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Precalculated phase equilibrium models for geophysical properties of the crust and mantle as a function of composition

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[1] The use of phase equilibrium calculations to compute physical properties of rocks has become commonplace in geophysical modeling. Typically, the phase equilibrium calculations are used to construct two-dimensional tables of rock properties as a function of pressure and temperature. We document a computer program that can be used to assemble a three-dimensional table that accounts for compositional variations from such two-dimensional tables. A user-selected interpolation scheme is used to recover data from the tables as continuous function of its independent variables. We illustrate the utility of the program using two examples. The first explores the effect of water content of an average continental crust composition. As water content is the primary parameter controlling the amount of melt and/or low-density fluid present in the crust, this model provides a basis for assessing the impact of fluids on the geophysical properties of the crust. In the second example, we model the mantle composition as a mixture between harzburgitic and basaltic end-members. We show that for purposes of seismic velocity calculations, the continuum model is well approximated by interpolation from a table in which the compositional variable is sampled at 10% intervals. The tables for both examples are provided electronically as ready-to-use geophysical tools.

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1. Introduction

[2] The use of free energy minimization codes to calculate the proportions and compositions of minerals and consequently bulk rock properties has become commonplace in geophysical modeling [e.g., *Kuskov and Panferov*, 1991; *Sobolev and Babeyko*, 1994; *Saxena*, 1996; *Connolly and Kerrick*, 2002; *Connolly*, 2005; *Stixrude and Lithgow-Bertelloni*, 2005; *Ricard et al.*, 2005; *Khan et al.*, 2006]. The free energy minimization code may be implemented dynamically within the larger framework of a geo-

physical code [e.g., *Khan et al.*, 2006; *Tirone et al.*, 2009; *Hebert et al.*, 2009], or statically via tables that are calculated prior to the solution of the geophysical application [e.g., *Petrini et al.*, 2001; *Gerya et al.*, 2001; *Xu et al.*, 2008]. The virtue of dynamic implementations are that they do not require the range of physical parameters to be anticipated in advance, but such implementations are costly and may lead to numerical instabilities [*Connolly*, 2009], making static implementations preferable when practical. The definition of practical in this context is dependent on the amount of memory required to store the tabulated data; however, present-day computational standards are such that there is effectively no limit on the resolution of a three-dimensional parameter space, e.g., defined by pressure (*P*), temperature (*T*) and a compositional parameter (*C*). Here, we describe a simple program, PHEMGP, for assembling three-dimensional tables (*P*, *T* and *C*) from two-dimensional tables (*P*, *T*) and for the recovery of data from the resulting three-dimensional table by interpolation. Our intention is to provide a simple program that can be easily modified to change interpolation schemes or to allow combination of phase equilibrium data with nonthermodynamic properties for the estimation of transport properties such as thermal conductivity and viscous rheology. To illustrate the utility of the program we construct seismic models for the crust and mantle as a function of pressure, temperature and a compositional parameter.

[3] For the seismic model of the mantle we define the local mantle composition as a binary mixture of harzburgitic and basaltic components [e.g., *Nakagawa and Tackley*, 2005; *Xu et al.*, 2008]. In this context, *Xu et al.* [2008] suggest two limiting models that they differentiate as mechanical mixing and equilibrium. In the mechanical mixing model aggregate mantle properties are computed as the Voigt-Reuss-Hill (VRH) average [*Watt et al.*, 1976] of the equilibrium mineralogies of the harzburgitic and basaltic end-member lithologies, while in the equilibrium model properties are based on the stable mineralogy computed directly at the composition of interest. Both models are implemented here.

[4] The purpose of the crustal model is to predict the physical conditions at which geophysical properties are likely to be reduced by the presence of fluids, i.e., low-density aqueous fluid or silicate melts. As bulk water content is the first-order parameter dictating the stability of fluids, we compute crustal seismic velocities for a single nonvolatile bulk chemistry [*Taylor and McLennan*, 2009] as a function of water content, pressure and temperature.

2. Precalculated Tables

2.1. Two- and Three-Dimensional Tables

[5] In the present context, two-dimensional tables are a digital representation of stable phase equilibria sampled at regular intervals for two independent variables, hereafter taken to be pressure and temperature. Three-dimensional tables are formed by combining two or more tables calculated at different values of a third variable, which is taken here to be composition. The purpose of the program PHEMGP is to combine an arbitrary number of two-dimensional tables to form a three-dimensional table and to extract phase equilibrium data and/or related geophysical properties from it as a continuous function of the table variables by interpolation.

