

Carbon cycle box model derivation

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Introduction

Here we will walk through the steps for deriving a simple box model of the geologic carbon cycle. The basic mathematical framework can be applied to box modeling in general. The parameterizations and assumptions are inspired by *Kump and Arthur, 1999 (Chemical Geology)* and formulations from *Jeremy K Caves Rugenstein's* C cycle model, CLiBeSO (*submitted*).

The basic model framework will include two differential equations: (1) an equation for the change in the mass of the reservoir (inorganic carbon on Earth's surface) and (2) an equation for the change in the isotopic composition of that reservoir. I have built in parameterizations for phosphorus recycling, mountain uplift, silicate weathering, and some other “knobs” to play around with. (*Note:* the phosphorus recycling parameterization requires a simple, third differential equation solving the mass of the phosphorus reservoir).

The end result will be a discretized solution to a one-box model for time-dependent analyses. Along with this derivation the R-script that runs the model can be found on my github page.

The isotope ODE

We start with a simple equation stating that any change in the mass of our single box (M_0) can be quantified by the balance between the fluxes into the box and the fluxes out.

$$\frac{dM_0}{dt} = F_w + F_{volc} - (F_{b,org} + F_{b,carb}) + F_{extra} \quad (1)$$

Here, dt denotes the time derivative and the fluxes into the box are F_w , the weathering flux of carbon, F_{volc} , the volcanic flux, and F_{extra} will be used to define a perturbation (input or subtraction) of carbon to the system ($F_{extra} = 0$ as an initial condition). The fluxes out of the box are the burial of organic and carbonate carbon, $F_{b,org}$ and $F_{b,carb}$ respectively.

Next we solve for the isotopic composition of the carbonate reservoir (which is a function of the isotopic compositions of its constituent fluxes). This step involves an assumption and a simplifying step. *First*, we assume that the weathering products are isotopically indistinguishable from the volcanic flux, allowing us to lump these fluxes together ($F'_w = F_w + F_{volc}$). *Second*, we simplify the isotopic composition of organic carbon so it is written as a function of carbonate carbon ($\delta^{13}C_{org} = \delta^{13}C_{carb} + \Delta_B$).

Plugging in these relations and distributing $F_{b,org}$, we get:

$$\frac{d}{dt}(M_0\delta^{13}C_{carb}) = F'_w\delta^{13}C_{volc} - F_{b,org}\delta^{13}C_{carb} + F_{b,org}\Delta_B - F_{b,carb}\delta^{13}C_{carb} + F_{extra}\delta^{13}C_{extra} \quad (2)$$

The end goal of this section is an equation for $\frac{d\delta^{13}C_{carb}}{dt}$. To arrive there, we use the product rule to split up M_0 and $\delta^{13}C_{carb}$ on the left side of equation 2. This gives us:

$$\frac{d}{dt}(M_0\delta^{13}C_{carb}) = \delta^{13}C_{carb}\frac{dM_0}{dt} + M_0\frac{d\delta^{13}C_{carb}}{dt} \quad (3)$$

We can now set the right side of equation 3 equal to the right side of equation 2. Then, subtracting both sides by $\delta^{13}C_{carb}\frac{dM_0}{dt}$ helps isolate the time derivative of the carbonate isotope composition such that:

$$M_0\frac{d\delta^{13}C_{carb}}{dt} = F'_w\delta^{13}C_{volc} - F_{b,org}\delta^{13}C_{carb} + F_{b,org}\Delta_B - F_{b,carb}\delta^{13}C_{carb} + F_{extra}\delta^{13}C_{extra} - \delta^{13}C_{carb}\frac{dM_0}{dt} \quad (4)$$

Things are starting to get messy, we'll clean that up soon. But let it get worse for just a moment. Notice that the last term in equation 4 (dM_0/dt) is the same as the left side of equation 1. So plugging equation 1 into 4 (and using $F'_w = F_w + F_{volc}$) we get:

$$M_0\frac{d\delta^{13}C_{carb}}{dt} = F'_w\delta^{13}C_{volc} - F_{b,org}\delta^{13}C_{carb} - F_{b,org}\Delta_B - F_{b,carb}\delta^{13}C_{carb} + F_{extra}\delta^{13}C_{extra} - \delta^{13}C_{carb}(F'_w - (F_{b,org} + F_{b,carb}) + F_{extra}) \quad (5)$$

Now things start to settle down. After we distribute the $\delta^{13}C_{carb}$ to the fluxes at the end of equation 5 two terms cancel out: $F_{b,carb}\delta^{13}C_{carb}$ and $F_{b,org}\delta^{13}C_{carb}$. Meaning we are left with:

$$M_0\frac{d\delta^{13}C_{carb}}{dt} = F'_w\delta^{13}C_{volc} - F'_w\delta^{13}C_{carb} - F_{b,org}\Delta_B + F_{extra}\delta^{13}C_{extra} - F_{extra}\delta^{13}C_{carb} \quad (6)$$

Finally, re-arranging and dividing through by M_0 leaves us with a differential equation describing the change in $\delta^{13}C_{carb}$ over time:

$$\frac{d\delta^{13}C_{carb}}{dt} = \frac{F'_w(\delta^{13}C_{volc} - \delta^{13}C_{carb}) + F_{extra}(\delta^{13}C_{extra} - \delta^{13}C_{carb}) - F_{b,org}\Delta_B}{M_0} \quad (7)$$

In a later section we will go through discretization and assigning functional forms to the fluxes and Δ_B . Next, we derive the differential equation for the mass of the inorganic carbon reservoir.

