Terra Nova

doi: 10.1111/ter.12109

# To conserve or not to conserve (mass in numerical models)

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## ABSTRACT

**Mass conservation is a fundamental physical law. Yet, computer models aiming to simulate Earth evolution commonly fail to respect it. Indeed, most geodynamic models implement phase transitions of rocks – such as metamorphism (solid–solid phase change) or melting (solid–liquid phase change) – following a simplifying assumption dating back to 1897 which is conserving volume rather than mass. The underlying problem is present at different scales, illustrated here by three examples: metamorphism in the continental crust, phase changes in the mantle transition zone and melt crystallization during columnar jointing. These illustrate that phase changes may become a driving force of a system's deformation and point to important differences with respect to simplified models. Developing and applying mass-conserving approaches in future modelling tools are therefore not an option, but a necessity.**

Terra Nova, 26, 372–376, 2014

## Introduction

Part of the richness of the Earth, and hence of Earth Sciences, is the heterogeneity in composition of materials, as well as the broad variability in the physical properties of each material. These attributes are the origin of numerous short- and long-term processes occurring on Earth, including geological and meteorological phenomena. To simulate these and their time evolution, Earth scientists commonly use computer models. These models include physical and chemical laws related to the target problem and – for scientific, technical or computational reasons – a number of simplifying assumptions.

One of the primary principles is the law of mass conservation, first alluded to by ancient Greek philosopher Parmenides, stated in fluid dynamics by Euler (1757) and formulated for chemical reactions by de Lavoisier (1789) following Lomonosov's work. One formulation of this law states that in a given spatial domain, any temporal variation of mass-density $\rho$ has to be compensated by in- or outflow of material at velocity $v$:

$$\partial\rho/\partial t + \nabla \cdot (\rho v) = 0$$

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In solid Earth Sciences, such as geology and geophysics, when researchers aim to numerically simulate the dynamics of a system they very often simplify this law using the so-called Boussinesq approximation. French scientist Joseph Valentin Boussinesq (1897) derived that, in the case of sufficiently small density variations, the above equation can be simplified to

$$\nabla \cdot v = 0$$

meaning that the flow of material is incompressible, i.e. volume rather than mass is conserved. While this approximation is valid in many engineering cases, it is a strong assumption in geology, where large spatial and time-scales are considered, and, as I illustrate below, it is rarely valid. In the early age of numerical simulations, such strong assumptions were common and judged reasonable, especially given the computer capacities for solving more complex and/or lengthy problems; however, it is now time to retrace our steps and to fully respect the law of mass conservation.

## A simple example

A simple demonstration of the nature of the problem related to the Boussinesq approximation can be given using the example of $H_2O$ along with a home experiment (Fig. 1). $H_2O$ is a key agent and all of its three phases – ice, water and water vapour – are present in and interact with our life. The volume difference between its solid and liquid phases causes stresses large enough to fracture the surrounding material. The density difference at the liquid-to-solid *phase transition* is about −8.3% at 0 °C and atmospheric pressure (Table 1). Conversely, any given weight of ice, when melted at 0 °C, occupies *c*. 8.3% less volume (Fig. 1b). This corresponds to the commonly referred to disappearing 'tip of the iceberg'.

Liquid water also changes density with varying temperature. Beyond a peculiar maximum at 4.0 °C, it becomes progressively less dense with increasing temperature. The overall *thermal expansion* of water from its melting point to its boiling point is 4.1% (Fig. 1a) (Table 1).

From this, it is clear that any model simulating the physical behaviour of $H_2O$ that takes into account its thermal expansion should also take into account its density and volume changes at its phase transitions as they correspond to first-order variations within the system.

Surprisingly, the great majority of current solid Earth Science computer models that aim to simulate different phases of materials fail at this point.