2.2. Algorithm

[6] The PHEMGP code for constructing and manipulating three-dimensional tables is written in standard Fortran 2003 and Python. For a specified *P-T-C* condition, or range of conditions, PHEMGP can be used to extract the properties of individual stable phases or the aggregate properties of the stable phases (i.e., rock properties). To extract a property at an arbitrary *P-T-C* coordinate within the parametric space of a table, PHEMGP (1) finds the two *P-T* tables closest to the *C* value of interest, (2) obtains the individual phase properties by bilinear interpolation from the phase properties at the four nodes of the table closest to the *P-T* coordinate in each of these *P-T* tables, and (3) computes aggregate properties, other than elastic moduli, as the volumetrically weighted arithmetic mean of the individual phase properties. The averaging of the elastic properties of individual phase properties to obtain aggregate elastic properties is done, at the users option, by one of two methods. For the mechanical mixture model [*Xu et al.*, 2008], the aggregate properties are computed as the VRH average [*Watt et al.*, 1976] of the properties of the entire collection of stable phases identified in the relevant *P-T* tables. Alternatively, the aggregate properties are computed by VRH averaging in each *P-T* table and linear interpolation is used to obtain aggregate properties as a function of the *C* coordinate. In the limit that the *C* increment between the *P-T* tables is sufficiently small, this latter method corresponds to the equilibrium method of

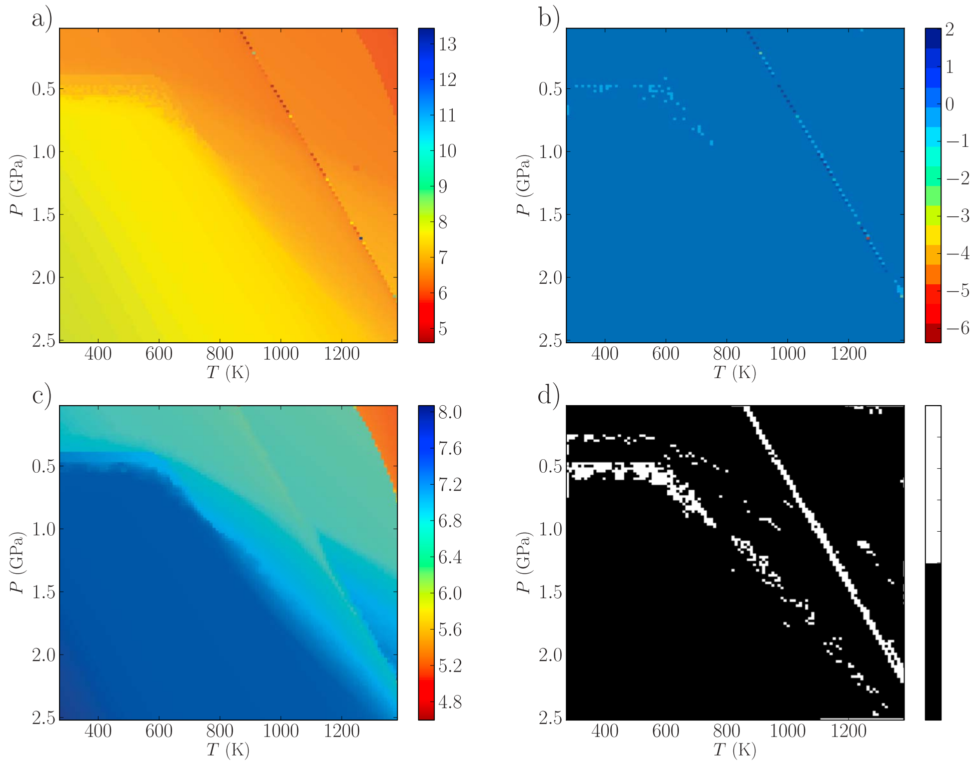

Figure 1. An application of the median filter to V_P data computed from tables. (a) Original data resulting from thermodynamical computations. (b) Difference between initial and filtered data set. (c) Final result after applying our filtering procedure. (d) Modified pixels after filtering procedure are in white; unmodified pixels are in black.

Xu et al. [2008], i.e., the properties obtained are identical to those which would be obtained by doing a free energy minimization calculation at the P-T-C condition of interest.

[7] The results are output to an ASCII file, which can be read by any high-level language (e.g., Python) for plotting or further manipulation. We provide a simple Python script to generate maps of density and seismic body wave speeds (V_P and V_S) given a table of data as input. The program and the tables described in this paper are available at http://www.perplex.ethz.ch/phemgp/.

2.3. Spurious Data

[8] The possibility of a spurious result is an inescapable feature of numerical phase equilibrium calculations. While spurious results may be due to the numerical methods, it is not uncommon that thermodynamic equations of state have mathematical singularities. These singularities can cause pathological problems in either, or both, the computation of stable phase assemblages or, more commonly, in the computation of physical properties of the stable phases. At the users option, the following procedure is implemented within PHEMGP to empirically detect and correct spurious results: (1) apply a median filter to the raw data set, (2) compute the difference between the filtered and original data as

$$t_{i,j} = \frac{|X^M_{i,j} - X_{i,j}|}{|X_{i,j}|} \tag{1}$$

where $X_{i,j}$ is the original data set and $X^M_{i,j}$ is the filtered data set, and i, j are array indexes, and (3) replace values from the original data where $t_{i,j}$ is greater than an empirically determined tolerance (Figure 1d) with values obtained by interpolation using a natural-neighbor algorithm (Figure 1c).

