimate the parameters of the environment, such as porosity and degree of saturation from the velocities of elastic and electromagnetic waves. This formulation was tested in the treatment of acquired data in a chemical plant in the city of São Paulo/Brazil, in a contaminated area by NAPL. Physicochemical analyzes of soil and water samples were taken to characterize the area and seismic data (P and S waves) and electromagnetic (GPR) were acquired for the characterization of NAPL contamination. As a result, we have concluded that the joint inversion velocity attribute retrieves the porosity parameters and degree of DNAPL saturation of the environment impacted by contaminants, as long as they integrate the information obtained from seismic and GPR.

Introduction

Contamination of groundwater and soils by hydrocarbon derivatives occurs mainly by spills and accidents during exploration, refining, transportation and storage operations, forming a contamination plume that normally grows in the direction of groundwater flow.

The fact that changes in physical, chemical, hydraulic and hydrogeochemical occur in the environment in the transport process and permanence of contaminants allows the use of shallow seismic reflection and ground penetrating radar - *Ground Penetrating Radar* (GPR) in the analysis and diagnosis areas contaminated by hydrocarbon derivatives (ESTHER; BRADFORD, 2015; JORDAN et al., 2004; CASTRO; BRANCO, 2003; WADDELL; DOMORACKI; TEMPLES, 2001; DEHAINI, 2001; KIM et al., 2000; JEFFERSON et al., 1998; DANIELS; ROBERTS; VENDL, 1995; BREWSTER; ANNAN, 1994).

In this paper, we have studied the problem of soil contamination and groundwater under the elastic and electromagnetic point of view, based on the formulation described by Paixão, Prado and Mendonça, 2007, who have formulated a direct problem by setting the mineralogical fractions of the environment and their elastic and electromagnetic parameters, porosity percentage and water saturation and DNAPL, so that, then, the P, S wave velocities could be obtained, as well as from the radar in the environment. The solution of the problem proposed by them (the determination of porosity and degree of saturation in DNAPL (S_{DNAPL})) was obtained by minimizing an objective function (inverse problem), defined as the difference between the velocities actual values (obtained for the initial model) and velocities calculated for different porosity and saturation ratios in water and DNAPL in a fully saturated environment.

Basing on the assumption that from the study of the inversion of the velocity fields of elastic and electromagnetic waves, it is possible to estimate the porosity and the degree of soil saturation non-aqueous phase liquids - Non-aqueous Phase Liquids NAPL[1], we conducted geophysical surveys in an area contaminated by hydrocarbon derivatives. These results were compared with the analysis of soil and water samples collected on site.

Methodology

- Area Characterization

The area chosen for the geophysical survey belongs to a chemical plant in the city of São Paulo/Brazil.

The geophysical line was located in the area diagnosed as the most contaminated. In order to describe the lithology and quantify the contamination in the area, we conducted survey hole drilling, well installation for carrying out geophysical tests between the holes, and collect samples of water and soil. To make the boreholes, we used the mixed system of mechanical rotary auger and percussion to collect soil samples. These samples laboratory tests were performed to describe and measure: particle size, apparent density and natural moisture (standard of the *Brazilian Association of Technical Standards* - ABNT 6502/95); hydrogen potential (pH) and redox potential (Eh) (standard EPA 9045C and 2580B);

[1] The Non-aqueous Phase Liquids (NAPL) are hydrocarbons classified as immiscible in water. The NAPL are typically classified into non-aqueous Light Phase Liquids (LNAPL) - e.g, benzene, toluene, ethyl benzene, and xylene with lower density than water (0.80 g/cm^3 - 0. 91 g/cm^3) and Dense Non-aqueous Phase Liquids (DNAPL) - e.g, dichloroethane, trichloroethane, carbon tetrachloride, methylene chloride, chloroform, tetrachlorethylene and trichlorethylene with densities higher than water (1.25 g/cm^3 - 1.62 g/cm^3) (EPA, 2000).

concentrations of benzene, toluene, ethyl benzene, p-xylene, m-xylene and o-xylene (BTEX) through gas chromatography and mass spectrometry techniques (head-space technique) and by the EPA 8260 method.

Particle size analyzes were made from separation sieves, where material has been split according to the grain size: gravel and others; coarse sand; medium sand; fine sand; silt and clay. The classification of sediments was performed according to ternary diagram of Shepard (1954). From the values of apparent density and natural moisture content, we determined the porosity and the degree of saturation of the medium valid for partially saturated media (Vadose Zone - VZ). The porosity values and degree of saturation of the medium presented uncertainties, as they were obtained from the apparent density (soil disturbed samples), since it had not been possible to obtain the actual density of the medium, which would depend on the collection of undisturbed samples in trenches.