## Approximations in geological models

While geological and geophysical simulations usually account for density and volume changes related to thermal expansion, they 'simplify' the system when it comes to phase transitions. They either do not change density and volume at phase transitions (Fig. 2a) (e.g. Poliakov

**Table 1** The density of $H_2O$ as a function of temperature, at 101 325 Pa pressure (Haynes, 2012).

| Temperature (°C) | Density (kg m$^{-3}$) |
|---|---|
| 99.974 (liquid) | 958.37 |
| 4 (liquid) | 999.9749 |
| 0.1 (liquid) | 999.8495 |
| 0.0 (liquid, supercooled) | 999.8 |
| 0.0 (solid) | 916.7 |

*et al.*, 1993; Avouac and Burov, 1996) or they update the density of the material from pre-calculated tables, but do not update its volume (Fig. 2b) (e.g. Kaus *et al.*, 2005; Yamato *et al.*, 2007; Rey and Müller, 2010), thereby artificially creating or removing mass. In the above simple example of $H_2O$, the first case would see water turn into ice at constant density and constant volume; the second case would see density change correctly at 0 °C, but the volume of the considered $H_2O$ would remain the same. Consequently, volumetric effects and therefore any mechanical interaction (stress- and strain-change) with the surrounding media are totally neglected in both simplifying cases. The second simplifying case prescribes suppression of mass. On a planet with such physical laws, there would be no fractures created by ice and no associated erosion, and there would be no need to empty garden taps for the winter. In the first simplifying case, there would be no icebergs.

Although the $H_2O$-system described above behaves in an unusual way – its liquid phase is denser than its solid phase, the opposite of most materials, including rocks – the concept and reasoning given above demonstrate very well the problem related to modelling rocks and their behaviour in the Earth's solid shell and interior. There, the volumetric effect of thermal expansion is of the order of 1% (thermal expansion coefficient $\alpha \approx 10^{-5}$ K$^{-1}$ multiplied by temperature differences of $\Delta T \approx 10^2$–$10^3$ K), while the density variations related to solid-solid phase transitions (metamorphic reactions) can easily reach 10–20% (e.g. Holmes, 1965; Liu, 1978); i.e., an order of magnitude larger. These density variations play a key role in global geodynamics by, for example, increasing and localizing the driving force for the subduction of slabs (e.g. Jeanloz, 1985). Also, locally, depending on the properties of the surrounding medium, volumetric changes may cause deformation, stress changes or (in most cases) both. Therefore, numerical models that aim to provide a sound physical explanation for processes including any kind of phase transition should step back from the Boussinesq approximation, which violates the conservation of mass, and should implement techniques that fully respect mass continuity by coupling density variations to volume variations (Fig. 2c). Three examples at different scales are presented below with the aim of drawing attention to this issue and to new perspectives in this research domain.

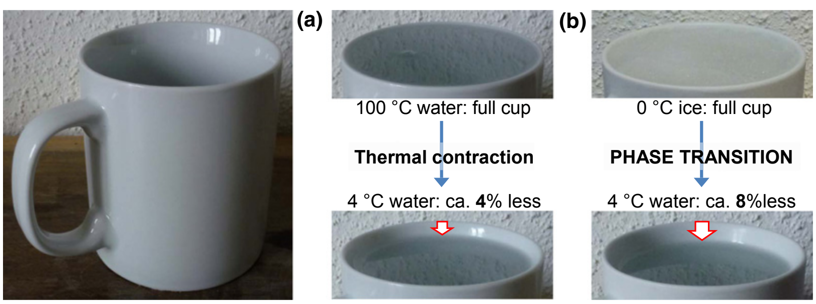


**Fig. 1** A simple experiment with $H_2O$ carried out at home in a cup, showing the importance of phase transition with respect to thermal expansion. (a) Thermal expansion/contraction: a full cup of boiling water occupies *c.* 4% less volume when cooled to 4 °C. (b) Phase transition: a full cup of ice occupies *c.* 8% less volume when molten. The volume changes of $H_2O$ are apparent as the thermal expansion of the cup is comparatively negligible.