[9] The utility of this strategy is that it smooths poorly behaved data with minimal impact on the remaining data. The procedure is illustrated by a phase equilibrium model for V_P as a function of P and T (Figure 1). The raw data (Figure 1a) include spurious points, the vast majority of which coincide with the alpha-beta quartz transition. In this particular case, the origin of the spurious velocities is a singularity that causes the heat capacity function of

Table 1. Solution Models and Thermodynamic Data Sources for the Crustal Model[a]

Phase	Formula	Source
biotite	$K[Mg_xFe_yMn_{1-x-y}]_{3-w}Al_{1+2w}Si_{3-w}O_{10}(OH)_2$, $x + y \leq 1$	1
mica	$K_yCa_xNa_{1-x-y}(Mg_{1-v}Fe_v)_zMg_wTi_wAl_{3+x-w-z}Si_{3-x+z}O_{10}(OH)_2$, $x + y \leq 1$, $w + z \leq y$,	2, 3
plagioclase	$Na_xCa_{1-x}Al2 - xSi_{2+x}O_8$	4
sanidine	$Na_xK_{1-x}AlSi_3O_8$	5
clinopyroxene	$Na_y[CaMg_xFe_{1-x}]_{1-y}Al_ySi_2O_6$	6
melt	Na-Mg-Al-Si-K-Ca-Fe hydrous silicate melt	7, 8
clinoamphibole	$Ca_{2-2w}Na_{z+2w}[Mg_xFe_{1-x}]_{3+2y+z}Al_{3-3y-w}Si_{7+w+y}O_{22}(OH_2$, $w + y + z \leq 1$	9, 10
garnet	$Fe_{3x}Ca_{3y}Mg_{3z}Mn_{3(1-x-y-z)}Al_2Si_3O_{12}$, $x + y + z \leq 1$	11
staurolite	$Mg_{4x}Fe_{4y}Mn_{4(1-x-y)}Al_{18}Si_{7.5}O_{48}H_4$, $x + y \leq 1$	11
chlorite	$[Mg_xFe_wMn_{1-x-w}]_{5-y+z}Al_{2(1+y-z)}Si_{3-y+z}O_{10}(OH)_8$, $x + w \leq 1$	12
chloritoid	$Mg_xFe_yMn_{1-x-y}Al_2SiO_5(OH_2$, $x + y \leq 1$	13
cordierite	$Mg_{2x}Fe_{2y}Mn_{2(1-x-y)}Al_4Si_5O_{18}\cdot(H_2O)_z$, $x + y \leq 1$	11
spinel	$Mg_xFe_{1-x}Al_2O_3$	11
orthopyroxene	$[Mg_xFe_{1-x}]_{2-y}Al_{2y}Si_{2-y}O_6$	6

[a] Unless otherwise noted, the compositional variables *w*, *x*, *y*, and *z* may vary between zero and unity and are determined as a function of the compositional variables by free energy minimization. Thermodynamic data, except for shear moduli, for stoichiometric phases and end-member compositions from *Holland and Powell* [1998]. Shear moduli from the compilation of *Connolly* [2005]. Solution model sources: 1, *Powell and Holland* [1999]; 2, *Auzanneau et al.* [2010]; 3, *Coggon and Holland* [2002]; 4, *Newton et al.* [1980]; 5, *Waldbaum and Thompson* [1968]; 6, *Holland and Powell* [1996]; 7, *Holland and Powell* [2001]; 8, *White et al.* [2001]; 9, *Wei and Powell* [2003]; 10, *White et al.* [2003]; 11, *Holland and Powell* [1998]; 12, *Holland et al.* [1998]; 13, *White et al.* [2000].

quartz to become infinite at the transition. The additional noise in the raw data, which is particularly notable at low pressure and temperature, is due to the numerical resolution specified for the free minimization method and/or the methods used to compute the physical properties from the phase equilibrium data. The tolerance used to identify poorly behaved data is adjusted empirically until the final result of the procedure (Figure 1c) is judged to be adequate. It should be remarked that there is no completely robust recipe for identifying poorly behaved data and that any filtering procedure introduces the risk of eliminating strong, but real, gradients in data. This risk can be minimized by using densely populated tables, but at the cost of computer memory. Thus, grid spacing and the numerical tolerance used for filtering cannot be prescribed and must be determined by trial and error to meet the demands of a particular application.

3. Models for Crust and Mantle Studies

[10] To illustrate the utility of PHEMGP we present phase equilibrium models for geophysical properties of the crust and mantle. The raw data for these models consist of tables that summarize the proportions and properties of the stable phases computed as a function of pressure and temperature for a specified composition. From these tables, PHEMGP is then used to obtain geophysical properties for any arbitrary *P-T-C* section or condition. In these models we ignore attenuation effects, but such effects are easily implemented [e.g., *Khan et al.*, 2011].

