

# Solving 2D gravity inversion problems using a PDE model in geophysics exploration

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## ABSTRACT

Inverse modeling is one of the useful solutions to create a logical model with relationships between observed and measured values. In geophysical and subsurface investigations such as cavities or mineral explorations, solving inverse problems using problem physics in a partial differential equation (PDE) system is very important. In this research, COMSOL multiphysics' optimization interface, combined with a PDE or physics interface, was used to solve inverse-modeling problems. Also, a framework is presented to solve undetermined inverse problems using COMSOL multiphysics' optimization. COMSOL multiphysics does not include a gravity calculation module. However, since Poisson's equation governs gravity and electrostatics, a gravity model can be created in the electrostatics module by changing the electrical permittivity value. We present a general adjoint state formulation that may be used in this framework and allows for faster calculation of sensitivity matrices in a variety of commonly encountered underdetermined problems. First of all, 2D inversion of gravity data has been run and validated in COMSOL multiphysics software using one synthetic model and synthetic data in a forward modeling process. Afterward, using real gravity data surveyed along a cross-section of the sinkholes in the NW of Abarkuh, the lateral structure and subsurface cavities were estimated. The inverted gravitational acceleration values, then cross-correlated with observed gravity data and available surface pieces of evidence such as sinkholes and circular structures. The results indicated that our COMSOL-based routines for the solution of PDE-based inverse problems using adjoint states, while high in computational speed, can be used in modeling a wide range of physical systems governed by the partial differential equation laws and also can accurately discriminate between low-density contrast regions and background

**Keywords:** 2D Gravity inversion, Geophysics, Comsol multiphysics, Adjoint operator, Sinkhole.

## 1. Introduction

Inverse modeling is useful in understanding the physical phenomena on Earth and applies to various fields of earth science, including geophysical exploration, groundwater hydrology, and seismology. In forward modeling, we assume that all physical parameters are known, and various models can be simulated through physical laws and scientific relationships. Despite the direct measuring of unknown parameters in inverse modeling, we would like to know their spatial distribution. In this paper, gravity forward modeling will be implemented by solving Poisson's equations with the appropriate boundary conditions, and then a methodology is presented for solving gravity inversion problems using COMSOL Multiphysics. Previously, Zhang et al. (2004) and Farquharson and Mosher (2009) used the numerical solution of Poisson's equation to determine the gravitational acceleration. COMSOL Multiphysics (COMSOL Multiphysics User's Guide, 2009) is a general finite-element modeling environment capable of numerical solving the governing equations in various physics systems [1, 2]. The COMSOL Multiphysics [3] determines many parameters such as electrical resistivity, density, induced polarization (IP), magnetic and hydraulic conductivity [4-10].

The gravity method measures the vertical component of the acceleration at the Earth's surface. The Earth's gravity field is affected by the density of different rocks and structures. Therefore, this method can be used in mineral exploration or studying the subsurface cavities and structures such as bedrocks, channels, and dikes. COMSOL does not include a built-in gravity calculation module, but since gravity and

electrostatics are governed by Poisson's equation, Butler and Sinha, 2012 created a gravity model by changing the electrical permittivity value. Cardiff and Kitanidis, 2008, presented a framework for solving the underdetermined inverse problems using COMSOL Multiphysics [4]. They used the adjoint operator to reduce the computational burden of inverse problems. Despite the most inversion codes designed for a particular application, this method applies to a broad range of physical systems governed by PDEs [5]. The mathematical formulation of most problems involving rates of change with respect to two or more independent variables, usually representing time, length, or angle, leads either to a partial differential equation (PDE) or to a system of such equations. Partial differential equations can be significantly more challenging than ordinary differential equations, since we may not be able to split the computation into discrete (time-)steps and have to approximate the entire solution at once. Special cases of the two-dimensional second-order partial differential equation:

$$A \frac{\partial^2 \varphi}{\partial x^2} + B \frac{\partial^2 \varphi}{\partial x \partial y} + C \frac{\partial^2 \varphi}{\partial y^2} + D \frac{\partial \varphi}{\partial x} + E \frac{\partial \varphi}{\partial y} + F \varphi + G = 0 \quad (1)$$

where A, B, C, D, E, F, and G may be functions of independent variables x and y and a dependent variable  $\varphi$ , occur more frequently than any others, because they are often the mathematical form of one of the conservation principles of physics.

