Box modeling the chemical evolution of geophysical systems: case study of the Earth's mantle

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Abstract. Geochemical measurements have been widely used for understanding geophysical dynamic systems. Fluid mechanics and box models are quantitative tools for testing the reliability of these interpretations. We present here the connection between these two methods, especially in the case of the Earth's mantle. We show that box models implicitly assume a chemical diffusivity inversely proportional to the number of boxes. From fluid dynamics considerations we suggest that at least 15 boxes should be used to model the mantle. Then, we compare the results of a simple convective geochemical model with box models to illustrate a way to incorporate dynamical constraints in them.

Introduction

Modeling the chemical evolution of dynamic systems is of interest in various fields of planetary sciences: oceanography, atmospheric and solid Earth sciences. The fully-dynamical description is the most straightforward approach: in the case of Earth's mantle, it consists in solving the convection equations and advecting chemical tracers [*Gurnis and Davies*, 1986; *Kellogg and Turcotte*, 1990; *Christensen and Hofmann*, 1994]. However, the difficulties of modeling some physical processes (turbulence for the atmosphere and ocean, or generation of plate tectonics), and the computational cost of this technique, make box models an alternative method.

Box models refer to the computation of the chemical evolution of structural units exchanging elements. These units are homogeneous boxes (in some cases defined by mean and rms concentrations [*Allègre and Lewin*, 1995]). The example of mantle geochemistry shows that it is difficult to design coherent and realistic box models. The same data has led to contradictory views: *Albarède* [1998], *Coltice and Ricard* [1999] argue for whole mantle convection, *Jacobsen and Wasserburg* [1979] for a separation between upper and lower mantle, and *Anderson* [1982] for an even more complicated layering. These conflicts are essentially due to the choice of the number of boxes and the difficulties for incorporating dynamical constraints [*Garçon and Minster*, 1988].

The goal of this paper is to describe quantitatively the framework of an accurate box modelisation. The results presented are applied mostly to the chemistry of the Earth's mantle, which is at the center of conflicts between geochemists and geophysicists [see *Hofmann,* 1997, for a review].

Assumptions of box models

Equations

To describe the equations used in chemical box models, we use the same formalism as in *Albarède* [1998]. The mass conservation for a reservoir i reads

$$\frac{dM_i}{dt} = \sum^{j\neq i} Q_{j\to i} - \sum^{j\neq i} Q_{i\to j}, \tag{1}$$

where M_i is the mass of the box i, t the time and $Q_{i\to j}$ the mass flux from box i to box j.

The conservation of the chemical element k with concentration C_i^k in the reservoir i is

$$\frac{dC_i^k}{dt} = -(\lambda^k + \frac{\sum^{j\neq i} Q_{i\to j}K_{i\to j}^k}{M_i} + \frac{\sum^{j\neq i}(Q_{j\to i} - Q_{i\to j})}{M_i})C_i^k + \frac{\sum^{j\neq i} Q_{j\to i}K_{j\to i}^k}{M_i}C_j^k + \lambda^{k-1}C_i^{k-1}, \tag{2}$$

where $K_{i\to j}^k$ is the enrichment factor due to the fractionation of element k upon transfer from box i to box j. The element k can be produced by the parent $k-1$ and produces the daughter element $k+1$ with radioactive decay constants λ^{k-1} and λ^k.

Equation (2) implicitly states that the concentration in each reservoir is homogeneous. A simple example will show how the size at which a fluid can be considered homogeneous can be linked to, or estimated from the flow pattern in this fluid.

A simple example: the plug flow

The most obvious characteristics of convection with internal heating is that there is only one thermal boundary layer, the cold lithosphere. The downwellings are intense and very localized, the hot return flow is very slow and diffuse. A possible zero-order model of the mantle flow might be a 1-D plug flow: the material that has reached the surface is brought back by subduction to the bottom of the mantle and then rises slowly back to the surface. To model this scenario with boxes, we can divide the mantle into n superposed boxes with masses M/n where M is the mass of the mantle. These boxes are crossed by a uniform mass flux $Q = \rho v_z S$ where ρ is the density, S the surface between two boxes, and v_z the vertical return velocity.

The easiest case to model is the transport of an inert gas. The n equations to solve are of the form

$$\frac{M}{n}\frac{dC_i}{dt} = Q(K_{i-1}C_{i-1} - K_iC_i), \tag{3}$$

where all K_i are equal to 1 (mass transport) except for the top box where $K_n = K_{top}$ (degassing) and for the bottom box (reinjection) where $K_0C_0 = K_{bottom}C_n$ (implicitly the atmosphere box accounts for mass conservation of the degassed species).

