Multi-observable thermochemical tomography: a new approach to an old problem

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SUMMARY

The past ten years have been marked by dramatic advances in four seemingly isolated research fields: Thermodynamic modelling of minerals and rocks at high PT conditions, numerical simulation of the thermomechanical behaviour of the Earth's interior, efficient decomposition techniques to solve complex simulation-based problems, and probabilistic data analysis and inversion methods. All these disciplines/techniques have individually created true "revolutions" in the way we understand and model natural systems, including the interior of the Earth. Nevertheless, a more profound understanding is still ahead of us from the formal combination of these disciplines/techniques into a single operational framework to study the physical state of the Earth's interior.

In this contribution, I will present and discuss the concept of multi-observable probabilistic tomography or "thermochemical tomography". This new kind of tomography is particularly designed for studies of the fundamental thermodynamic variables of the Earth's lithosphere, namely temperature, pressure and chemical composition. Once these variables are known, all physical parameters of interest (e.g. seismic velocities, density, viscosity, conductivity, etc), as well as traditional tomography images, are also retrieved in a thermodynamically-consistent way. The method is built on a simulation-based inversion technique where multiple satellite (e.g. gravity gradients, geoid height, etc) and land-based (e.g. seismic, plate motions, heat flow, etc) datasets can be jointly inverted to maximize the physical consistency of the resulting Earth model. Assembling this large problem required a collaborative effort between thermodynamicists, mineral physicists, geophysicists and geochemists, and marks the first step towards a full coupling between geophysics, geodynamics, thermodynamics, and geochemistry. I will present results for both synthetic and real case studies, which serve to highlight the advantages and limitations of this approach.

Key words: lithosphere, multi-observable thermochemical tomography, probabilistic inversion.

INTRODUCTION

There are two main sources of information available to constrain the present-day physical state and chemical composition of the Earth's lithosphere and sub-lithospheric upper mantle: the interpretation of geophysical observables (e.g., gravity anomalies, travel time data, surface heat flow, etc.) and studies on exhumed mantle samples (e.g., xenoliths, tectonically exposed mantle bodies). Experimental petrology/mineralogy and numerical simulations offer an important complement, but they cannot constrain the present-day compositional and temperature structure of the upper mantle *per se*. Both geophysical observables and exhumed mantle samples have their own set of, virtually independent, advantages and limitations when used to make inferences about the upper mantle. Geophysical observables offer a larger and more continuous spatial coverage, but their conversion into estimates of composition and temperature is populated with difficulties. Exhumed mantle samples, on the other hand, represent direct evidence of the compositional and thermal structure of the upper mantle at the time of exhumation. However, their spatial and temporal coverage are highly discontinuous, their original compositions may have been modified by or during the exhumation process, and there may be an inherent bias in that large mantle samples (>40– 60 cm in diameter) may be too heavy for transportation to the surface by magmatic events. Ideally, these sources should be used together to provide a more complete picture of the thermochemical state of the Earth's upper mantle than that resulting from the evaluation of them individually.

The main question is then how to combine both sources of information into an internally consistent, general, and objective inverse framework. Probabilistic formulations (statistical inference) of inverse problems are particularly well suited for the task at hand, simply because the actual solution to the problem is probabilistic in nature. Since (i) the available information from geophysical measurements and/or exhumed mantle samples is always incomplete and subject to uncertainties, (ii) the physical theories we use to make predictions may be imperfect, and (iii) the sensitivity of our measurements to variations in some of the parameters of interest are nonlinear and relatively weak, any inference made on the physical state of the Earth's mantle is necessarily probabilistic. In other words, the best one can, and should, achieve is to obtain a probability density over the parameters of interest, rather than a single, necessarily non-unique solution.