The main benefit of COMSOL for solving inverse problems is that, once a user is comfortable with the software, it can solve a wide range of physical problems. Additionally, COMSOL's "Multiphysics" capabilities allow coupling intrinsically to several physical equations.

This paper presents the forward and inverse modeling theories, followed by running and validating a 2D inversion of gravity synthetic

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data forward-modeled in COMSOL software. Afterward, subsurface cavities were estimated using real gravity data surveyed along cross-sections in a part of sinkhole areas in Abarkuh plain. Finally, the inverted density values were cross-correlated with existing surface pieces of evidence.

## 2. Methods and theory

COMSOL multiphysics does not include a gravity calculation module. However, since Poisson's equation governs gravity and electrostatics, a gravity model can be created in the electrostatics module by changing the electrical permittivity value. Poisson's equation of gravitational potential is:

$$\nabla^2 U = -4\pi G\rho \quad (2)$$

Where  $U$  is gravitational potential in  $J\ kg^{-1}$ ,  $\rho$  is mass density distribution in  $kg\ m^{-3}$ , and  $G = 6.67 \times 10^{-11}\ J\ m\ kg^{-2}$  is the universal gravitational constant (e.g., [11]).

Poisson's equation of electrical potential ( $V$ ) in  $V$  is

$$\nabla^2 V = \frac{-\rho_c}{\epsilon} \quad (3)$$

Where  $\rho_c$  is the charge density distribution in  $C\ m^{-3}$ , and  $\epsilon$  is the electrical permittivity [12].

By substituting  $\epsilon = 1/4\ \pi\ G$ ,  $\rho_c = \rho$ , and  $V = U$ , a gravitational potential energy model can be easily created [4].

In order to test the model in 3D, Butler, and Sinha, 2012 used a cylinder with radius,  $a = 1000\ m$ , and density contrast with the surrounding  $\Delta\rho = 100\ kg\ m^{-3}$  previously (Fig. 1.a). For comparison, we used a 2D model the same 3D model with similar specifications (Fig 1. b). In this model, a circle with radius,  $a = 1000\ m$ , and density contrast with the surrounding material,  $\Delta\rho = 100\ kg\ m^{-3}$ , in a square solution domain that is  $10\ km$  on a side was used. The outer rectangular prisms of thickness  $2\ km$  are "infinite elements" that place the outer boundary virtually at infinity.

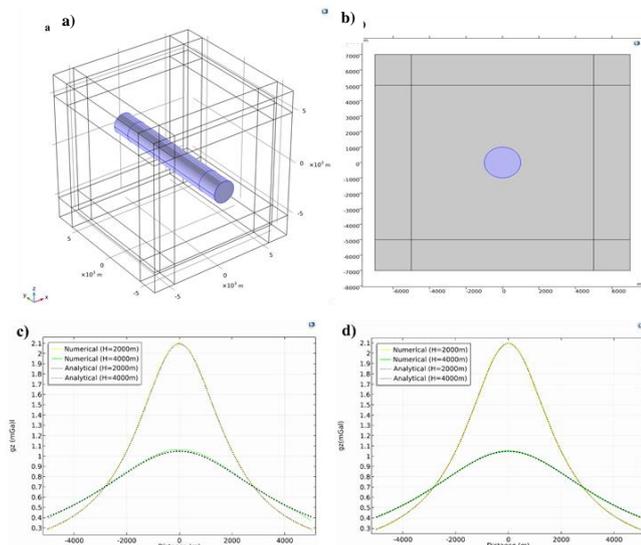


Fig. 1. Geometry solution: the central cylinder (a) and circle (b) has anomalous density  $\Delta\rho$ . The outer rectangular prisms of thickness  $2\ km$  are "infinite elements" that place the outer boundary virtually at infinity. c) and d) Profiles of  $g_z$  at heights  $2$  and  $4\ km$  above the cylinder and circle along the  $x$ -axis over the cylinder and circle's centers. Solid and dotted lines indicate numerical solutions and analytical solutions, respectively.

Profiles of the gravitational acceleration vertical component, perpendicular to the cylinder's long axis, above the cylinder and circle's centers in the  $x$ -direction at  $2$  and  $4\ km$  height, are plotted in Fig.1.c and Fig 1.d, respectively. The red and green solid lines are numerical solutions, and the black dotted lines are the analytical solution. As can be seen, the numerical solution with infinite elements agrees very well with the analytical solution at both  $z = 2$  and  $4\ km$ . The numerical

solution with infinite elements agrees very well with the analytical solution at both  $z = 2$  and  $4\ km$ . The numerical solutions of both models ( $2$  and  $3$  space dimensions) are quite similar.