By a second order Taylor expansion in z,

$$C_{i-1} = C_i - \frac{\partial C}{\partial z}\Delta z + \frac{1}{2}\frac{\partial^2 C}{\partial z^2}\Delta z^2 \tag{4}$$

($\Delta z = \frac{L}{n}$ where L is the mantle thickness), equation (3) becomes

$$\frac{\partial C}{\partial t} + v_z\frac{\partial C}{\partial z} = \frac{v_z \Delta z}{2}\frac{\partial^2 C}{\partial z^2}, \tag{5}$$

where the concentration $C(z,t)$, is now a function of both depth and time.

The two boundary conditions read, at the surface

$$\frac{\partial C}{\partial t}(top) + v_z\frac{\partial C}{\partial z}(top) = \frac{v_z}{\Delta z}(1 - K_{top})C(top), \tag{6}$$

and at the core mantle boundary

$$C(bottom) = K_{bottom}C(top). \tag{7}$$

The physical meaning of a box model representation is clearly shown by equation (5). Implicitly this type of box model assumes that the transport is characterized by an advection term and a diffusion term. The latter has an equivalent diffusivity $v_z\Delta z/2$. When the number of boxes increases to infinity ($\Delta z \to 0$), the equivalent diffusivity goes to zero and the concentrations are purely advected by the flow. Fig. 1 depicts various concentration profiles computed either with equation (3) (thin line) or with equation (5) (thick line). The good agreement between the two computations increases with the number of boxes (5 on the left, 25 in the middle, 100 on the right). Fig. 1

The return velocity imposed by slab subduction v_z is around 1 mm yr^{-1} (the flux of slab divided by the Earth's surface). When geochemical data are explained by a two reservoir mantle, a diffusivity coefficient of 25.10^{-6} m^2 s^{-1} is implicitly assumed. We will see in the following that this implicit diffusivity coefficient is not related to that of solid state chemical diffusivity. The latter is $\sim 10^{-20}$ m^2 s^{-1} [*Allègre and Turcotte*, 1986], hence a diffusivity 14 orders of magnitude smaller than that of a 2 box model.

The fluid dynamicist point of view

Modeling the evolution of concentration in a convection model where the incompressible velocity field is $\vec{v}$, only consists in solving

$$\frac{\partial C}{\partial t} + (\vec{v}.\vec{\nabla})C = 0, \tag{8}$$

assuming a negligible chemical diffusivity.

Following the reasoning of *Taylor* [1921], the dispersion of particles around a mean position in a mixing flow is similar to a diffusive behavior in Lagrangian coordinates. The convective velocity can be divided into a large scale, slowly varying velocity, $\vec{V}$ and a remaining velocity $\vec{u}$. Taylor has shown that equation (8) can be recast as

$$\frac{\partial C}{\partial t} + (\vec{V}.\vec{\nabla})C = \bar{u}^2 \tau \nabla^2 C, \tag{9}$$

where τ is the correlation time of the velocity field, i.e. the time after which the memory of the initial field has vanished, and $\bar{u}$ some average of $||\vec{u}||$. Intuitively the advection by a small scale, time dependent flow that is responsible for chaotic mixing is equivalent to diffusion at a larger scale.

Equation (9) has been mostly used for turbulent flows [i.e., *Pedlosky,* 1987] and in hydrology where this Taylor diffusivity is called dispersivity [*Bear and Bachmat,* 1990]. However the idea that transport at a given scale appears as diffusion at a larger scale can be extended to most complex flows. When Taylor's idea of modeling sub-scale transport by diffusion does not hold, mixing cannot be understood without the computation of the finest scales of the flow, and hence the interpretation of transport by box model becomes impossible.

By comparison of equations (5) and (9), one sees that modeling convective mixing with box models requires a number of boxes given by

$$n = \frac{L}{2\bar{u}\tau}, \tag{10}$$

where we assume comparable amplitudes for $\vec{V}$ and $\vec{u}$.

Putting numbers in (10) is certainly hazardous, our goal is only to show that the number of boxes can, in principle, be deduced from the space and time characteristics of mantle convection. Lower mantle velocities are around 1 mm yr^{-1}. The mantle has a memory of about 100 Myrs, a value that has been estimated from convection models [*Ricard et al.,* 1993; *Bunge et al.,* 1998]. In this case, a box model would require at least 15 boxes to predict the results of a convection code (i.e., boxes with sizes comparable to that of the boundary layers of the mantle), a number larger than what is commonly assumed. This corresponds to a diffusivity of $\sim 3.10^{-6}$ m^2 s^{-1}, an order of magnitude smaller than that corresponding to a simple two box model.

