Geodynamics and dissolution processes: The Good, the bad, the ugly

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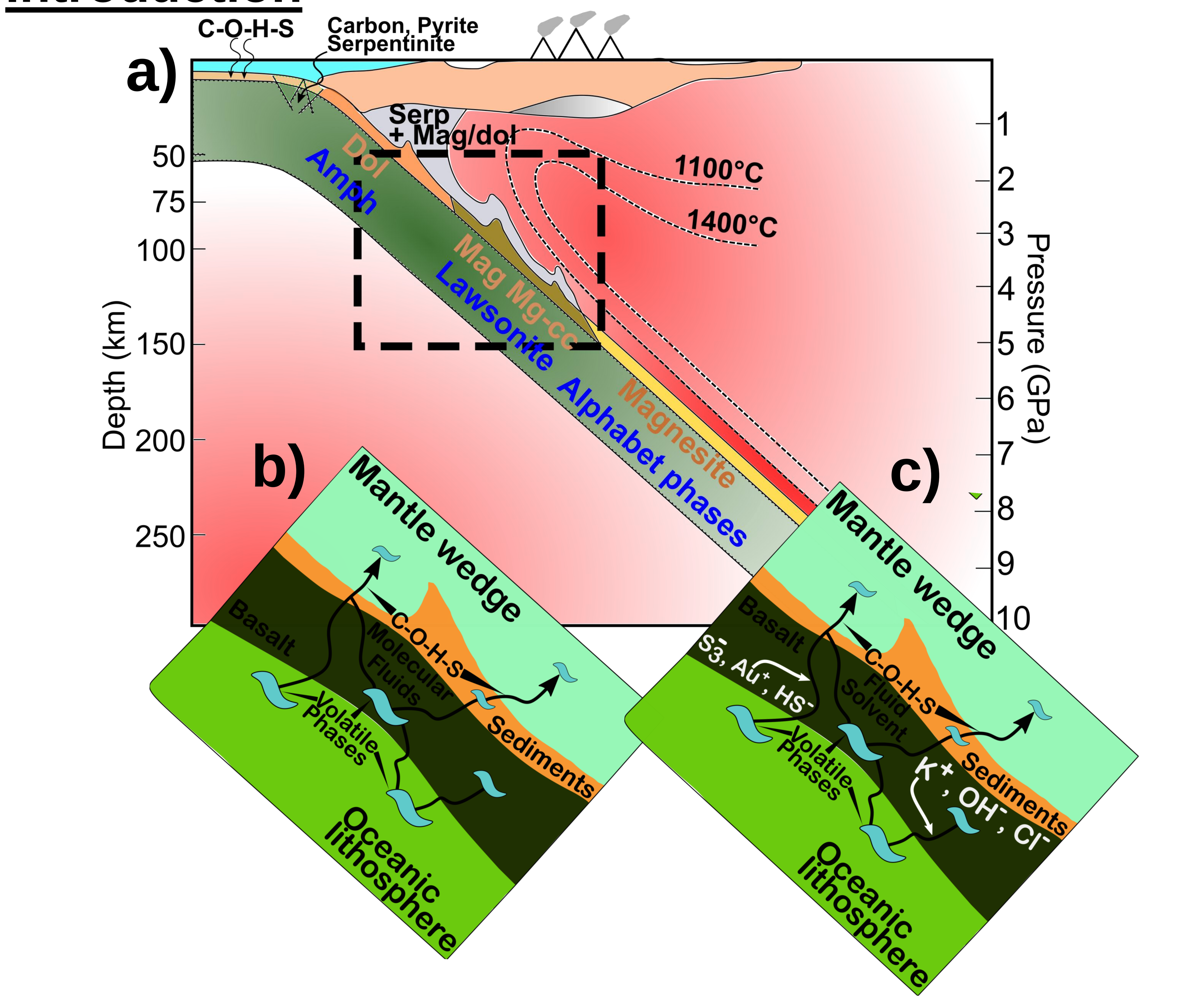
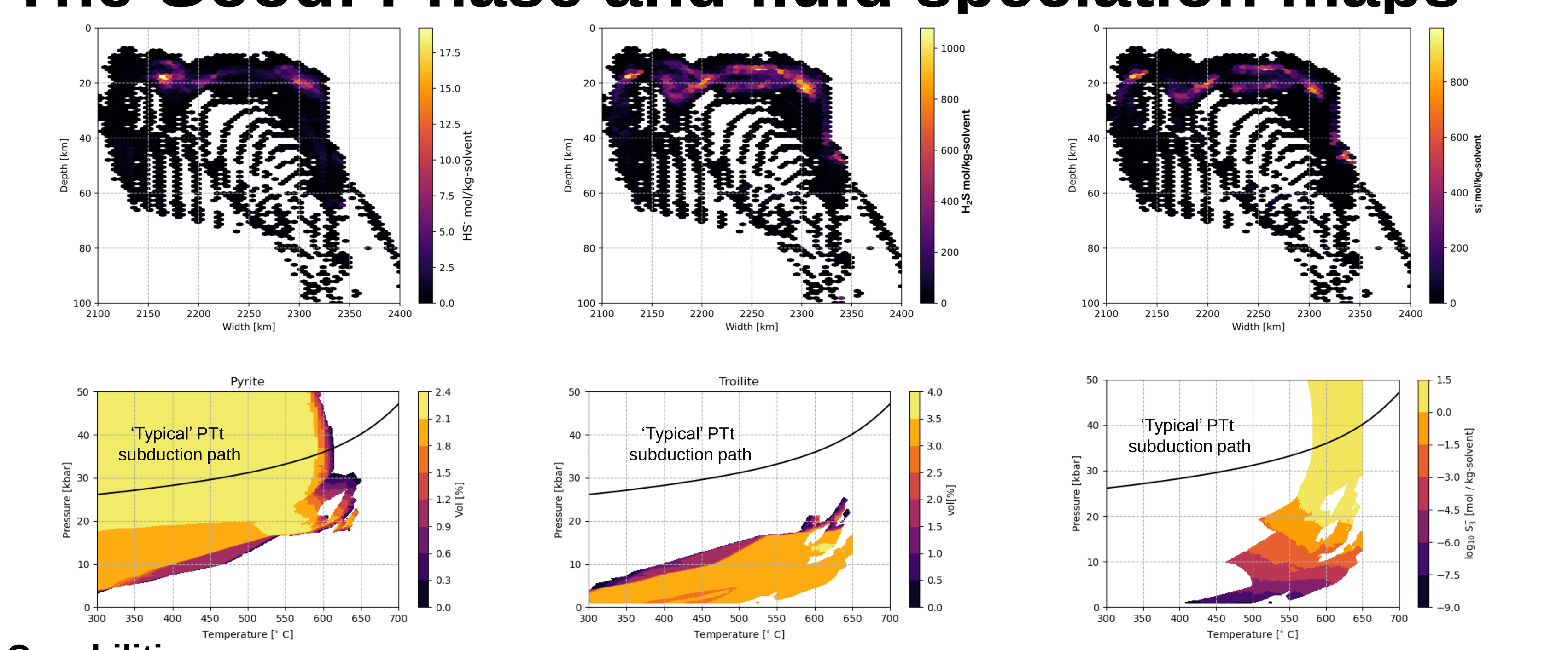
Introduction