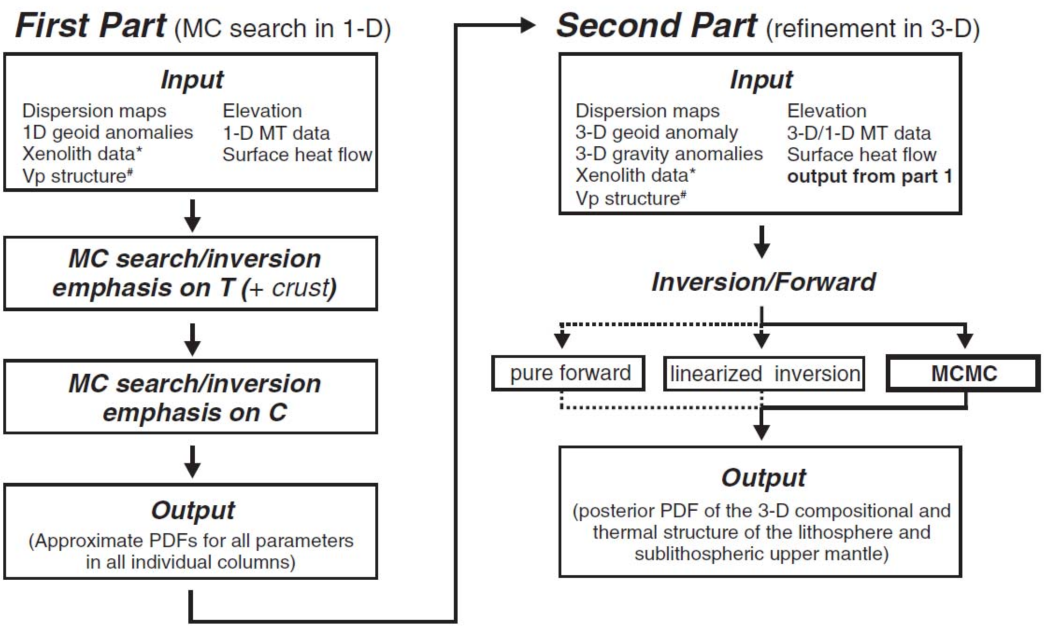
METHOD AND RESULTS

As explained in Afonso et al. [2013b], the entire inversion involves two main stages: In the first stage, we subdivide the 3D volume into individual 1D rectangular columns and invert a subset of the entire data vector in each column using those observables that are most sensitive to the 1D subsurface structure (e.g. surface-wave dispersion curves, geoid height under a 1D approximation, surface heat flow, receiver functions). We set the initial parameter space large enough to include all plausible parameter configurations. Since most of the observables used in this stage are strongly sensitive to the main model parameters (e.g. temperature structure, Moho depth, etc), the initial parameter space is greatly reduced once the first inversion stage is completed. During this first stage, we use the Delayed Rejection Adaptive Metropolis algorithm [Haario et al., 2006] to obtain a population of acceptable models (i.e. realizations) that are compatible with the abovementioned data. Numerous tests indicate that, at this stage, ~ 300,000 realizations per column are enough to reach stationarity of the chain. To be conservative, a total of 400,000 realizations were run for each column; a typical acceptance rate at this stage is ~ 35-40.

Once the first stage is completed, we use the resulting population of acceptable models as priors in the second full 3D stage ("refinement stage" of Afonso et al., 2013b), where the entire data vector (gravity anomalies, 3D geoid anomalies, gravity gradients, body-wave travel-times, etc) is inverted using a standard Metropolis-Hastings algorithm. Effectively, this process "updates" our previous belief (the previous posterior) by adding new information to the problem. The final posterior distribution (i.e. a joint probability function in the parameter and data space) obtained after this second stage therefore represents our best "state of knowledge" and constitutes the most general solution to our inverse problem. A step-by-step description of the entire procedure is included in Fig. 1. The total number of realizations run during this stage is ~ $7x10^6$, with a typical acceptance rate of ~ 30-35%.

In contrast to traditional tomography techniques, the primary variables in our inversion are temperature, major-element composition, and pressure rather than e.g. seismic velocity, electrical conductivity or density. These "secondary parameters" are obtained for each specific realization of the primary variables (i.e. a specific thermochemical Earth model) by solving a Gibbs free-energy minimization problem [Afonso et al., 2013a,b]. Therefore, traditional tomographic images (e.g. S-wave velocity structure) become a ubiquitous by-product of our inversion rather than the main result; with the important difference that our tomographic images explain a large number of independent observations. Note also that since we use a Bayesian approach, the solution to the inversion problem is represented by a posterior probability density function rather than a single model.