Box vs. geodynamic models: case studies

We compare the two approaches using a 2D circulation model in a rectangular domain of aspect ratio 3. We do not solve the whole convection system including the heat equation : the flow is only driven by a surface forcing simulating two plates diverging from a ridge, and by an internal forcing corresponding to two associated slabs [see *Ferrachat and Ricard,* 1998]. The ridge moves sinusoidally and sweeps the whole surface every 180 Myrs. The viscosity increases by a factor 100 in the lower $2/3^{\mathrm{rd}}$ of the box. During 3 Gyrs, 300,000 tracers are advected carrying ^{3}He and U with an initially homogeneous concentration.

To model melt fractionation and outgassing at ridges, we compute the running average over 3,000 tracers of the He and U contents of the tracers that enter a semi circular area beneath the ridge (mimicking a magma chamber of radius 150 km). As soon as a new tracer enters the magma chamber, a tracer is released, either in the crust (7 km thick) with probability 1/10, or in the underlying lithosphere (63 km thick) with probability 9/10. This tracer is degassed with respect to the magma chamber by a factor 1/1000 in the crust, or 1/50 in the lithosphere. Similarly its U-content is enriched by 9.91 in the crust or depleted by 1/100 in the lithosphere.

From the velocity field, we compute the rms vertical flux (horizontally- and time-averaged) $< Q(z) >$. We also monitor the horizontally averaged ^{3}He and U concentrations as a function of time and depth.

Case one: ^{3}He degassing

We investigate two opposite organizations of the fluxes in the box models. In the first case we consider that each horizontal box only exchanges with adjacent boxes. We call this model the "diffusive" model. In the second case, we consider that the down-going mass fluxes are very localized, as downwellings carry directly the concentrations from the top boxes. Therefore we add fluxes from the uppermost boxes where toward lower boxes (see Fig. 2). We call this model the "localized" model. Fig. 2
Results from the convective code and from the "diffusive" and "localized" box models are depicted in Fig. 3, Fig. 3
for different numbers of boxes. The upward fluxes in the box models at each box interfaces are exactly those of the circulation model, $< Q(z) >$.

The horizontally averaged content of ^{3}He of the convection model (thick line) shows that 60% of the mantle is degassed. Despite of the rather high viscosity jump, the mantle is surprisingly homogeneous in agreement with previous studies [*van Keken and Ballentine,* 1999]. The only acceptable box model is the "localized" model, independently of the number of boxes. In this model, each layer has roughly the same input flux of degassed material from the near surface which results in a homogeneous mantle. In the "diffusive" model, the signal of degassing is diluted with depth so that the deepest boxes are kept undegassed. According to equation (5), more diffusion occurs in models with a low number of boxes.

Case two: U trapping in D"

The only way with our simple convection model to obtain a significant depth dependence of element concentrations is to artificially impose the segregation of the oceanic crust which enters the lowermost 200 km [*Hofmann and White,* 1982]. Storing the U-rich crust into an isolated D" layer depletes the lower mantle [*Coltice and Ricard*, 1999].

In the box model, crustal segregation implies that only depleted material enters the boxes in the bottom 200 km, because U-enriched crust is removed from the budget. This effect is introduced in the "localized" model by an enrichment coefficient K^U_{bottom} =0.01 from the top box toward the lower-most boxes.

Fig. 4 depicts the U concentration computed with the convective model after 3 Gyrs of simulation (thick line). As for ^{3}He, the horizontally averaged U content is relatively constant with depth, except near the bottom where it is depleted by segregation. The D" layer is not represented and has stored 1/10 of the initial amount of U. The box model results are shown by thin lines for various numbers of boxes. The box model predicts the vertical structure of the convective model fairly well for a number of boxes larger than 20. With a smaller number, the equivalent diffusivity is too large and the whole mantle is depleted.

Fig. 4

Conclusions

Although ultimately, chemical exchanges will have to be modeled by a fully dynamical description, this goal is presently out of reach for several reasons that make box model of particular interest. We have shown that the box model equations are equivalent to advection-diffusion equations with a diffusivity related to the mixing properties in a fluid dynamics analysis. Then, the topology and the number of boxes must be deduced from a flow analysis, that would give, for mantle convection, a number of boxes larger (~ 15) than what is commonly considered.

