Using reactive transport models to predict the geophysical responses of alteration

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Introduction

Geophysical responses, such as gravity, total magnetic intensity or seismic reflections, result from spatial variations in physical properties, such as density, magnetic susceptibility or acoustic impedance, of the present-day subsurface. The physical properties of the subsurface are a function of prior geological history of the region; in basement terranes, where most mineral deposits are located, the physical properties are primarily controlled by the mineralogy of the rocks in the subsurface. This mineralogy, in turn, is controlled by primary lithology as well as a chemical alteration overprint.

The pmd*RT reactive transport (RT) modelling code, through its simulations of heat and fluid flow, and chemical reactions, produces models of mineralogy that vary both spatially and temporally (Hornby et al., 2008). These models of mineralogy can be used to produce physical property models and hence predict the geophysical response of the alteration system which has been simulated by the chosen reactive transport model.

This summary describes a method that can be used to calculate the geophysical response of a reactive transport model, and provides a simple example of applying this method to a model simulating gold deposition (Cleverley et al., 2006). More detailed analysis of the possible geophysical signatures of this model are given by Chopping (2008); a comparison of these signatures with a known mineralised region are discussed by Chopping et al. (2008).

Symbology

i	Arbitrary mineral index, assuming an array of minerals; subscript on various properties relates to that property for a given mineral
n	Number of minerals that constitute the mineralogy of a cell in the RT model
k	Magnetic susceptibility
v	Seismic velocity
v_p (or v_s)	P- (or S-) wave velocity

Creating physical property models from an RT model

A number of methods to calculate physical properties from mineralogy exists in the published literature. We will discuss some of these methods for three key physical properties: density, magnetic susceptibility and seismic velocity.

Density

Density, defined as the mass per unit volume of material, is the simplest physical property to calculate, and thus is not discussed in the literature. If the calculation of

density does not include porosity, then the calculated density is the bulk or material density (Emerson, 1990). For the purposes of using gravity surveys in the exploration of mineral deposits, the bulk density is the property required for calculating the gravity response.

Reactive transport models specify the mineralogy of the solid phases in terms of the number of each mineral. Defined in the chemical system specification of the model is the molar volume and mass for each mineral, which can be used to calculate the mass and volume of each mineral component of the mineralogy. The density of any given point within the RT model is thus:

$$bulk\ density = \sum_{i=0}^{n} \frac{mass_i}{vol_i}$$

The gravity response depends also on the density contrast with respect to the entire crust. Most gravity maps are based on the Bouguer corrected gravity, which assumes a constant crustal density of 2670 kgm^{-3} (Telford et al., 1990). To produce a physical property model which would simulate the Bouguer response, the bulk density calculated using the above formula needs to be corrected to the Bouguer density:
Bouguer density contrast = bulk density – 2670 kgm^{-3}.

Magnetic susceptibility

Magnetic susceptibility is a dimensionless constant that relates the inducing magnetic field to the magnetic field due to a magnetic material. Although it is dimensionless, it has a different scale in SI compared to cgs units: Susceptibilities for cgs units are 4π smaller than SI susceptibilities (i.e. 1 cgs unit = SI unit / 4π: Whiting, 1986, Telford et al., 1990).

Magnetic susceptibilities are predominantly influenced by magnetite, ilmenite and/or pyrrhotite content, which are the three most ferromagnetic minerals. Some paramagnetic materials, such as quartz, have negligible to negative magnetic susceptibilities. Generally, for modelling magnetic response these are assumed to be particularly small, that is, $k_{quartz} \sim 10^{-7}$ to 10^{-9} in SI units (Williams and Dipple, 2006).

The simplest method to calculate the magnetic susceptibility from mineralogy is to assume that it is a linear average, weighted by the volumetric proportion of each mineral, of the magnetic susceptibility of each mineral:

$$k = \sum_{i=0}^{n} \frac{vol_i}{\left(\sum_{i=0}^{n} vol_i\right)} \times k_i$$

This formula is appropriate for concentrations of magnetite up to ~ 20% by volume. Above this, the magnetic domains do not combine linearly (Shandley and Bacon, 1966; Fannin et al., 1990).

Other empirically derived formulae exist to calculate magnetic susceptibility based on magnetite content (e.g. Werner, 1945; Mooney and Bleifuss, 1953; Grant and West, 1965; Parasnis, 1973). These methods can be applied to the proportion of all magnetic

minerals by using magnetite-equivalent volumes (Shandley and Bacon, 1966):
$vol_{magnetite\ equivalent} = vol_i \times (k_i/k_{magnetite})$.
This magnetite-equivalent volume may then be used in place of the magnetite volume in any method that is only based on the volume proportion of magnetite.