The collection of samples allowed the assessment of the degree of the medium contamination, both for the interpretation of the area, and for the definitions of the initial parameters for the modeling study. Analyses of hydrogenionic potential (pH) and redox potential (Eh) supported the evaluation of contamination.

Figure 1 shows the particle size description. Samples were collected every 1 m to a depth of 15 m, not exceeding that horizon to prevent the generation of a preferred path of the contaminants to the water level. We observed that the most surface horizons (up to approximately 5 m) have the highest percentages of clay, and from this depth, the maximum depth (15 m), the horizons become predominantly sandy-silty. Surface horizons are associated with landfill materials, used in waste disposal and flatwork, and the others, with the residual and saprolite soils.

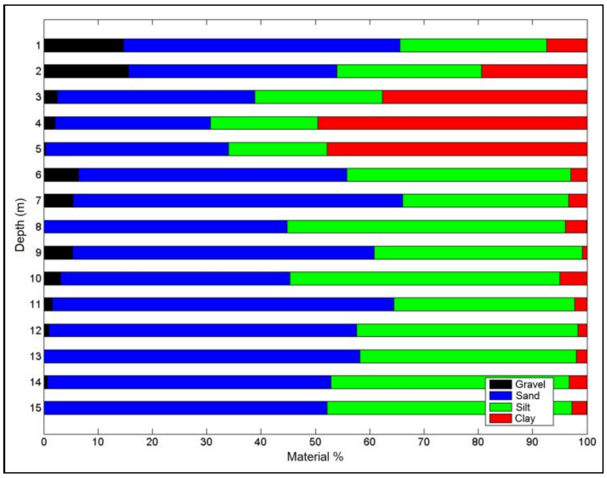


Figure 1 - Particle size description of geophysical line

In Figure 2 we have the density profiles, moisture, porosity and line degree of saturation. The horizons < 4m have the lowest density values; high porosity and high degree of saturation due to the higher volume of voids present in them.

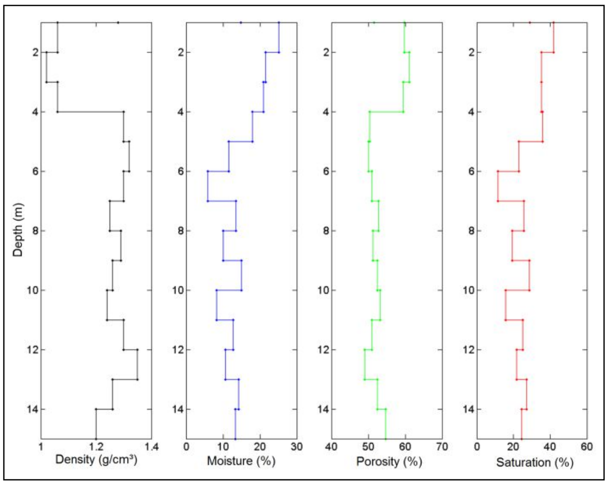


Figure 2 - Density profiles, moisture, porosity and degree of saturation of geophysical line

The results (Figure 3) tests for the concentrations of LNAPL - BTEX - analysis confirmed that the levels are much higher than the industrial intervention scale of CETESB[2] (Benzene = 1 mg/kg, Toluene = 130 mg/kg Ethyl benzene = 50 mg/kg and Xylenes = 25 mg/kg).

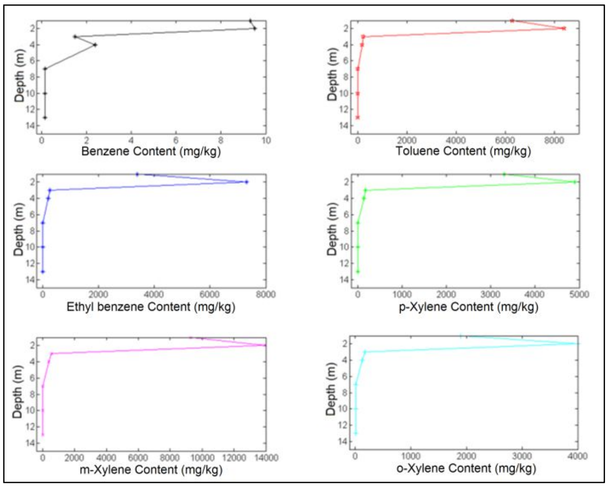


Figure 3 - Saturation profile of BTEX

The physicochemical analyses of the area of all horizons could be characterized as acid (pH < 7) with positive Eh values, characteristic of media that are able to oxidize.