Rocks are recycled into and out of the Earth's interior at subduction zones. They are unique areas concentrating mass and energy into the overlying crust and mantle. Understanding volatile cycles is critical to better understanding the evolution of planetary bodies, atmospheric regulation, life, and in the formation of major mineral deposits [1].

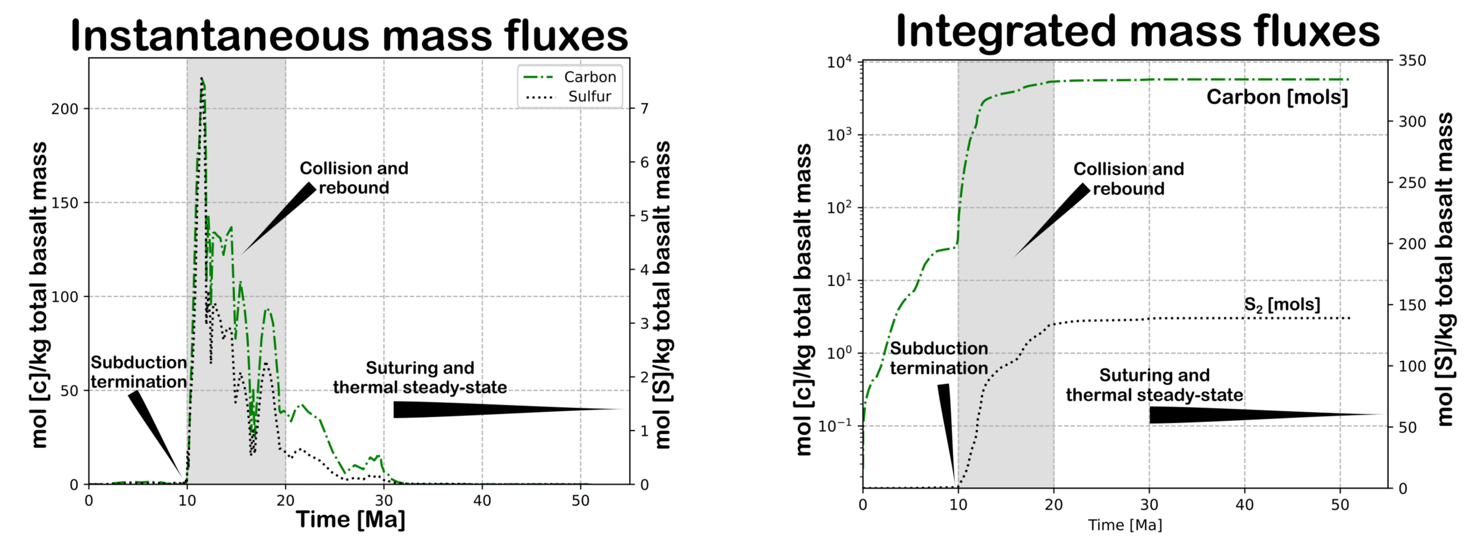
Increasing evidence for the role of ionic aqueous species (e.g., S_3^-, HS^-, CO_3^{-2}) in mass transfer and as a catalyst in the deposition of large deposits. Diamond inclusions show evidence of important role of charged species dissolved from molecular solvents as the fluid moves through the rocks and into the mantle wedge. S_3^- complexes with gold to concentrate it within hydrothermal fluids for increased mobility [2]. This work aims to capture pivotal moments during geodynamic processes within a mechanical framework to illustrate the importance that dynamics have in devolatilization volatile and aqueous species that supply giant ore deposits.

The Good: Phase and fluid speciation maps



Capabilities:
The models are capable of reconstructing compositions and stable phases for each of the aqueous speciations derived from the DEW model. **Fig. 3a-c** show calculated heat maps with integrated sums for retrograde mélange as the exhumed rocks resurface. The sulfur species represent critical complexing agents for transporting gold within ore deposits. Stable mineralogy **Fig. 3d-e** is also possible and may be reduced to 1-D paths for steady-state conditions.

The Good: Mass conservative fluid fluxes



Capabilities:
Elemental mass flux calculations are impact global carbon and water budgets. Long term climate cycles are regulated by the efficacy of recycling. These figures illustrate the importance of geodynamic processes (e.g., rollback, collision, breakoff; **Fig. 2**) and the impact on the return of fluxes to metasomatized units in the crust/mantle or returned as volatiles into the atmosphere through hydrothermal systems or volcanism. These can be easily tracked and incorporated into the post-processing process.