Seismic Velocity

Similarly to magnetic susceptibilities, the seismic velocity of an arbitrary mineralogy can be calculated using linear averaging, weighted by the volume of the minerals:

$$v = \sum_{i=0}^{n} \frac{vol_i}{\left(\sum_{i=0}^{n} vol_i\right)} \times v_i$$

Another method, generally named the time-averaged method (Wyllie et al., 1956), is to linearly average the slowness ($1/v$) of each of the minerals:

$$\frac{1}{v} = \sum_{i=0}^{n} \frac{vol_i}{\left(\sum_{i=0}^{n} vol_i\right) \times v_i}$$

More elaborate schemes exist for calculating seismic velocity from mineralogy, such as Voigt-Reuss-Hill (in Berryman, 1995) or Hashin-Shtrikman (in Watt, 1988); these methods utilise the elastic moduli of the minerals. For minerals of mantle origin, the elastic moduli are well defined - they are required inputs to chemical understandings from regional and whole-earth seismic tomography – they are not well defined for crustal minerals. The linear and time-averaged methods produce similar results, with some subtle differences; our preferred choice is slightly simpler to conceptualise linear averaging method to calculate seismic velocity.

Calculating the model's geophysical responses

Calculating the gravity and magnetic response can be performed using the forward-modelling components of the University of British Columbia – Geophysical Inversion Facility (UBC-GIF) potential field inversion codes *grav3d* (Li and Oldenburg, 1998) and *mag3d* (Li and Oldenburg, 1996). To calculate the gravity, or magnetic, response, the RT model must be sampled on a regular grid[1]. A suitable interpolation method to best preserve the resolution and to limit the introduction of artefacts is the natural neighbour algorithm (Owen, 1992).

For 2D RT models, the regular grid must be extended into the third dimension to adequately calculate the gravity response. There may also be edge effects that result from mass changes off to the side; in this case, it is desirable to mirror the physical property model on either side.

[1] The voxels within the 3D property distribution need not be cubic for the *grav3d* and *mag3d* codes. They can have rectangular sizes, and the cells can be of variable size throughout the property volume. To preserve the spatial resolution of the RT model, however, it is generally advisable to have cells with side lengths similar to the spacing of the closest nodes in the RT model.

The seismic response of the RT model is considerably more complex to forward-model than the gravity or magnetic responses. One simple method to image where reflections may arise from an arbitrary acoustic impedance model is to examine a vertical reflection profile. To calculate this, the reflection coefficient of each cell is related to the acoustic impedance of a cell (depth *z*, horizontal position *xy*) and the cell immediately below it (depth *z+1*, horizontal position *xy*):

$$R_{xyz} = \frac{Z_{xyz} - Z_{xyz+1}}{Z_{xyz} + Z_{xyz+1}}$$

To interpret the vertical reflection coefficient model, reflection coefficients greater than 0.06, in general, will result in a very strong positive reflection, and a reflection coefficient smaller than -0.06 will result in a very strong negative reflection (assuming vertical incidence, Salisbury et al., 2000). More complex methods to calculate the seismic response of an RT model are beyond the scope of this summary report (for a possible scheme see Hobbs, 2003).

An example: the gravity response of an RT model

For this example, we used the listric fault model of Cleverley et al. (2006), created physical property distributions, and then calculated the density response for a gold deposit presently sitting at the base of 100 m of constant low-density (2000 kgm^{-3}) material, to simulate the regolith. The initial RT model was used to simulate an unaltered architecture, and the RT model after chemical alteration and fluid transport was used to simulate an architecture after alteration. This model also has been compared to the known gravity response over a mineralised region (Chopping et al., 2008).

The general pattern of the gravity response over this model is that alteration has increased the density laterally away from the site of gold deposition, and has reduced the gravity response directly above the zone of gold deposition. This decrease of gravity response above the site of gold deposition is approximately 8% of the unaltered response for the same region, which has the potential to be able to be detected in a gravity survey, for station spacings which are at least 1km apart (Chopping et al., 2008).

Conclusions

The prediction of geophysical responses for geochemical simulations provides a new tool to explore, especially in undercover regions. The calculations are likely to be fast enough to be implemented directly in the RT modelling code, although currently they are utilised by calculating on completed RT model time steps. By using these methods on a simple reactive transport model, there is the potential to generate geophysical targets directly from geochemical simulations. These targets compare favourably with known mineralisation at the Victory-Defiance region of the St Ives Gold Mine (Chopping et al., 2008).