In inverse problems, if the number of unknown parameters is more than that of measurement values, the inverse problem is underdetermined. The objective function for an underground inverse problem is the sum of a fitness and penalty term [5]:

$$L(y, s) = L_{fitness}(y, s) + L_{penalty}(s) \quad (4)$$

The first term in (4) is equivalent to a weighted data-fitting criterion, and the second term measures the smoothness of the field relative to the given variogram.

$$L_{fitness}(y, s) = (y - h(s))^T R^{-1} (y - h(s)) \quad (5)$$

Where  $y$  is an  $m$ -dimensional row vector of measurement values;  $s$  is an  $n$ -dimensional row vector of parameter values;  $h: R_n \rightarrow R_m$  is the forward model, and  $R$  is an  $m$ -by- $m$  covariance matrix of the measurement errors. Assuming that the measurement errors are independent and identically distributed with variance  $\sigma_R^2$ , it that  $R = \sigma_R^2 I$ , where  $I$  denotes the  $m$ -by- $m$  identity matrix [5].

In the gravity method, the density values are calculated from measurements of the vertical component of the acceleration at the Earth's surface. Therefore,  $y$  in equation (5) is an  $m$ -dimensional row vector of the vertical component of the acceleration, and also,  $s$  is an  $n$ -dimensional row vector of density values.

The vertical component of the acceleration measurements are assumed to be independent and have accuracy on the order of  $\Delta H = 0.01\ mG$ , resulting in the fitness term (Equation 5):

$$L_{fitness}(y, s) = \frac{\|y - h(s)\|^2}{\sigma_H^2} \quad (6)$$

To make use of the experimental data, we must reduce the infinite number of degrees of freedom in the density field to a finite number of unknown parameters. To this end, decompose the quadratic domain into an  $A$ -by- $B$  grid of rectangle (or square), assuming that the density takes a constant value in each rectangle. The number of parameters characterizing the aquifer is then  $A \times B$ , which gives a well-defined underdetermined inverse model that can be solved quickly.

To calculate the penalty term or covariance matrix, the spatially distributed parameters follow a geostatistical distribution defined by some parametrized variogram that is a common assumption in the geological sciences, was used. This COMSOL model uses an exponential variogram of the form  $\gamma = \partial^2 (1 - e^{-\frac{h}{r}})$  with variance  $\partial^2 = 1$  (the sill parameter) and correlation length  $r$  (the range). Since the covariance must approach zero as the distance between samples increases, this implies a simple covariance function  $q(|X_i - X_j|) = q(h) = e^{-\frac{h}{r}}$ . Thus, for the penalty term, the elements of the covariance matrix  $Q$  are easy to evaluate.

The penalty term distinguishes between solutions with comparable fitness values in problems where the number of parameters,  $n$ , exceeds the number of measurement values,  $m$ . Through geostatistical reasoning, Kitanidis ([13]) arrived at the penalty term

$$L_{penalty} = (s - X\beta)^T Q^{-1} (s - X\beta) \quad (7)$$

where  $Q$  is covariance matrix by the following formula:

$$Q = E[(s - X\beta)(s - X\beta)^T] \quad (8)$$

$X$  is an  $n$ -dimensional row vector with every element equal to one, and  $\beta$  denotes the scalar constant mean of the parameter field. The covariance matrix elements are only a function of the distance between the corresponding points in space:

$$Q_{i,j} = q(|X_i - X_j|) \quad (9)$$

The dependence of  $q$  is expressed by the following variogram that can be fitted on the data.

$$\gamma(X_i - X_j) = q(0) - q(|X_i - X_j|) \quad (10)$$

Therefore, for the penalty term, the covariance matrix elements of  $Q$  are easily calculated using variography of input data and determining

the spatial geostatistical data indices. Despite calculating the  $Q^1$  matrix, which will increase the computation time and expense, the penalty term can be split into two distinct parts.