The results of box models are highly dependent on the flux configuration: a box model assuming localized downwellings ("localized" model) reproduces our fluid dynamics results whereas a box model assuming symmetrical upwellings and downwellings ("diffusive" model) does not. However, a good prediction requires ~ 20 superposed boxes.

These conclusions leave apart the fact that the fluid dynamics code also predicts large scale lateral variations that have not been considered by our depth-dependent box model, and the fact that 3 D mixing properties might not be easily extrapolated from simple 2 D models [*Ferrachat and Ricard,* 1998].

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Figure 1. Concentration profiles, $C(t)/C(0)$, as a function of normalized depth ($K_{top} = 10$, $K_{bottom} = 0.2$, $t = 1.8$ Gyrs, $v_z = 1$ mm.yr^{-1}).

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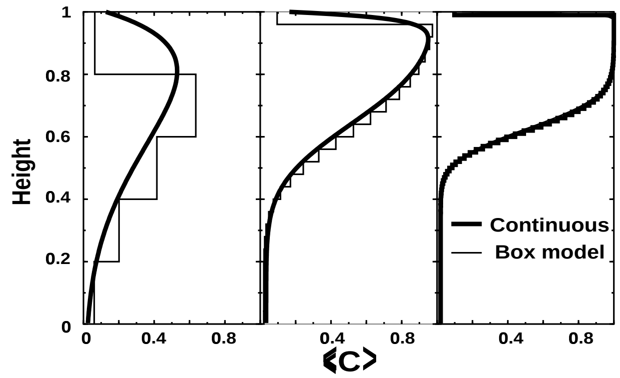

Fig 2

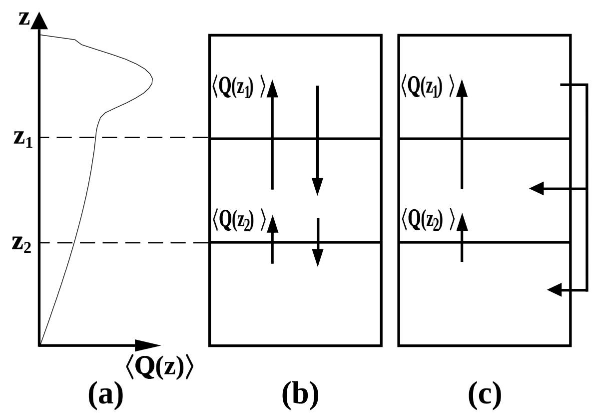

Fig 3

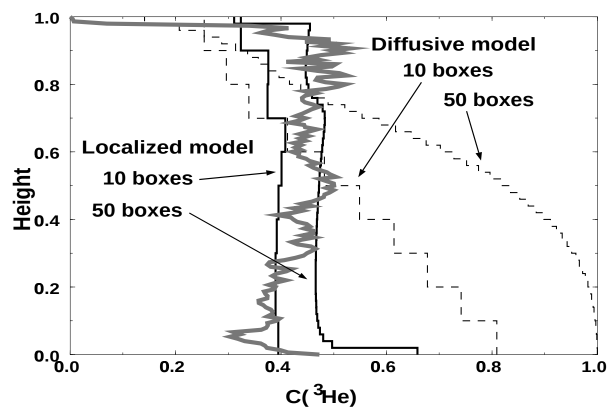

Fig 4

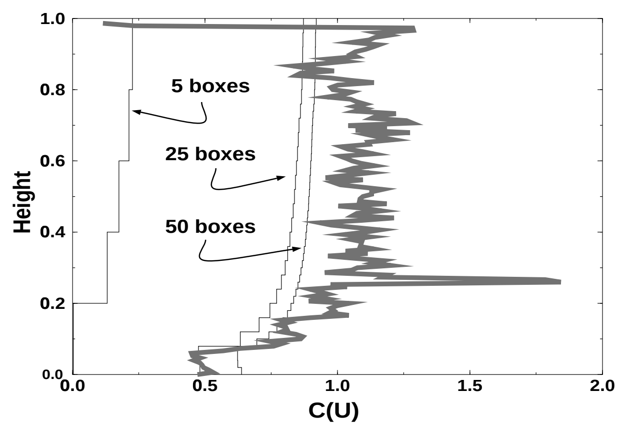

Figure 5.

Figure 5.

N. COLTICE, S. FERRACHAT AND Y. RICARD: BOX MODELS OF THE EARTH'S MANTLE

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