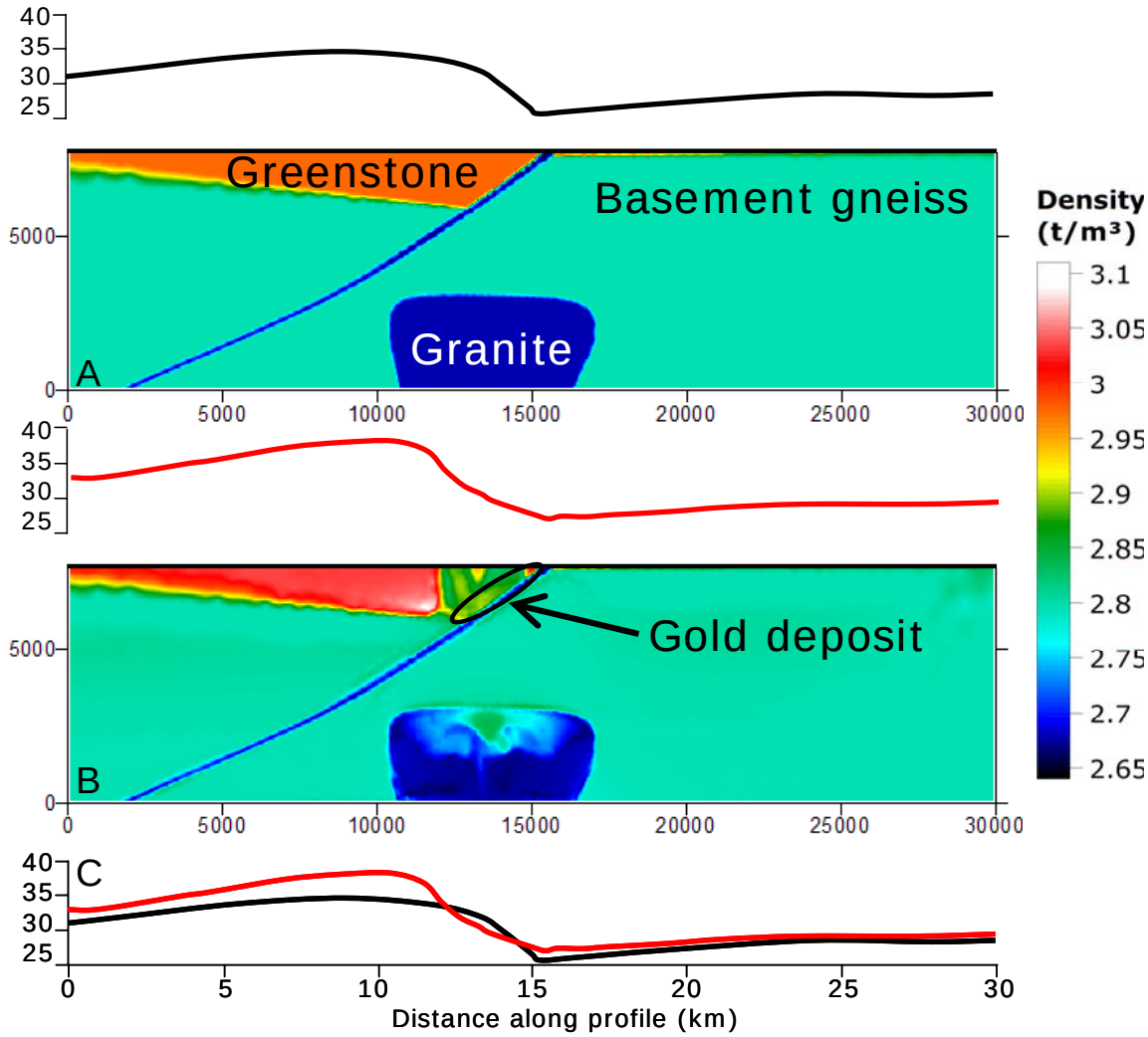

Figure 1: Physical property models, after simulation of erosion and regolith formation, of an unaltered (A) and altered (B) gold mineral system. The profiles above each density model is the corresponding gravity response for that model. In general, alteration has increased the density of the greenstone package in the hangingwall of the fault. The density also haso been increased, although by a smaller amount, in the footwall basement gneiss. The density has been decreased from the unaltered density in the vicinity of the gold deposit (oval); this includes alteration associated with the 'chimeny' directly above the gold deposit. This decrease in density is caused by an increase in carbonate, quartz and some feldspar in this outflow zone. Correspondingly, there are increases in the gravity response, with respect to the unaltered gravity response, on either side of the deposit, and a decrease in gravity response directly above the position of the gold deposit. These differences are apparent when the two gravity profiles are plotted on the same graph (C).

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