The mass ODE

After deriving the isotope ODE this step is easy. All we are doing is re-writing the fluxes so that they capture processes that we care about. For example, we will want to separate the weathering of carbonate and organic carbon such that:

$$F_w = F_{w,carb} + F_{w,org} \quad (8)$$

The reason we want this distinction is so that we can make a crucial assumption that allows us to include the silicate weathering feedback. The silicate weathering feedback is theorized to be responsible for the regulation of Earth's climate on geologic timescales. It does not appear in equation 1 because the silicate weathering flux is simply a flux of one inorganic carbon phase (CO_2) to another (HCO^-).

But we can include the silicate weathering feedback if we make one simplifying assumption: that bicarbonate is buried the moment it is weathered. This is a reasonable assumption because response time of carbonate burial to a flux imbalance is an order of magnitude faster than the that of M_0 . So we can assume it happens instantaneously in our model. This assumption allows for:

$$F_{w,carb} + F_{w,sil} = F_{b,carb} \quad (9)$$

So in order to include the silicate weathering feedback we must explicitly partition the burial flux of carbonate carbon into its contributions from the weathering of carbonate rock ($F_{w,carb}$) and silicates ($F_{w,sil}$).

By including this assumption, we can re-write equation 1 to include the silicate weathering flux by:

$$\frac{dM_0}{dt} = F_{w,org} + F_{volc} - F_{b,org} - F_{w,sil} + F_{extra} \quad (10)$$

Note that here, we do explicitly include the notation $F'_w = F_{volc} + F_w$ (which was included in the isotope ODE). This is okay. The notation is independent of the assumption to which it was applied. The assumption only affects the isotopic signatures of the fluxes, not the fluxes themselves. Since there are no isotopes in equation 10, and all weathering and volcanic fluxes are accounted for ($F_{w,carb}$ was canceled out), there is no need to use F'_w notation. In fact, with this notation we could not include the silicate weathering flux because it requires separating out organic and carbonate components.

Equation 10 is the differential equation for the change in the mass of the system over time. Next we will discuss parameterizations of the terms in both the mass ODE (equation 10) and the isotope ODE (equation 7).

Parameterizations

First, we include a relationship linking pCO_2 to the mass of the inorganic carbon reservoir. This term is more conceptually useful and will help parameterize other aspects of the model, including the isotopic fractionation between carbonate and organic carbon. Following Kump and Arthur (1999) we use:

$$pCO_{2,t} = \left(\frac{M_{0,t}}{M_{0,init}} \right)^2 pCO_{2,init} \quad (11)$$

This is a scaling relationship that tells us the pCO_2 level at timestep= t is proportional to the fractional change in the mass of the system squared and the original pCO_2 level. With this equation, if the mass of inorganic carbon in the box doubles, the pCO_2 value will increase by a factor of 4.

Now that we have a way to calculate pCO_2 we can also calculate Δ_B , the fractionation factor between organic and inorganic carbon, which depends on pCO_2 . Following Kump and Arthur (1999):

$$\Delta_B = \frac{159.5[PO_4] + 38.39}{0.034pCO_2} - 33 \quad (12)$$

A number of assumptions are required to arrive at this equation. See Kump and Arthur for a discussion of these assumptions and references for further reading.

Functional forms

In order for the box model to include feedbacks—a control on the system that responds to and modifies the state of the system itself—we must allow the fluxes of carbon to be a function other fluxes

and/or the size of the reservoir. Prescribing feedbacks often requires some thoughtful decision-making because it is not always possible to know the functional form of a feedback from data or theory.

Here, I'll walk through a couple examples of flux parameterizations that operate as feedbacks in the C cycle model associated with these instructions.

Perhaps the most well-known feedback of the geologic carbon cycle is the silicate weathering feedback. This is the feedback between climate and rock weathering by which climate warming can strengthen the water cycle, thus weathering more rock and sequestering more CO_2 to shift the climate back to a colder state.

The true functional form of this feedback is not known (and may very well have changed through geologic history). But one way to express it is:

$$F_{sil} = F_{sil,init} \left(\frac{pCO_{2,t}}{pCO_{2,init}} \right)^n \quad (13)$$

This equation tells us that the flux of silicate weathered-carbon is scaled with the change in pCO_2 at the first timeslice, raised to the n , and multiplied by the silicate weathering flux at that timeslice. This is a simple formulation with just one tunable parameter: n . Thus, n effectively determines the strength of the silicate weathering feedback (the change in silicate weathering flux per change in pCO_2).