3.1. Example 1: Continental Crust as a Function of Water Content

[11] The model for continental crust accounts for the influence of water content by means of a three-dimensional physical property table as a function of pressure, temperature and water content. The bulk composition of the crust with respect to all components other than water is taken to be the old generic crust composition of *Taylor and McLennan* [2009]. For PHEMGP the input consists of two-dimensional tables as a function of pressure and temperature computed for water contents from 0 wt% to 5 wt% in steps of 1 wt%. In each table, temperature ranges from 273 to 1400 K and pressure ranges from 0.02 to 2.5 GPa, with *P*, *T* increments of 0.02 GPa and 10 K, respectively. The phase equilibrium computations account for the presence of

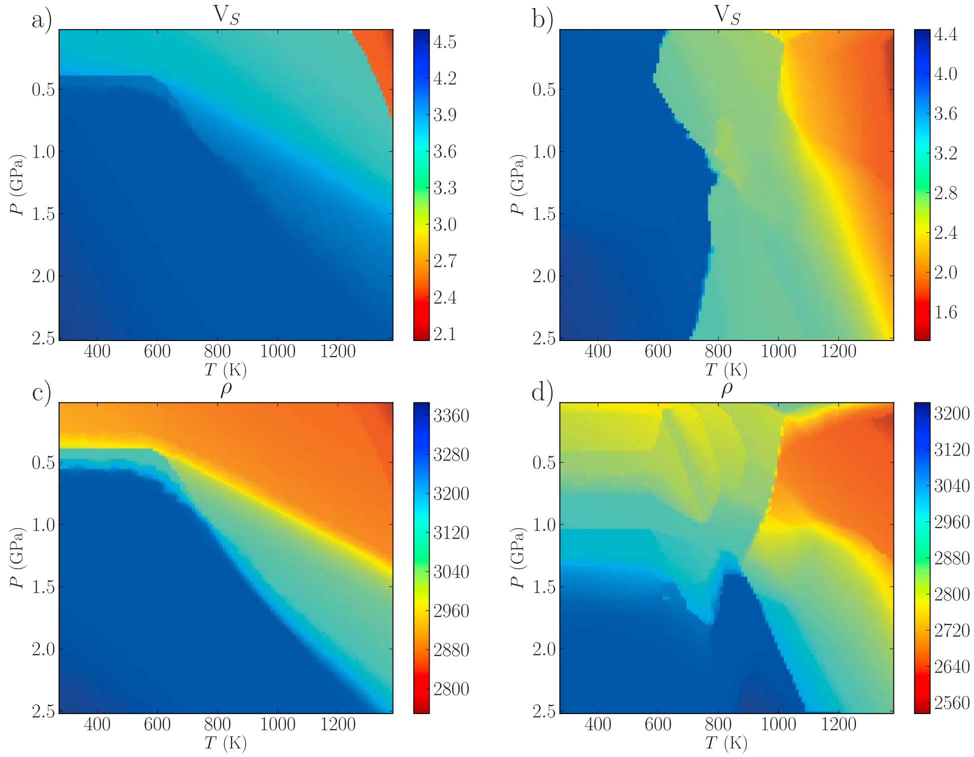

Figure 2. Crustal seismic properties and density for two different water contents. (a and c) V_S (km/sec) and density (ρ, kg/m^3) for 0 wt% H_2O. (b and d) V_S and ρ for 3 wt% H_2O.

aqueous fluid and/or silicate melt. The thermodynamic data for the phase equilibrium computations are summarized in Table 1. The resulting physical property maps (Figure 2) illustrate the profound influence of water content on the geophysical properties of the crust.

3.2. Example 2: Mantle as a Function of Bulk Composition

[12] For the mantle model, the mantle composition is characterized as a binary mixture of basaltic (MORB) and harzburgitic components in the chemical system Na_2O–CaO–FeO–MgO–Al_2O_3–SiO_2. The compositions of these end-member components are specified as in the study by *Khan et al.* [2009]. The mantle phases and relevant thermodynamic data used for the phase equilibrium computations are as described by *Xu et al.* [2008]. In the model system, typical mantle compositions correspond to a basalt mass fraction of 20%–30%. The input for PHEMGP consists of two-dimensional tables at specified basalt fraction, similar to those presented by *Xu et al.* [2008], for pressure from 0 to 140 GPa at 0.05 increments and temperature from 500 to 4000 K at 10 K increments. An example of the mantle properties obtained by PHEMGP for a basalt fraction of 22.5 wt% (Figure 3) illustrates the influence of phase equilibria on mantle seismic structure and density. In particular, properties extracted with PHEMGP along a representative mantle geotherm (Figure 4) reveal the prominent effects of the olivine→wadsleyite (~13 GPa), wadsleyite→ringwoodite (~19 GPa), and ringwoodite+garnet→magnesiowüstenite+perovskite (~23 GPa) phase transitions. These transitions cause strong seismic velocity gradients that are thought to correspond to the so-called 410, 520 and 660 km seismic discontinuities [e.g., *Xu et al.*, 2008].