This method has been applied in a number of countries (e.g. China, US, Canada, South Africa) and provided fundamental information on the internal constitution of the crust, lithospheric mantle and upper mantle in general. An example in US is shown in Fig. 2; more examples will be shown and discussed in the presentation.



* When this information is reliable, it can be used to limit the compositional parameter space of specific compositional layers
# The present implementation uses ΔVp models only. Future implementations will include the inversion of teleseismic arrival time residuals (see text).

Figure 1: Flow chart illustrating the two-part inversion approach presented in this study. In this paper, we only describe the Markov Chain Monte Carlo inversion method (solid lines) for the second part. Other potential approaches, such as pure forward or linearized inversions (dashed lines), are simpler and more restrictive and therefore will not be discussed here (from Afonso et al., 2013b).

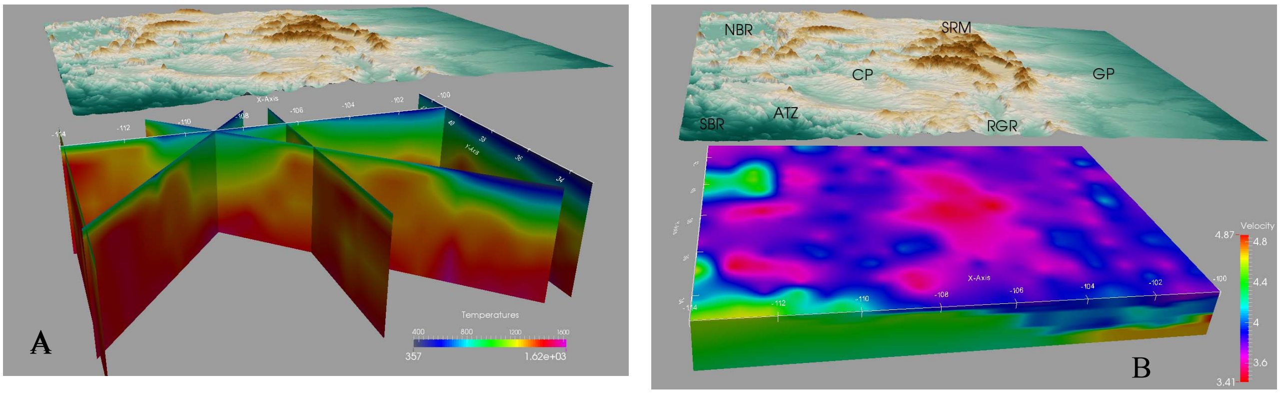


Figure 2: Temperature (A) and shear wave velocity (B) structures beneath the Colorado Plateau and surroundings obtained with the multi-observable probabilistic method of Afonso et al. (2013a,b). In A, the temperature cross-sections extend from 30 to 380 km depth. In B, the top and bottom of the velocity block are at 30 and 60 km depth, respectively.

CONCLUSIONS

The results reported here demonstrate that multi-observable thermochemical tomography offers a sound method to characterise the thermochemical structure of the lithosphere and upper mantle and opens new opportunities for deep-Earth imaging. In this method, all physical and chemical parameters defining an Earth's model are linked together by fundamental thermodynamic relations, rather than by ad hoc empirical assumptions. This allows as to directly invert for the fundamental variables defining the physical state of the Earth's interior, namely temperature, pressure and major-element composition using a multitude of datasets with complementary strengths: body wave teleseismic data, surface wave phase dispersion data, gravity anomalies, long-wavelength gravity gradients, geoid height, absolute elevation, and surface heat flow data. The final result is a multidimensional probability density function containing the entire population of thermochemical Earth models that are simultaneously compatible with all used constraining datasets. Consequently, a ubiquitous by-product of this type of inversion are traditional tomographic images of physical parameters such as seismic velocity. However, our tomographic images are, by design, also compatible with all the other inverted observables instead of satisfying one type of dataset only. This is important, as any model deemed representative of the real physical state of the Earth's interior should pass the test of explaining other geophysical datasets as well.

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