Methodology

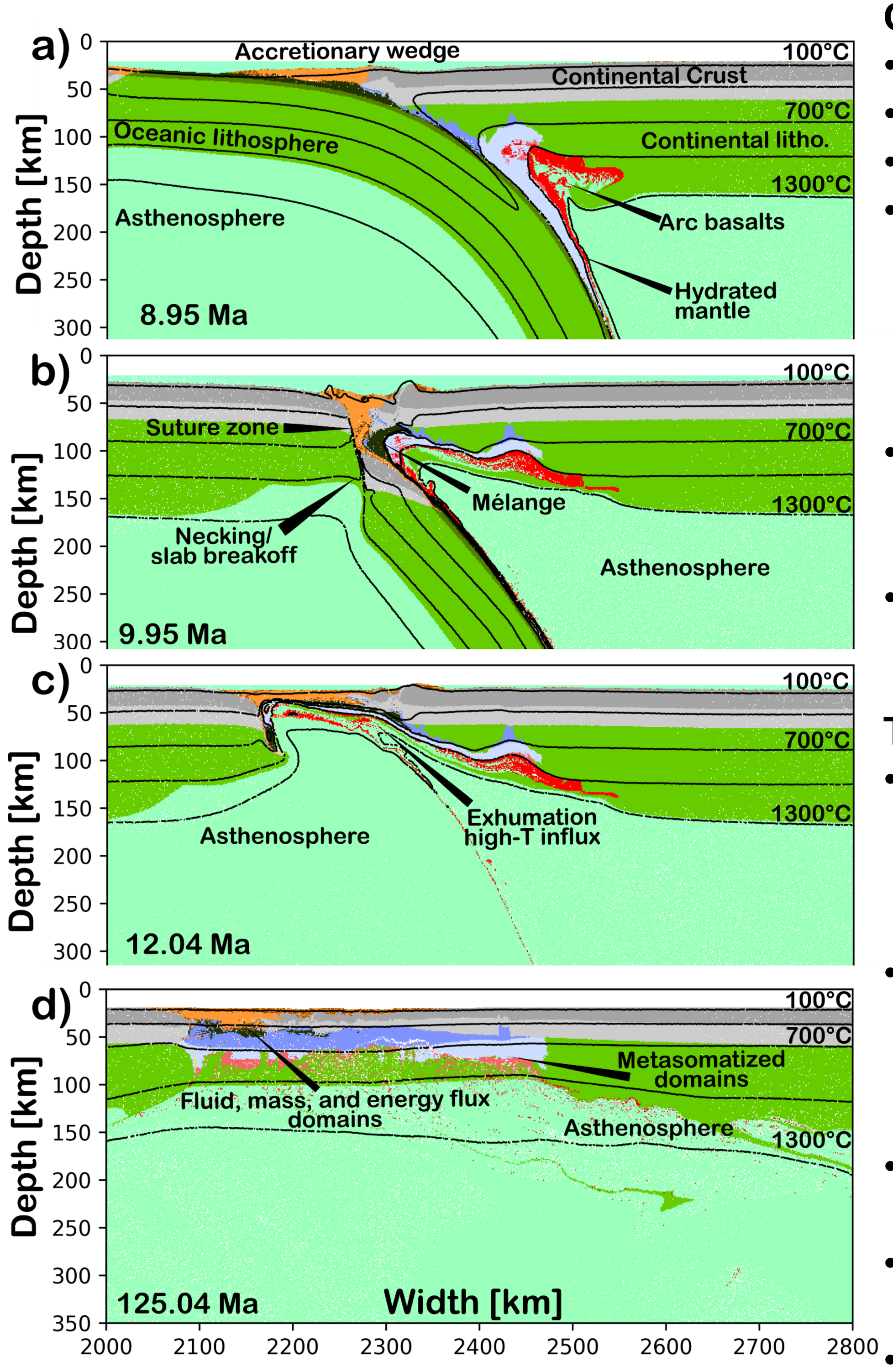


Figure 2: Typical model evolution for the prototype code. Plagioclase An_{75} used as lower crustal rheology. 5 cm yr^{-1} with an 80 Ma oceanic plate and a proton composition for the continental lithospheric mantle. Initial subduction for the first 7.5 Ma followed by slab-pull and buoyancy driven processes for the remainder of the models. Illustrates process of collision, asthenospheric upwelling, exhumation, and suturing.