4. Equilibrium Mixing Model With PHEMGP

[13] An advantage of the aforementioned mechanical mixture model [*Xu et al.*, 2008] for mantle properties is that only tables for its lithological end-members are required to compute properties as a continuous function of mantle composition. In contrast, the equilibrium model requires knowledge

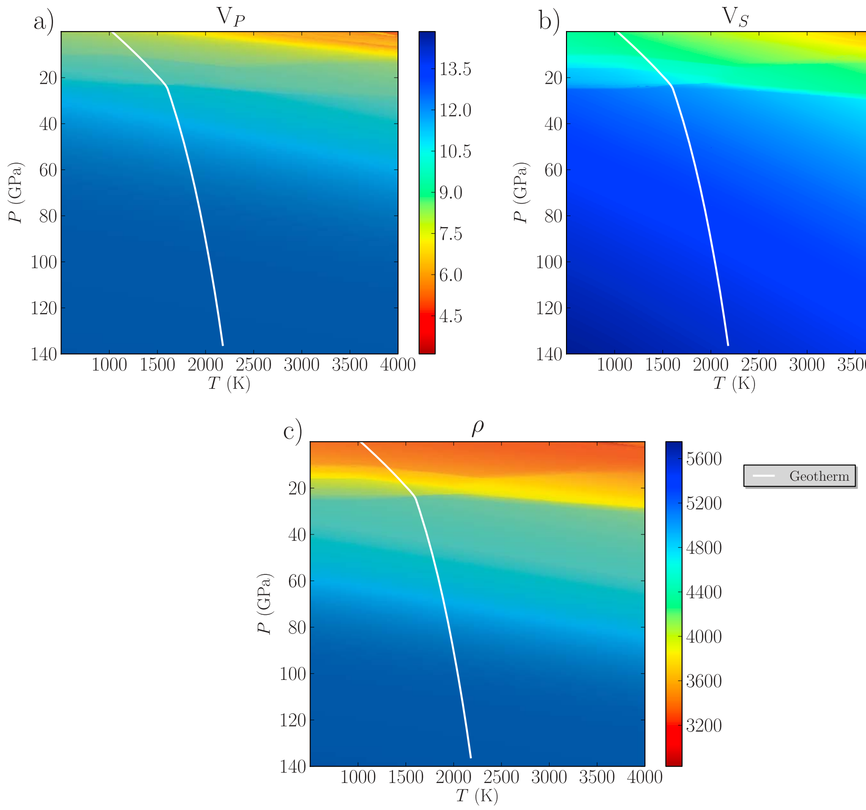

Figure 3. Mantle seismic properties and density computed for a mantle composition with a basalt weight fraction of 0.225. V_P and V_S are expressed in km/s, while ρ is in kg/m^3. The white line represents the geotherm [*Brown and Shankland*, 1981] used for the profile of Figure 4.

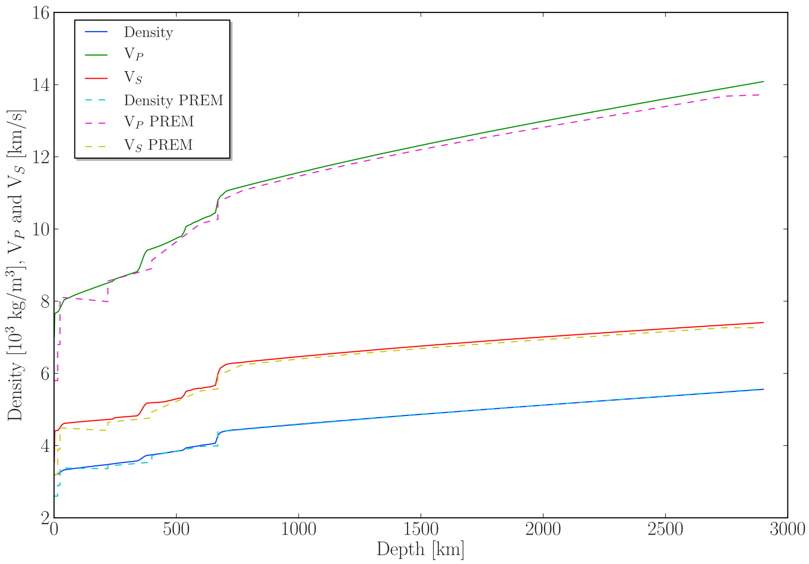

Figure 4. Comparison of one-dimensional profiles of density, V_P and V_S for a basalt weight fraction of 0.225 computed with PHEMGP by interpolation between tables computed for basalt weight fractions of 0.2 and 0.3. A basalt fraction of 0.225 corresponds roughly to pyrolite mantle model composition [*Ringwood*, 1975]. For comparison, PREM seismic reference model properties [*Dziewonski and Anderson*, 1981] are also shown.