A stronger feedback implies a greater change in F_{sil} per change in pCO_2 . So does that mean that the feedback is stronger with higher or lower values of n ? While it's easy to intuit, it may be worthwhile to explore the effect of that parameter in the model itself.

Another feedback that follows a more complicated path is that between nutrient availability, organic carbon burial, and climate. The burial of organic carbon represents the removal of CO_2 from our box. So this term can be an important negative feedback on Earth's climate (and there is good evidence for this mechanism playing a key role in global climate throughout geologic time). In order to allow organic carbon burial to feedback on climate, I have written the burial term as a function of nutrient availability. Then, nutrient availability is a function of climate because weathering is the primary nutrient input.

We can set the input flux of nutrients to be equal to the weighted average contribution of silicate, organic, and carbonate weathering. Then, the flux of nutrients to the box at time t can be written as:

$$F_{Nutrients,t} = F_{Nutrients,init} \left[x \left(\frac{F_{sil,t}}{F_{sil,init}} \right) + y \left(\frac{F_{w,carb,t}}{F_{w,carb,init}} \right) + z \left(\frac{F_{w,org,t}}{F_{w,org,init}} \right) \right] \quad (14)$$

Where $x + y + z = 1$ and the fractional changes in the contributing fluxes sum to a factor that is multiplied by the initial nutrient flux to calculate that of time t .

This links the nutrient flux to climate (because weathering increases in a warmer world). To complete the link to the burial of organic carbon, we write:

$$F_{b,org,t} = F_{b,org,init} \left(\frac{PO_{4,t-1}}{PO_{4,init}} \right)^{P_{exp,t}} \quad (15)$$

This equation tells us that the burial flux of organic carbon is related to the change in the reservoir size of nutrients (denoted here as phosphate, PO_4). This reservoir size was calculated in the previous time step using equation 14. It cannot yet be known for this time step (t) because the flux into the nutrient reservoir was only just calculated (equation 14) and to get the burial flux of nutrients we must first know the burial flux of organic carbon (equation 15).

You may have recognized that each flux at time t is a function of the initial flux multiplied by some scaling value, and that the scaling value includes the fractional change in the flux(es) or reservoir(s) that influence the flux. The final layer of complexity involves adding exponents or roots to the scaling value such that the feedbacks are non-linear (a fair assumption for the Earth system). For example, without an exponent in equation 15, $F_{b,org,t}$ would scale linearly with the nutrient reservoir. If the nutrient reservoir doubles in size, then so will the burial flux of organic carbon. It is a worthwhile exercise exploring the effects that different functional forms have on the output of your model (the response of the modeled reservoir to a prescribed perturbation).

Discretization

In earlier sections we derived differential equations for the change in the mass of the box's reservoir (equation 10) and the change in its isotopic composition (equation 7). In order to make these equations useful in R, we must discretize them so we can solve the mass and isotopic composition *at each time step*.

This is a relatively simple approach. While there are many different numerical solutions that one could use, I will demonstrate the forward difference approach here (sometimes called backwards difference... admittedly, I don't know which is correct).

The basic form of the forward difference is:

$$\frac{dC}{dt} = \frac{C_t - C_{t-1}}{dt} \quad (16)$$

This says that the change in some variable, C , is equal to the difference between its values at time t and at time $t - 1$ (the previous time step) divided by the size of the time step itself. As we loop through every time step in R, we will always know the value for C_{t-1} . At the first time step in our loop ($t = 2$; see script) we know $t - 1$ because it was prescribed. Then, within that time step we calculate the new fluxes so at $t = 3$ we can call the values from $t = 2$.

This means that our only unknown in equation 16 is C_t , the variable's value at the present time step. We can plug the right side of equation 16 into the left side of equations 7 and 10 (changing C to $\delta^{13}C_{carb}$ and M_0 , respectively). Then, after multiplying through by dt and adding C_{t-1} we arrive at the final equations that we will actively solve in our “for loops” in R.

For the isotopic composition of the inorganic carbon reservoir, this equation is:

$$\delta^{13}C_{carb,t} = \delta^{13}C_{carb,t-1} + \left(\frac{F'_w(\delta^{13}C_{volc} - \delta^{13}C_{carb}) + F_{extra}(\delta^{13}C_{extra} - \delta^{13}C_{carb}) - F_{b,org}\Delta_B}{M_0} \right) dt \quad (17)$$

And for the mass of inorganic carbon in our box:

$$M_{0,t} = M_{0,t-1} + (F_{w,org} + F_{volc} - F_{b,org} - F_{w,sil} + F_{extra}) dt \quad (18)$$

With these equations, and having solved their fluxes at time t earlier in the same iteration of the for loop, you will have completed your box model.

The general framework of these derivations is applicable to any single-box model but, of course, most of the assumptions are not (they are specific to this system).

Please contact me with any questions or concerns, or to set up a time to meet: *tykukla@stanford.edu*.

I wrote this pretty quickly, copying the derivation I wrote earlier. It is possible that there are mistakes. If you find any, please let me know!