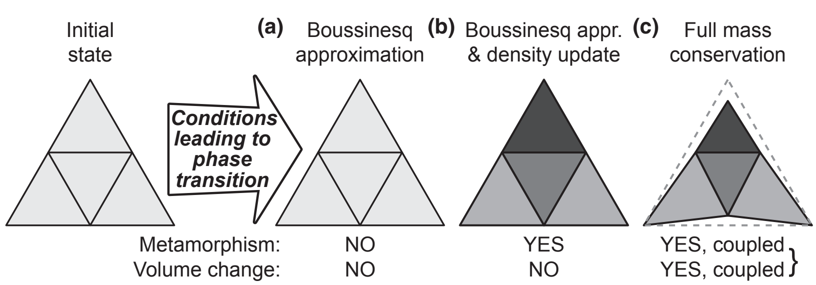


**Fig. 2** Implementations of phase transitions (metamorphism of rocks) and related volume changes (deformation) in numerical modelling tools. From an initial state of elements simulating rock evolution, three different approaches produce three different setups. (a) The Boussinesq approximation does not take into account metamorphism. (b) The same with density update of elements corresponding to rock equilibrium conditions does not apply volumetric changes and therefore does not conserve mass. (c) The fully mass-conserving approach couples density and volume changes. The greyness of elements is proportional to density.

## Metamorphism

At crustal and lithospheric scales metamorphism accounts for isochemical phase changes in a system. Due to varying pressure and temperature conditions, a rock undergoes mineralogical transformations. The consequent changes in physical properties (elastic parameters, thermal conductivity) can be measured in laboratory experiments. One of the primary effects is the variation in density, which can be measured but also computed for any composition, pressure and temperature, given the stable mineralogical phases (see methods, databases and software to compute petrogenetic grids: Perple_X (Connolly, 2005), Theriak-Domino (de Capitani and Brown, 1987; de Capitani and Petrakakis, 2010)). As mentioned above, the induced volumetric effect of metamorphism in the crust and lithosphere can easily reach 10–20%. When correctly implemented, models incorporating such density and volumetric variations show significant differences from Boussinesq approximated models, even if these are linked to petrogenetic grids. A finite-element modelling of an orogen's geodynamic evolution with lower crustal eclogitization demonstrates that the Boussinesq approximation may cause significant (approaching 100%) errors in characteristic measures of orogenic shape, such as relief and foreland basin depth, and that mass conservation errors amplify with model time (Hetényi *et al.*, 2011). The physically correct implementation shows enhanced deformation localization as a narrower and deeper crustal root develops beneath the mountain range. The induced stresses exceed the order of a few bars and are therefore large enough to create fractures or to trigger earthquakes. This underlines that implementing mass conservation is essential to understand both short- and long-term tectonic evolution and to properly assess the importance of different geodynamic processes.

## Mantle transition zone

The upper and lower compartments of the Earth's mantle are separated by the mantle transition zone (MTZ), bound by discontinuities at 410 and 660 km depth. The common view is that the MTZ discontinuities correspond to mineralogical phase changes. Depth variations of these discontinuities are detected by seismic waves and are usually interpreted in terms of temperature anomalies that deflect the phase change depths from their nominal values. These two statements hold true regardless of the assumed petrological composition end-members, i.e., pyrolite, piclogite, or a mixing of the two within relatively short distances (Cornwell *et al.*, 2011). Seismically, the variations in P- (resp. S-) wave velocity associated with the '410' and the '660', according to the *iasp91* model (Kennett and Engdahl, 1991), are 3.65% and 5.78% (resp. 4.11% and 6.25%), respectively. In the Primary Reference Earth Model (Dziewonski and Anderson, 1981) velocity changes are similar and density changes across the discontinuities are, respectively, *c.* 5% and *c.* 10%. These density changes are comparable to but spatially much more localized than those due to compressibility integrated throughout the upper mantle, and both outweigh those due to thermal expansion.