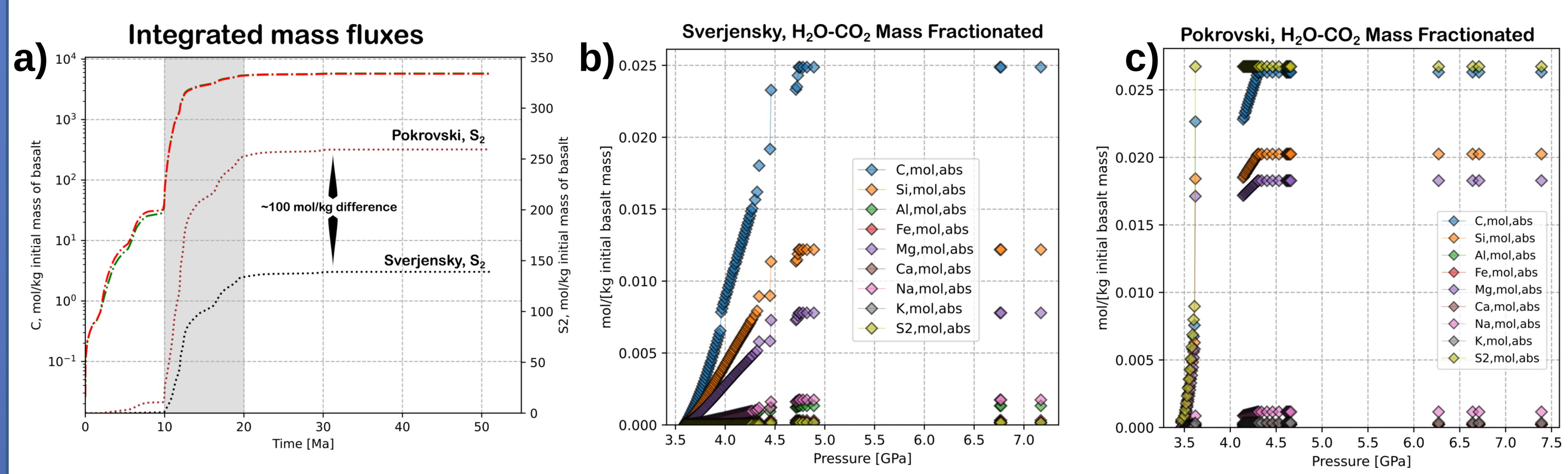
Geodynamics:

- Simulated continental collision
- Thermomechanical code I2VIS [3].
- Petrological implementations [4].
- Initial conditions:
  - **Dimensions**: 4000 x 1200 km
  - **Velocity**: 2.5, 5, 7 cm yr^{-1}
  - **Plate ages**: 20, 40, 60, 80 100 Ma
- Stable mineralogy: Perple_X look-up tables for density and bulk CO_2 and H_2O devolatilization [4].
- Melting: Only partial melting without extraction.

Thermodynamic speciation:

- Calculated using the Deep Earth Water (DEW) model [5] and a Helgeson-Kirkham-Flowers (HKF) Equation of state (EoS).
- Lagged speciation and stable mineralogy was calculated with Perple_X [6] with H_2O and H_2O-CO_2 solvents using a generic fluid EoS.
- Mass fractionated and becomes refractory if all fluid removed.
- Calculated for each initial bulk calculation of rock.
- Calculations computed for a carbonated basalts [4] and an addition 0.1 vol.% of pyrite for sulfur.

The Bad: Not all speciation models are equal



Limitations:

- Discrepancy between two experimental regressions of HKF coefficients for S_3^- demonstrate the fragility of experimental models. **a)** Shows integrated mass fluxes differences due to different calculated molar volumes from experimental work [2, 5]. This effect the mass fractionated components and the stability of sulfur during continental collision (**Fig. 2**).
- 1-D P-T-t paths for steady-state subduction (**Fig. 4 b&c**) reduce complexity to investigate elemental components. Nearly all sulfur is retained along the PTt path **(b)** vs. completely recycled in **(c)**.
- ***Not all bad:*** *Ab initio* studies (e.g., [7]) may guide the future path to thermodynamic wisdom. Thermodynamic properties, such as molar volumes, can be used to resolve discrepancies.

The Ugly: The implementation

- Much like this photo of Chris as a kid eating spaghetti, the implementation is a mess. The geodynamic code is written in C, the thermodynamic minimizations written in Fortran, and all held together in a venerable sauce of Python wrappers. It does scale as the geodynamic code implements C with OMP directives and Python.
- Scalability of the speciation calculations:
  - (6204 individual models) Total time: 25 hours (or 248 individual fractionation paths/hour on only 9 cores.
- Fractionation is still within a single chunk of rock. Further, implementations could consider reactive transfer.

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