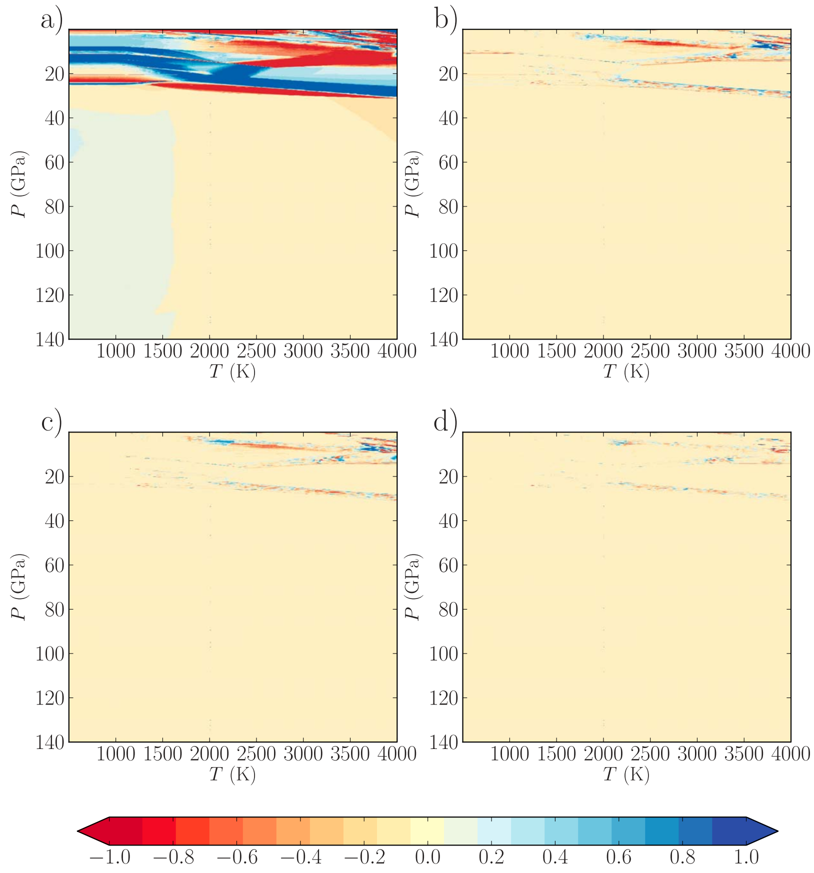

Figure 5. Discrepancy (%) between V_P computed directly by free energy minimization for a basalt fraction of 0.225 and V_P obtained at that composition by interpolation between tables computed for basalt fractions of (a) 0 and 1, (b) 0.2 and 0.3, (c) 0.2 and 0.25, and (d) 0.22 and 0.23.

of mantle properties, at least in principle, as a continuous function of composition and is therefore computationally costly. By interpolating between tables constructed at specified mantle compositions, PHEMGP offers a pragmatic means of incorporating the equilibrium model in computationally intensive geophysical calculations. The compositional spacing between tables necessary to reproduce the equilibrium model by interpolation is the critical factor controlling the feasibility of this approach. To establish this spacing in the context of the present mantle model, we compare (Figure 5) seismic velocities computed directly by the equilibrium model for a basalt fraction of 22.5 wt% (Figure 3), with velocities obtained with PHEMGP by interpolating between tables separated by various compositional increments. This comparison reveals that surprisingly low compositional resolution is required to reproduce velocities computed from equilibrium model with the accuracy required for typical geophysical models. For example, the discrepancies between the velocities of the true equilibrium model and those obtained by interpolation with PHEMGP from tables computed at basalt fractions of 20 and 30 wt% are generally less than 1% (Figures 5b–5d). These interpolation errors are substantially smaller than the differences between the mechanical and equilibrium mixing seismic models (Figure 5a). At face value, interpolation errors of this magnitude may seem unacceptable, however the largest errors occur where velocity gradients are also large. Thus, these errors would have relatively little influence on the depth resolution of a geophysical inversion. To illustrate this quantitatively we convert the interpolation error for $V_P(\epsilon_{V_P})$ of Figure 5 to a depth error (ϵ_d) by dividing ϵ_{V_P} by the velocity gradient $g\rho dV_P/dP$. The resulting depth errors (Figure 6) are generally below 10 km.

5. Conclusions

[14] We have presented a computer program that assembles three-dimensional tables of physico-