Geophysical Methods

In the same place where we collected soil and water samples the seismic geophysical well surveys and GPR were carried out. The values obtained from these tests supported the direct modeling of petrophysical

[2] Companhia Ambiental do Estado de São Paulo-CETESB

parameters and served as the input parameters for the inversion of the velocity fields for estimating the degree of contaminant saturation and porosity of the medium.

- Seismic test between holes (Crosshole) - V_P and V_S

Velocity profiles of the P and S waves of crosshole survey were obtained from reading the beginning of the wavelets observed in the seismic trace. With these times, using the distance between source and receiver, of 1 m, the velocities were calculated at each horizon profiled (Figure 4).

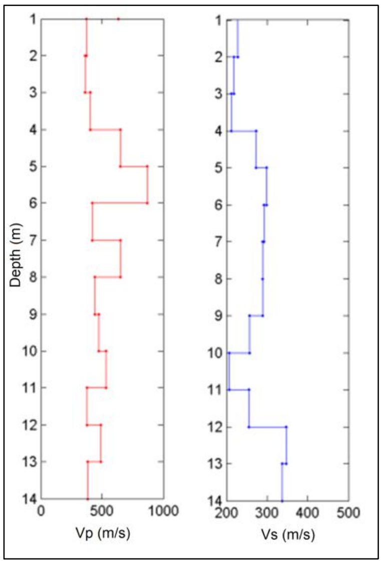


Figure 4-Velocity profile of the P and S waves (Crosshole) survey in geophysical line

- GPR - CMP Record

With the 100 MHz unshielded antenna, we recorded events corresponding to the direct ground wave by an offset of approximately 3 m (Figure 5), both with the transverse mode in the magnetic antenna as with the electrical. This event indicated a velocity of 0.105 m/ns for the electromagnetic wave. The red arrow in Figure 5 indicates the event concerning the direct ground wave propagation.

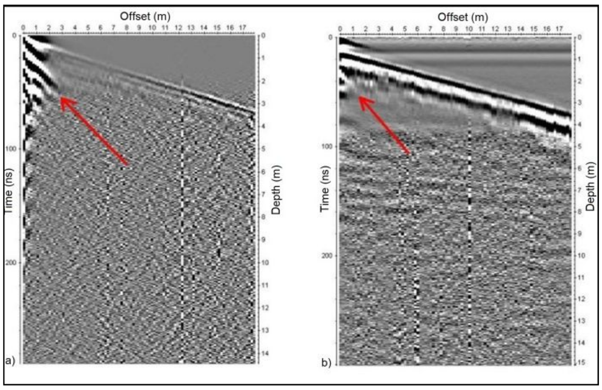


Figure 5 - Radargrams - unshielded 100 MHz modes antennas: a) electric transverse b) magnetic transverse

It was not possible to take an image of any reflector, due to the large signal attenuation. In this industrial area there are the highest rates of contamination, resulting in very high soil conductivity values, which explains the attenuation of GPR signal.

Inversion model

The sensitivity study proposed by Paixão, Prado and Mendonça (2007) and confirmed by Góis (2010) in her doctor degree thesis, showed that the velocity attribute is sensitive to variations of porosity and of S_{DNAPL} degree. Therefore, we set out to formulate an inverse problem in order to estimate the parameters of the medium - porosity and S_{DNAPL} degree - from the velocities of elastic and electromagnetic waves.

Studies of direct modeling formed the basis for the implementation of the object function tests, represented by the differences between actual and calculated data. The joining of the object functions provided for the elastic and electromagnetic waves enabled to estimate the percentage of porosity and the S_{DNAPL} degree of soil in the theoretical models, allowing the application of this methodology to the data of the chemical industry.

The field data were obtained from tests between holes (crosshole) for seismic survey and CMP for GPR.

The process of inversion of the study area data was compared to direct sampling (data collected to a depth of 4 m, representative of the most contaminated horizon of VZ).

We emphasize that in the shallow surveys reflection data for both methods (seismic and electromagnetic) are not easy to obtain because of environmental conditions (conductivity - GPR) and or safety conditions, so the velocity attribute is easier to obtain.