Early numerical models of mantle convection usually used the Boussinesq approximation for practical (computational) reasons (e.g. McKenzie *et al.*, 1974; Baumgardner, 1985; Cserepes *et al.*, 1988). A less restrictive formulation, the so-called anelastic approximation

$$\nabla \cdot (\rho v) = 0$$

was developed later (Solheim and Peltier, 1990) and is also often used (e.g. Tackley, 2008; Krien and Fleitout, 2010). The anelastic approximation allows for stratified density distributions in the Earth and therefore accounts for MTZ phase changes at constant depths. However, depth variations in the 410 and the 660, mapped at several different locations on Earth (e.g. Hetényi *et al.*, 2009; Lombardi *et al.*, 2009 and references therein), are not taken into account. These perturbations have been explained in terms of thermal anomalies due to cold subducted material or mantle plumes, kinetic effects of mineralogical reactions, varying water content across a discontinuity and reactions involving garnet across the bottom of the MTZ. Whichever is the cause, mantle convection models aiming to account for these large, up to 40 km, depth variations need to implement a fully mass-conserving approach because the material between the nominal and actual phase transition depths, with a density (and volume) different from its surroundings, will exert a non-negligible force on the downgoing slab and hence influence its dynamics. Although (to my knowledge) currently no such model exists, I expect that the effects are at least as large as those of introducing phase transition kinetics (Tetzlaff and Schmeling, 2009) or of pressure- and temperature-dependent thermal expansion and compressibility (Tosi *et al.*, 2013) investigated recently.

## Columnar jointing

Cooling of lava provides an example of the importance of mass conservation at a much smaller, outcrop (10–100 m) scale. It is well known that lava or magma cooling at specific rates develops a set of columnar joints, delimiting mostly hexagonal and pentagonal columns (e.g. Tomkeieff, 1940; Hetényi *et al.*, 2012) that are spectacular and attract tourists (e.g. Giant's Causeway). The common explanation for the development of this type of jointing is that the cooling igneous body shrinks and the rock fractures when the accumulated stress overcomes the tensile stress limit (Raspe, 1776). However, the joints between the columns usually account for only *c.* 0.5% of the body's volume reduction, whereas the total volume decrease exceeds 15% (Mattsson *et al.*, 2011). Thermodynamic and rheological modelling of the solidification process suggests rapidly varying composition and physical properties within a less than 200 K temperature decrease after emplacement. Combined with petrographic observations, a qualitative but mass-conservative mechanism for magma migration within the columns is proposed, which is driven by pressure gradients induced by the inhomogeneous cooling (Fig. 3; Mattsson *et al.*, 2011). However, there is currently no thermo-mechanical dynamic model that takes into account petrological and volumetric changes simultaneously. Such a model would be able to confirm (or refute) this mechanism and provide further insights into the process of columnar joint development.

## Future directions

Conservation of mass is a primary physical law. It has first-order effects on the evolution of geological processes, as demonstrated here by three examples at different scales. Comparisons of results from fully mass-conserving models with those from approximated approaches show significant errors in the latter group. The volumetric changes resulting from phase transitions cause large