$$L_{penalty} = (s - X\beta)^T u$$

$$u = Q^{-1}(s - X\beta) \quad (11)$$

Solving the linear equation  $Qu=s-X\beta$  is cheaper than inverting the  $Q$  matrix [5]. The Levenberg–Marquardt method was used for solving and optimizing the nonlinear least-squares problem. The Levenberg–Marquardt algorithm as implemented in the Optimization Module relies on two fundamental ideas: evaluation of an approximate Hessian and regularization of the Hessian approximation. The special structure of least-squares objective functions allows cheap evaluation of an approximate Hessian (matrix of second derivatives), which can in principle be used directly in a Newton iteration. However, least-squares problems are also often ill-conditioned, making the full Newton process unstable. Therefore, the Hessian is modified using a regularization parameter to guarantee its positive definiteness. This parameter is updated between iterations, based on the success or failure of the previous step [14]. For a better understanding of the forward and inverse modeling, see Fig 2.

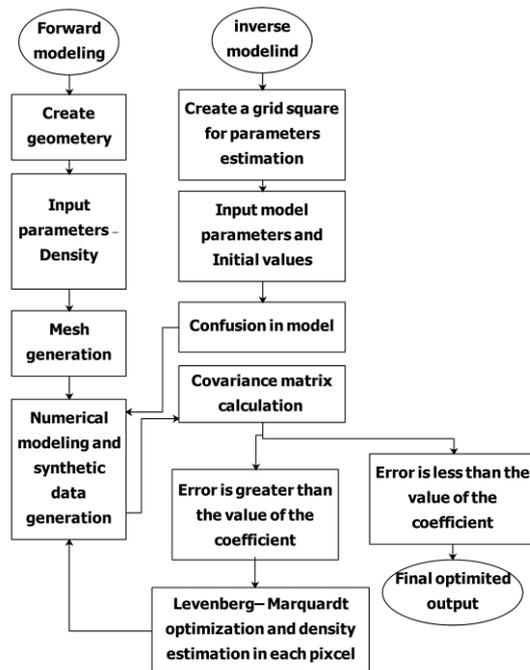


Fig. 2. Process flow diagram of Forward and inverse mod.

### 3. Creating the synthetic model and implementation in COMSOL

Previously, Cardiff and Kitanidis 2008, developed an adjoint state formulation for the general “coefficient form” PDE in COMSOL and presented an example of an inverse problem in the field of aquifer characterization and present results from the COMSOL as a forward model and an adjoint state solver [5]. In this section, we will apply this technique to a 2D synthetic gravity model using the AC/DC module of COMSOL. In the gravity field, a common inverse problem is estimating the density of subsurface structure given measurements from the vertical component of gravitational acceleration.

A synthetic model to generate the “field” data was created with two rectangles  $60 \times 40$  m and  $40 \times 20$  m and density contrast,  $\Delta\rho = 100 \text{ kg m}^{-3}$ , (Fig.3). The synthetic model confines domains with infinite boundaries. Also, a constant potential,  $U = 0$ , was imposed as a boundary condition on all the outer boundaries. The model mesh consists of 6840 domain

elements and 516 boundary elements. The synthetic data using forward modeling relations (equation (2) and (3)), was generated and the vertical component of gravitational acceleration in mGal was calculated on the surface (black point with ten meters apart in Fig. 3). Forward-calculating the solution used 859 Mbytes of physical memory, 1004 Mbytes of virtual memory, and took 1 s. Table 1 shows the properties of the numerical model.

The forwarded data  $\pm 5\%$  noise were used as observation in inverse modeling.

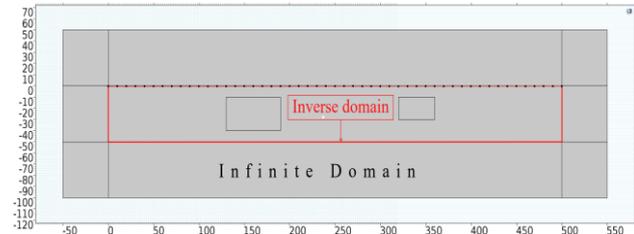


Fig. 3. Synthetic model for creating synthetic gravity data.

Table 1. Relevant synthetic forward model information.