- Construction of object functions and analysis of the error

The construction of the object functions for both elastic waves and electromagnetic wave followed the premise that the pores of the soil would be filled by water, air and DNAPL, totaling 100% of the fluid volume – VZ.

A three-dimensional problem was implemented, where for each value of porosity and degree of saturation a velocity value for each of the velocity fields was obtained (Expression 01).

$$f_{V_P} = \left(V_{P_{Field}} - V_{P_{Calculated}}\right)^2$$

$$f_{V_S} = \left(V_{S_{Field}} - V_{S_{Calculated}}\right)^2$$

$$V_{EMW} = \left(\frac{V_{EMW_{Field}} - V_{EMW_{Calculated}}}{1000}\right)^2 \qquad 01$$

where: $V_{P_{Field}}$, $V_{P_{Calculated}}$, $V_{S_{Field}}$, $V_{S_{Calculated}}$, $V_{EMW_{Field}}$ e $V_{EMW_{Calculated}}$ are the velocities of elastic and electromagnetic fields.

After the velocity fields were determined, that is to say, the field velocity and the calculated one for each combination of porosity and saturation degree, we determined the errors from the readings of linear events (specific for transmission of elastic and electromagnetic waves in direct trajectories) of both seismic data and the electromagnetic data that served as the link to the problem. We attributed errors of 5% of the true values of the velocities (or field) of the P and S waves, and 3% for the velocities of the electromagnetic wave. To determine the error associated with the degree of porosity and the S_{DNAPL} medium, we considered a coupled system in which the velocities of elastic and electromagnetic waves depended on the saturation percentage of fluids and porosity (Expression 02).

$$\sigma^2 = \mathrm{diag}[\bar{\mathrm{G}}^{\mathrm{T}}\bar{\mathrm{W}}\bar{\mathrm{G}}]^{-1} \qquad 02$$

where: $\bar{W} = (1/\sigma_i)^2$ e $\bar{G}_{3x2}\bar{m}_{3x2} = \bar{d}_{3x1}$

$\bar{G}_{3x2}$ is the sensitivity matrix in which the elements of the first row correspond to the derivatives of V_P in relation to porosity and S_{DNAPL}; the second row corresponds to the elements derived from V_S in relation to porosity and S_{DNAPL}; and the third row elements correspond to the elements derived from V_{EMW} in relation to porosity and S_{DNAPL} (for derivatives calculation, the increment for S_{DNAPL} and porosity was 1% of the initial value).

$\bar{W}_{3x3}$ is the weight matrix and the main diagonal elements equal the square of the inverse of the error of measurement compared to 5% of V_P, V_S and 3% V_{EMW}, and the other elements equal zero. Extracting the square root of the matrix main diagonal elements σ_{2x2}, we have the error associated with the porosity and degree of saturation, S_{DNAPL} of the contaminated soil.

Field data results

In the construction of the object function, we used the representative values of VZ for waves velocity fields: V_P - 406.25 m/s, V_S - 218.49 m/s and V_{EMW} - 1.05 x 10^8 m/s, all obtained from actual well data (seismic) and CMP (GPR). Assuming the errors in identification of seismic events and GPR and the order of 5% and 3%, respectively, we constructed contour lines in the region of minimum of the object functions (Figure 6). Thus, the parameter values in the minimum region were restricted to what was wished to obtain.

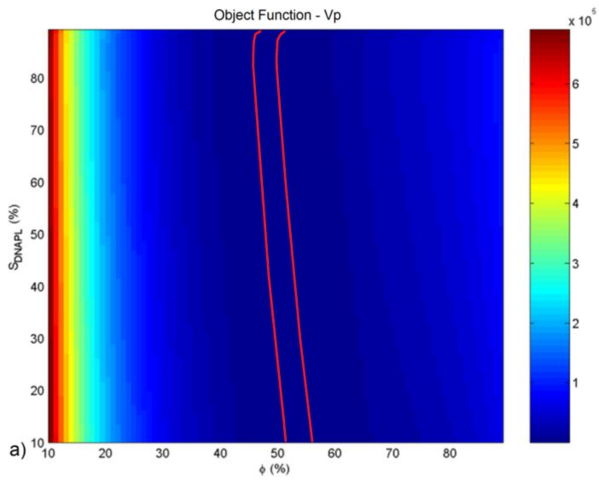
In Figure 6a, we have the object function for the P wave. One can observe that there are several combinations of the same porosity value with varying degrees of S_{DNAPL}. Therefore, the minimum region defines, reasonably well, the porosity, but the degree of saturation of the medium cannot be identified.