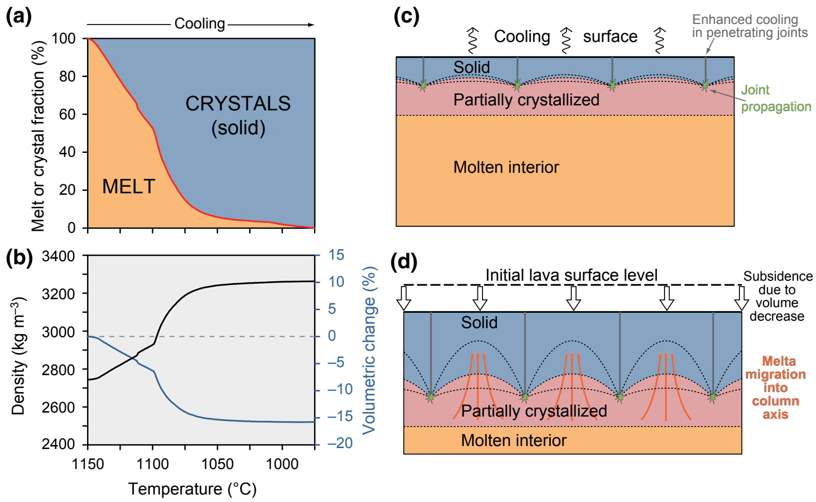


**Fig. 3** Solidification and shrinking of basalt during columnar joint formation (modified from Mattsson *et al.*, 2011). (a, b) Thermodynamic modelling of basalt melt solidification: the crystallization (liquid-to-solid phase transition) between 1150 and 975 °C increases the density and decreases the volume by more than 15%. (c) Initial stage: cooling of the lava flow (shown in cross-section) at its top surface and locally in the joints penetrating its freshly solidified crust. This setup causes concave isotherms in each column. Most of the lava is still molten; some of it is partially crystallized. (d) Advanced stage of column formation: a significant part of the lava has solidified. The overall volume decrease has caused subsidence of the lava surface. This translates into migration of the still molten lava into the columns' axes.

stresses, which initiate significant mechanical interaction with and deformation of the environment. All these aspects highlight the importance of respecting mass conservation, which should be accounted for in numerical models.

All models are a simplification of nature, and not all have to deal with phase changes with significant volumetric effects. Still, phase changes should be correctly incorporated when their effects are non-negligible in the general behaviour of the system. I propose two criteria to decide whether phase changes should be accounted for in a numerical model:

1 A rule of thumb that can be verified before computations: the relative volume change from phase changes ($\delta V_{PC}$) is non-negligible with respect to the volume change from thermal expansion of the system: $\delta V_{PC}/(\beta \cdot \Delta T_{max}) \geq 0.1$, where $\beta$ is the volumetric thermal expansion coefficient and $\Delta T_{max}$ is the largest temperature difference expected in the system.
2 A more time-consuming alternative is to run models both with and without phase changes incorporated and test whether the strain due to phase changes ($\varepsilon_{PC}$) is non-negligible with respect to the characteristic mechanical deformation of the system ($\varepsilon_0$): $\varepsilon_{PC}/\varepsilon_0 \geq 0.1$.

An additional challenge for future models will be the implementation of chemically open systems. In particular, the addition of water is likely to play an important role in both chemical and physical processes. Two examples are (1) melting and related density variations in magmatic systems (e.g. Ashworth and Brown, 1990; Sawyer *et al.*, 2011) and (2) metamorphic reactions involving significant amounts of water (e.g. Hacker *et al.*, 2003; Wada *et al.*, 2012) that induce stresses sufficient to trigger earthquakes. A good example is the dehydration reactions during eclogitization of the Indian lower crust beneath Southern Tibet, which spatially coincides with an earthquake swarm at 60–80 km depth (Hetényi *et al.*, 2007).

The aims of this paper are to (1) call for existing mass-conserving modelling tool users to manifest, (2) inspire existing tool developers and users to adapt to approaches that fully respect mass conservation, (3) motivate new modelling tool authors to implement mass conservation and (4) express the need to benchmark new codes on a well-formulated geological phenomena including non-negligible phase changes. Computational techniques and computer capacities are sufficiently developed to accommodate such changes. This is demonstrated by the – to my knowledge – so far four modelling tools applying fully compressible formulations (Gerya and Yuen, 2007; Warren *et al.*, 2008; Afonso and Zlotnik, 2011; Hetényi *et al.*, 2011), employing both Lagrangian and Eulerian-Lagrangian formalisms. The perspectives lying in this domain are demonstrated by the four different numerical implementations these authors use. Therefore, it is time to step back to a more-than-a-century-old simplifying assumption and then to move forward with the full mass-continuity equation.

## Acknowledgements

This work reflects numerous discussions with people formerly or currently at ENS Paris, at the University of Leeds and at ETH Zürich, as well as a session discussion at the EGU 2010 conference. They are all acknowledged for their input. I am very grateful to the reviewers: Stefan Schmalholz, Jean Chéry and Greg Houseman, as well as the Editor Jean Braun, for their constructive criticism, which definitely improved this manuscript.

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*Received 16 December 2013; revised version accepted 22 April 2014*