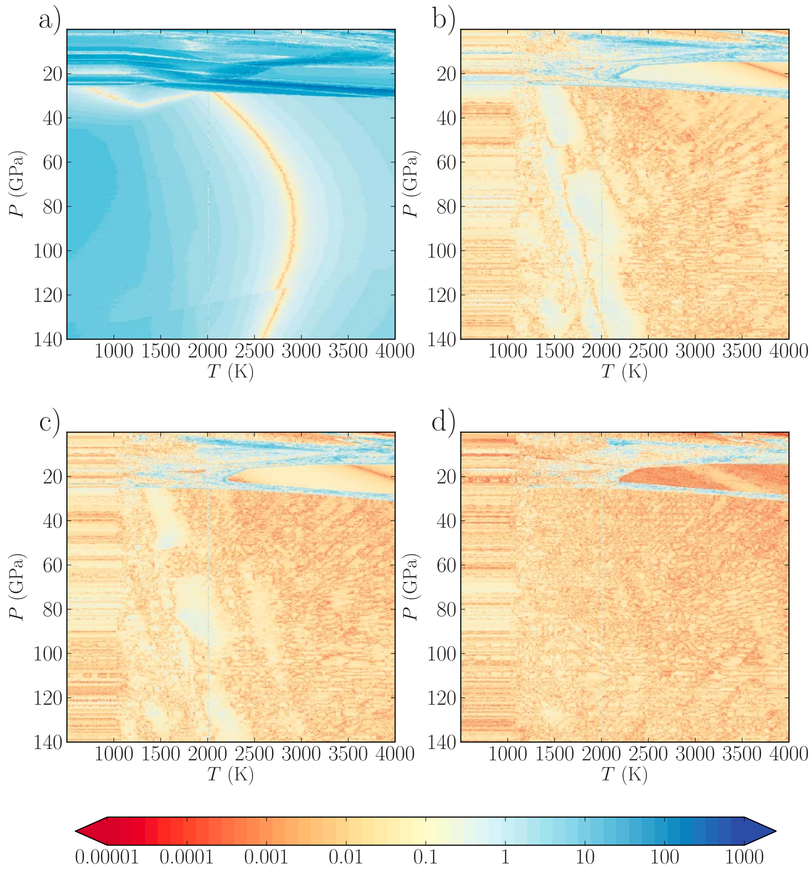

Figure 6. The error in depth (km) resolution corresponding to velocity errors depicted in Figure 5; the errors are for a comparison between velocities computed directly at a basalt fraction of 0.225, with those obtained at that composition by interpolation between tables computed for basalt fractions of (a) 0 and 1, (b) 0.2 and 0.3, (c) 0.2 and 0.25, and (d) 0.22 and 0.23.

chemical properties as a function of pressure, temperature and an arbitrary compositional parameter. The input for this program consists of two-dimensional tables generated as a function of pressure and temperature by free energy minimization.

[15] Our code extracts the information from tables and can also be used to convert the information to a form suitable for plotting or further analysis. A simple interpolation routine allows the user to recover information from the three-dimensional table as a continuous function of its independent variables. We anticipate that the program will be particularly useful for inverse problems, especially for Monte Carlo simulations, where speed of execution is an essential requisite.

[16] We have demonstrated the effectiveness of the method with examples for crust and mantle. For the latter, comparison of the properties obtained by interpolation with those obtained by direct calculation, shows that even with a relatively poor compositional resolution interpolation can be used as an adequate mean to represent geophysical properties.

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References

Auzanneau, E., M. W. Schmidt, D. Vielzeuf, and J. A. D. Connolly (2010), Titanium in phengite: A geobarometer for high temperature eclogites, *Contrib. Mineral. Petrol.*, *159*, 1–24.

Brown, J. M., and T. J. Shankland (1981), Thermodynamic parameters in the Earth as determined from seismic profiles, *Geophys. J. Int.*, *66*, 579–596, doi:10.1111/j.1365-246X.1981.tb04891.x.

Coggon, R., and T. J. B. Holland (2002), Mixing properties of phengitic micas and revised garnet-phengite thermobarometers, *J. Metamorph. Geol.*, *20*, 683–696.

Connolly, J. A. D. (2005), Computation of phase equilibria by linear programming: A tool for geodynamic modeling and its application to subduction zone decarbonation, *Earth Planet. Sci. Lett.*, *236*, 524–541.

Connolly, J. A. D. (2009), The geodynamic equation of state: What and how, *Geochem. Geophys. Geosyst.*, *10*, Q10014, doi:10.1029/2009GC002540.

Connolly, J. A. D., and D. M. Kerrick (2002), Metamorphic controls on seismic velocity of subducted oceanic crust at 100–250 km depth, *Earth Planet. Sci. Lett.*, *204*, 61–74, doi:10.1016/S0012-821X(02)00957-3.

Dziewonski, A. M., and D. L. Anderson (1981), Preliminary Reference Earth Model (PREM), *Phys. Earth Planet. Inter.*, *25*, 297–356.

Gerya, T. V., W. V. Maresch, A. P. Willner, D. D. Van Reenen, and C. A. Smit (2001), Inherent gravitational instability of thickened continental crust with regionally developed low- to medium-pressure granulite facies metamorphism, *Earth Planet. Sci. Lett.*, *190*, 221–235, doi:10.1016/S0012-821X(01)00394-6.

Hebert, L. B., P. Antoshechkina, P. Asimow, and M. Gurnis (2009), Emergence of a low-viscosity channel in subduction zones through the coupling of mantle flow and thermodynamics, *Earth Planet. Sci. Lett.*, *278*, 243–256, doi:10.1016/j.epsl.2008.12.013.

Holland, T., and R. Powell (1996), Thermodynamics of order-disorder in minerals. 2. Symmetric formalism applied to solid solutions, *Am. Mineral.*, *81*,1425–1437.

Holland, T. J. B., and R. Powell (1998), An internally consistent thermodynamic data set for phases of petrological interest, *J. Metamorph. Geol.*, *16*, 309–343.

Holland, T., and R. Powell (2001), Calculation of phase relations involving haplogranitic melts using an internally consistent thermodynamic dataset, *J. Petrol.*, *42*, 673–683.

Holland, T., J. Baker, and R. Powell (1998), Mixing properties and activity-composition relationships of chlorites in the system MgO-FeO-Al_2O_3-SiO_2-H_2O, *Eur. J. Mineral.*, *10*, 395–406.

Khan, A., J. A. D. Connolly, and N. Olsen (2006), Constraining the composition and thermal state of the mantle beneath Europe from inversion of long-period electromagnetic sounding data, *J. Geophys. Res.*, *111*, B10102, doi:10.1029/2006JB004270.