For the S wave (Figure 6b) the behavior of the object function is the same, defining porosity and not defining S_{DNAPL}. In the case of the GPR (Figure 6c) the porosity and S_{DNAPL} are not conclusive, but S_{DNAPL} has lower uncertainties than those observed for elastic waves.

In (Figure 6d), we have the object functions integrated with the intersections of the contours of the curves of the errors associated with the identification of seismic and GPR events. Even when jointly analyzed, the results for P and S waves show no uniqueness for answers regarding the degree of S_{DNAPL}, although a better definition for porosity occurs.

Joint analysis improves results, when compared to a single method separately. The region of intersection of the curves of the errors associated with each method provides porosity value ≅ 50% and S_{DNAPL} ≅ 53%−74%. These values, when compared to the direct measurements (Figure 2) indicate that the inversion process retrieves well the porosity, but also shows uncertainties regarding the estimation of the degree of contamination. We emphasize that the medium saturation measurement was made from undisturbed soil samples, which generate inaccurate results.

These results repeated the same pattern observed for the theoretical models (GOIS, 2010), e.g., in order to define the degree of saturation and porosity a joint analysis of elastic and electromagnetic waves is necessary.



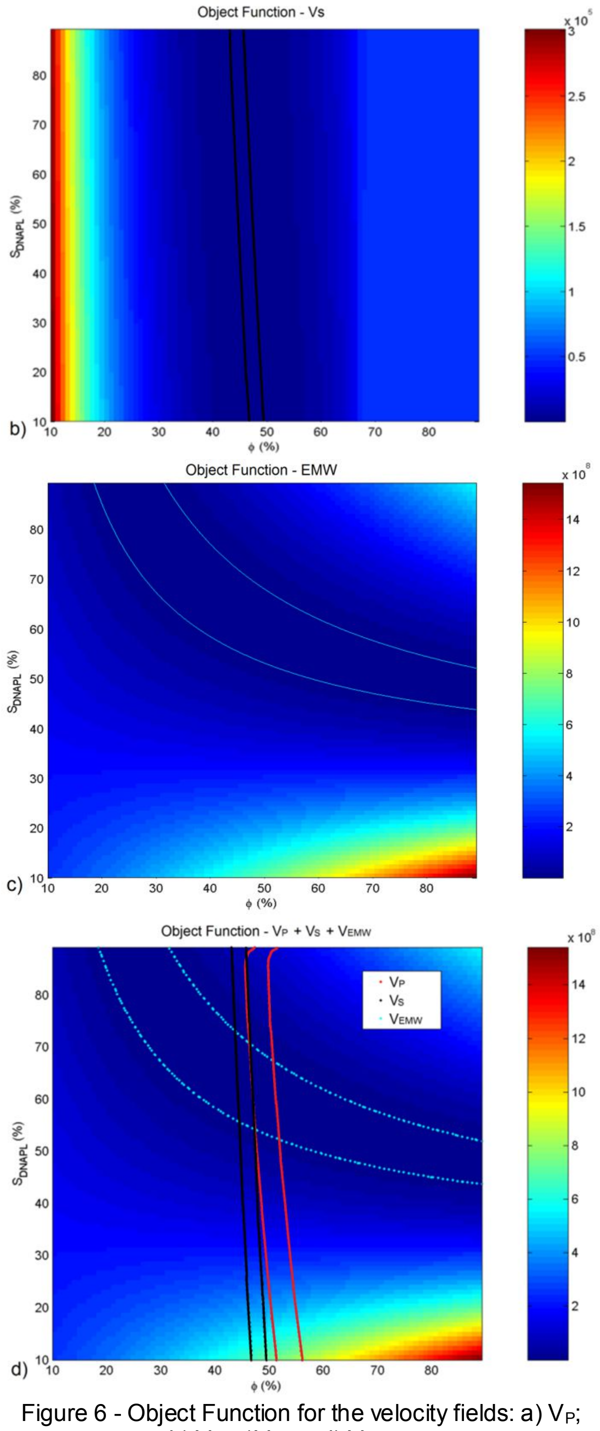


Figure 6 - Object Function for the velocity fields: a) V_P; b) V_S; c)V_{EMW}; d) $V_{Integrated}$

- Discussion of field data

As already mentioned, for the recovery of parameters (porosity and degree of S_{DNAPL}) seismic integration is required with the GPR because only one of the methods does not provide unique information on the degree of porosity nor of S_{DNAPL}. For unconsolidated media (high porosity) and quite saturated with D_{NAPL}, the error associated with the porosity and degree of S_{DNAPL} is small. For media with low porosity and little saturated, the error associated with the porosity is low, but high in the degree of S_{DNAPL} (PAIXÃO; PRADO; MENDONÇA, 2007).