Dimensions	2D
Geometry	Two rectangles anomalous $60 \times 40$ m and $40 \times 20$ m in a rectangle background $500 \times 50$ m surrounded by 50 m buffer (minimizes effects of boundary conditions on gravitational acceleration)
Density contrast	$\Delta\rho = 100 \text{ kg m}^{-3}$
Outer boundary conditions (BCs)	Dirichlet
Out-of-plane thickness	10m
Total # of Gravity stations	51
Station intervals	10 m
Measurements	gravitational acceleration
Time solution	1 s
Mesh elements	6892 domain elements 568 boundary elements
Memory	Physical memory: 0.859 GB Virtual memory: 1.004 GB

All calculations were done for  $10 \times 10$  m pixels in the red area of Fig. 3 (Inverse domain), and bulk densities ( $\text{kg/m}^3$ ) were detected for all pixels. The least-squares nonlinear method using Levenberg–Marquardt optimization was applied to solve the inverse equations. Resulted of inverse modeling is shown in Fig. 4. The lateral and vertical separation is acceptable (Fig. 4. up), as well as the agreement between the observed and measured values (dashed black and solid red lines, respectively, in Fig. 4. down). As can be seen in Fig.4, the black dashed line is the values obtained from the forward modeling. These data with the addition of  $\pm 5\%$  noise that were used as observation in inverse modeling, denoted by the black dotted line and calculated values in inverse modeling are shown with the solid red line.

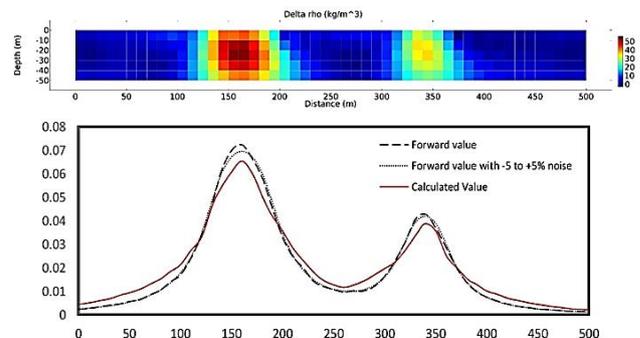


Fig. 4. Detected density for  $10 \times 10$  pixel using inverse modeling (up) and comparing between observed and measured values (dashed black and solid red lines, respectively).

#### 4. Case study (Sinkholes area in Abarkuh plain)

The study area is located in Abarkuh plain at SW Yazd province. In this area, subsidence has occurred due to groundwater over-pumping during the last two decades. Also, some big sinkholes have occurred in the land-subsided area that could have a devastating collapse effect on urban settings because of their proximity to the Abarkuh city. Deep cracks, cavities, and circular structures on the ground (Fig. 5) near Abarkuh city are some pieces of evidence of sinkholes or land subsidence occurrences.



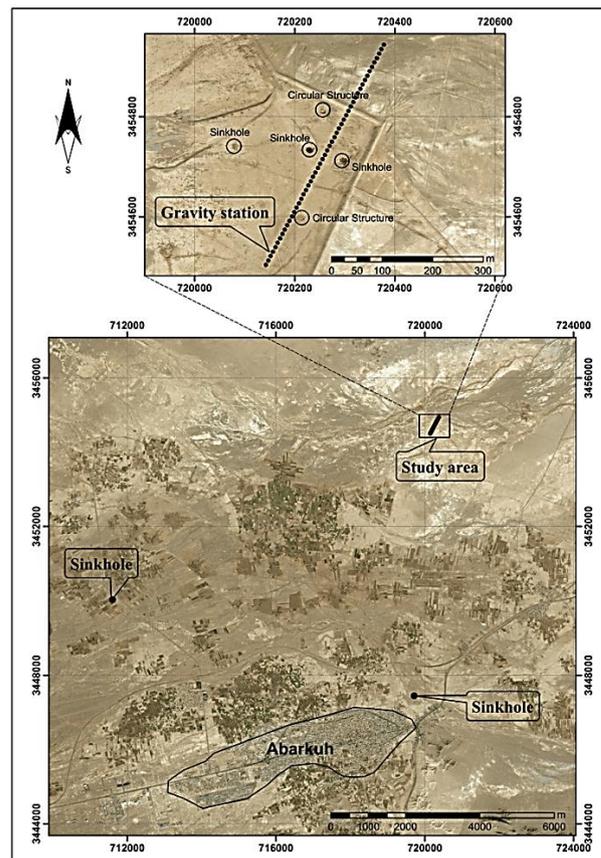
**Fig. 5.** Creating deep cracks, cavities, and circular structures on the ground around Abarkuh as pieces of evidence of sinkhole occurrence.

The study area is about 7km to the NW Abarkuh (Fig 6). There are three big sinkholes, and two circular structures close together in the region. Fig. 7 shows some of these sinkholes.