Khan, A., L. Boschi, and J. A. D. Connolly (2009), On mantle chemical and thermal heterogeneities and anisotropy as mapped by inversion of global surface wave data, *J. Geophys. Res.*, *114*, B09305, doi:10.1029/2009JB006399.

Khan, A., L. Boschi, and J. A. D. Connolly (2011), Mapping the Earth's thermochemical and anisotropic structure using global surface wave data, *J. Geophys. Res.*, *116*, B01301, doi:10.1029/2010JB007828.

Kuskov, O. L., and A. B. Panferov (1991), Phase-diagrams of the FeO–MgO–SiO_2 system and the structure of the mantle discontinuities, *Phys. Chem. Miner.*, *17*, 642–653.

Nakagawa, T., and P. J. Tackley (2005), Deep mantle heat flow and thermal evolution of the Earth's core based on thermo-chemical multiphase mantle convection, *Geochem. Geophys. Geosyst.*, *6*, Q08003, doi:10.1029/2005GC000967.

Newton, R. C., T. V. Charlu, and O. J. Kleppa (1980), Thermochemistry of the high structural state plagioclases, *Geochim. Cosmochim. Acta*, *44*, 933–941.

Petrini, K., J. A. D. Connolly, and Y. Podladchikov (2001), A coupled petrological-tectonic model for basin evolution: The influence of metamorphic reactions on the tectonic subsidence of sedimentary basins, *Terra Nova*, *13*, 354–359.

Powell, R., and T. Holland (1999), Relating formulations of the thermodynamics of mineral solid solutions: Activity modeling of pyroxenes, amphiboles, and micas, *Am. Mineral.*, *84*, 1–14.

Ricard, Y., E. Mattern, and J. Matas (2005), Synthetic tomographic images of slabs from mineral physics, in *Earth's Deep Mantle: Structure, Composition, and Evolution*, *Geophys. Monogr. Ser.*, vol. 160, edited by R. D. van der Hilst et al., pp. 285–302, AGU, Washington, D. C.

Ringwood, A. E. (1975), *Composition and Petrology of the Earth's Mantle*, McGraw-Hill, New York.

Saxena, S. K. (1996), Earth mineralogical model: Gibbs free energy minimization computation in the system MgO–FeO–SiO_2, *Geochim. Cosmochim. Acta*, *60*, 2379–2395.

Sobolev, S. V., and A. Y. Babeyko (1994), Modeling of mineralogical composition, density, and elastic-wave velocities in anhydrous magmatic rocks, *Surv. Geophys.*, *15*, 515–544.

Stixrude, L., and C. Lithgow-Bertelloni (2005), Thermodynamics of mantle minerals: I. Physical properties, *Geophys. J. Int.*, *162*, 610–632, doi:10.1111/j.1365-246X.2005.02642.x.

Taylor, S. R., and S. M. McLennan (2009), *Planetary Crusts: Their Composition and Evolution*, 378 pp., Cambridge Univ. Press, Cambridge, U. K.

Tirone, M., J. Ganguly, and J. P. Morgan (2009), Modeling petrological geodynamics in the Earth's mantle, *Geochem. Geophys. Geosyst.*, *10*, Q04012, doi:10.1029/2008GC002168.

Waldbaum, D. R., and J. B. Thompson (1968), Mixing properties of sanidine crystalline solutions: II. Calculations based on volume data, *Am. Mineral.*, *53*, 2000–2017.

Watt, J. P., G. F. Davies, and R. J. O'Connell (1976), The elastic properties of composite materials, *Rev. Geophys. Space Phys.*, *14*, 541–563.

Wei, C. J., and R. Powell (2003), Phase relations in high-pressure metapelites in the system KFMASH (K_2O-FeO-MgO-Al_2O_3-SiO_2-H_2O) with application to natural rocks, *Contrib. Mineral. Petrol.*, *145*, 301–315.

White, R. W., R. Powell, T. J. B. Holland, and B. A. Worley (2000), The effect of TiO_2 and Fe_2O_3 on metapelitic assemblages at greenschist and amphibolite facies conditions: Mineral equilibria calculations in the system K_2O-FeO-MgO-Al_2O_3-SiO_2-H_2O-TiO_2-Fe_2O_3, *J. Metamorph. Geol.*, *18*, 497–511.

White, R. W., R. Powell, and T. J. B. Holland (2001), Calculation of partial melting equilibria in the system Na_2O-CaO-K_2O-FeO-MgO-Al_2O_3-SiO_2-H_2O (NCKFMASH), *J. Metamorph. Geol.*, *19*, 139–153.

White, R. W., R. Powell, and G. N. Phillips (2003), A mineral equilibria study of the hydrothermal alteration in mafic greenschist facies rocks at Kalgoorlie, Western Australia, *J. Metamorph. Geol.*, *21*, 455–468.

Xu, W., C. Lithgow-Bertelloni, L. Stixrude, and J. Ritsema (2008), The effect of bulk composition and temperature on mantle seismic structure, *Earth Planet. Sci. Lett.*, *275*, 1–2, doi:10.1016/j.epsl.2008.08.012.