Of the various analyzes that were made, we observed that the error associated with the porosity is small, both with small and high porosity media. On the other hand, the degree of error for the S_{DNAPL} for porous media is smaller when compared to the media that have a low porosity. This is confirmed by the results of object functions. The application of the methodology to actual data (crosshole and CMP test) was satisfactory through the inversion process for the recovery of porosity and uncertain to the degree of saturation of DNAPL. These uncertainties are related to the sensitivity level of the elastic attributes for DNAPL the degree of saturation, e.g. to the scenarios that depict the VZ replacement of fluids, air and water contaminants by contaminant brings no significant differences in the degree of DNAPL saturation.

Acknowledgments

To Professors Doctors Renato Prado and Liliana Diogo; the Instituto de Astronomia, Geofísica e Ciências Atmosféricas-IAG/USP- Departamento de Geofísica; Conselho Nacional de Desenvolvimento Científico e Tecnológico-CNPq and Fundação de Amparo à Pesquisa do Estado de São Paulo-Fapesp (process 2006/01350-1). The entrepreneur and owner of the chemical industry who provided the location for data acquisition.

References

BREWSTER, M. L.; ANNAN, A. P. Ground-Penetrating radar monitoring of a controlled DNAPL release: 200 MHz radar. Geophysics, v. 59, n. 8, p. 1211–1221, august 1994.

CASTRO, D. L. de; BRANCO, R. M. G. C. 4-D Ground Penetrating Radar Monitoring of a Hydrocarbon Leakage Site in Fortaleza (Brazil) During its remediation Process: A Case History. Journal of Applied Geophysics, v. 54, p.127–144, november 2003.

DANIELS, J. J.; ROBERTS, R.; VENDL, M. Ground penetrating radar for the detection of liquid contaminants. Journal of Applied Geophysics, v. 33, p. 195–207, 1995.

DEHAINI, J. GPR Aplicado a Estudos de Contaminação por Hidrocarbonetos. Tese (Doutorado) — Instituto de Geociências - IGc/USP, 2001. 100 f.

EPA, E. P. A. NAPL: Simulator Documentation. [S.l.], 2000.

ESTHER, B.; Bradford, J. H. Reflection waveform inversion of ground-penetrating radar data for characterizing thin and ultrathin layers of nonaqueous phase liquid contaminants in stratified media. Geophysics 80.2, 2015.

GÓIS, M. S. Análise de atributos de dados sísmicos e eletromagnéticos para o diagnóstico de áreas contaminadas por derivados de hidrocarbonetos. Tese

(Dourado) – Instituto de Astronomia, Geofísica e Ciências Atmosféricas – IAG/USP, 2010. 201 f.

JEFFERSON, R. et al. Effects of soil-moisture content on shallow seismic data. Geophysics, v. 63, n. 4, p. 1357–1362, july-august 1998.

JORDAN, T. E. *et al*. Using amplitude variation with offset and normalized residual polarization analysis of ground penetrating radar data to differentiate an *NAPL* release from stratigraphic changes. Journal of Applied Geophysics, v.56, p. 41-58, 2004.

KIM, C. et al. Residual Hydrocarbons in a Water-Saturated Medium: A Detection Strategy Using Ground Penetrating Radar. Environmental Geosciences, v. 7, n. 4, p. 169–176, december 2000.

PAIXÃO, M. S. G.; PRADO, R. L.; MENDONÇA, C. A. Análise da sensibilidade na determinação da porosidade e grau de saturação em DNAPL a partir da inversão das velocidades das ondas P, S e de Radar. Tenth International Congress of the Brazilian Geophysical Society, 2007.

SHEPARD, F. P. Nomenclature based on sand-silt-clay ratios. Journal Sedimentary Petrology, v. 24, p. 151–158, 1954.

WADDELL, M. G.; DOMORACKI, W.; TEMPLES, T. J. Non-Invasive Determination of the Location and Distribution of Free-Phase Dense Nonaqueous Phase Liquids (DNAPL) by Seismic Reflection Techniques. [S.l.], 2001.