The dissolution of clay in alluvium deposits is the main reason for sinkhole occurrence in this region. These types of sinkholes tend to occur in clay because clay holds the soil together like glue, and by leaching the soil into an underground cave, because of the rainwater, a large cave is created, and then, all of a sudden, it cannot support the overburden weight and collapses.

The circular structures might be related to sinkholes around the subsurface cavities. For estimation of subsurface cavities, 51 gravity stations were surveyed ten meters apart along a cross-section across the sinkholes and circular structure occurrences. Gravity data were collected using a CG5 gravimeter with a standard resolution of one microGal. After applying the topography, latitude, and Bouguer corrections, the residual gravity data were implemented as observation value input to COMSOL multiphysics. The resulted in subsurface estimated density values for  $10 \times 10$  pixels and comparing the correlation between observed and measured values are shown in Fig. 8 (The solid red line illustrates the calculated gravity from the inverse modeling and the dashed black

line shows the measured surface data).



**Fig. 6.** The study area and some big sinkholes occurred around Abarkuh.



**Fig. 7.** Some sinkholes with about 10m radius and 17m depth in the study area.

The maximum and minimum difference between estimated density changes from  $-164 \text{ kg/m}^3$  for soil containing empty spaces to  $116 \text{ kg/m}^3$  for compact soil and clay. Sinkholes and circular structures are projected on the gravity cross-section in Fig. 8. The results of inverse modeling indicate that the estimated subsurface cavity (the solid circular shape in Fig.8 up) can be related to sinkholes and circular structures.

## 5. Conclusions

Undetermined inverse problems in which the unknown parameters are more than the measured values can be solved using problem physics in the partial differential equation (PDE) system. This research presented a template to solve undetermined inverse problems of 2D gravity data using COMSOL multiphysics' optimization applying in 2D

or 3D modeling of a wide range of different underdetermined inverse geophysical problems. Also, we present a general adjoint state formulation that may be used in this framework and allows for faster calculation of sensitivity matrices in a variety of commonly encountered underdetermined problems. First of all, 2D inversion of gravity data has been run and validated in COMSOL multiphysics software using one synthetic model and synthetic data in a forward modeling process. Afterward, using real gravity and geoelectric data surveyed along a cross-section of the sinkholes in the NW of Abarkuh, the lateral structure and subsurface cavities were estimated. Finally, the inverted density values were cross-correlated with existing surface pieces of evidence.

The results indicated that this method, while high in computational speed, can accurately discriminate between low-density contrast regions and the background. Flexible and fast processing is an advantage of this method.

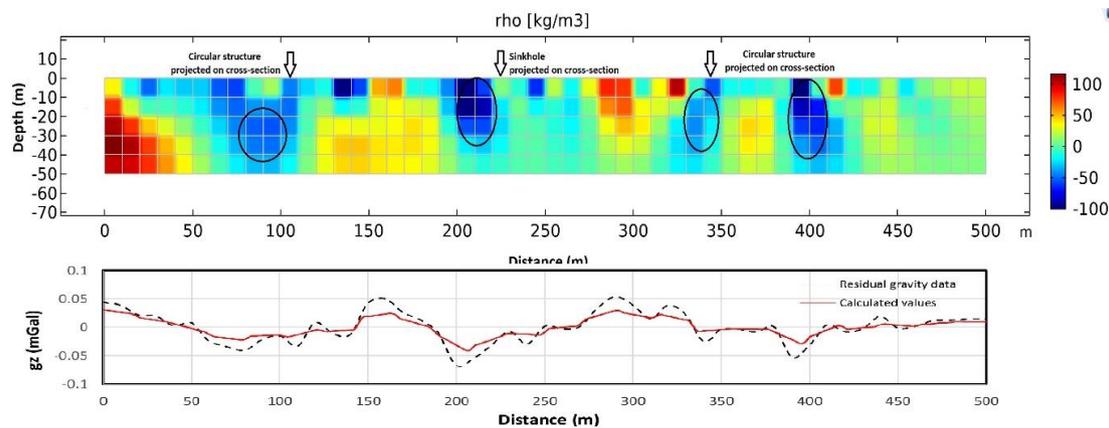


Fig. 8. Gravity value estimated using inverse modeling in Comsol in  $\text{kg/m}^3$  (up) and comparing the correlation between observed and measured values (down).

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