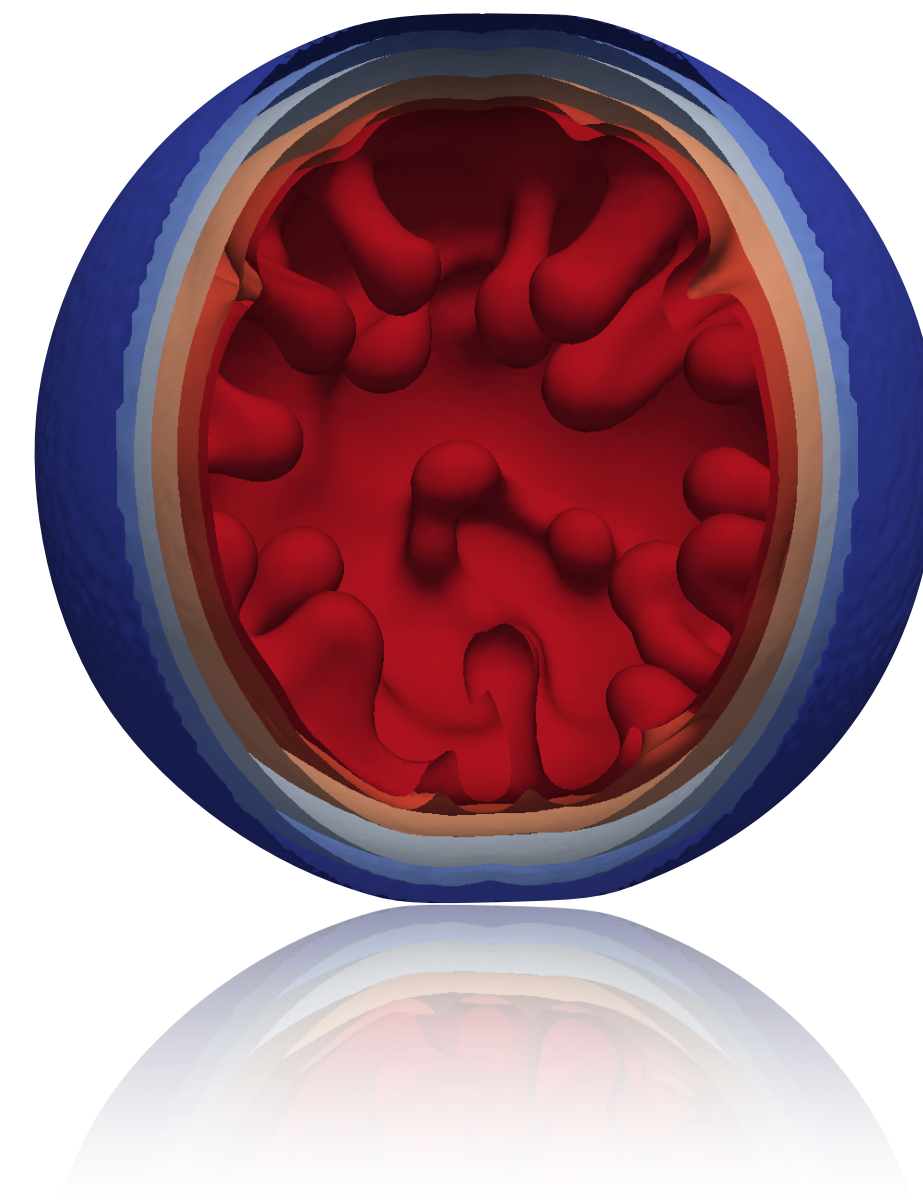


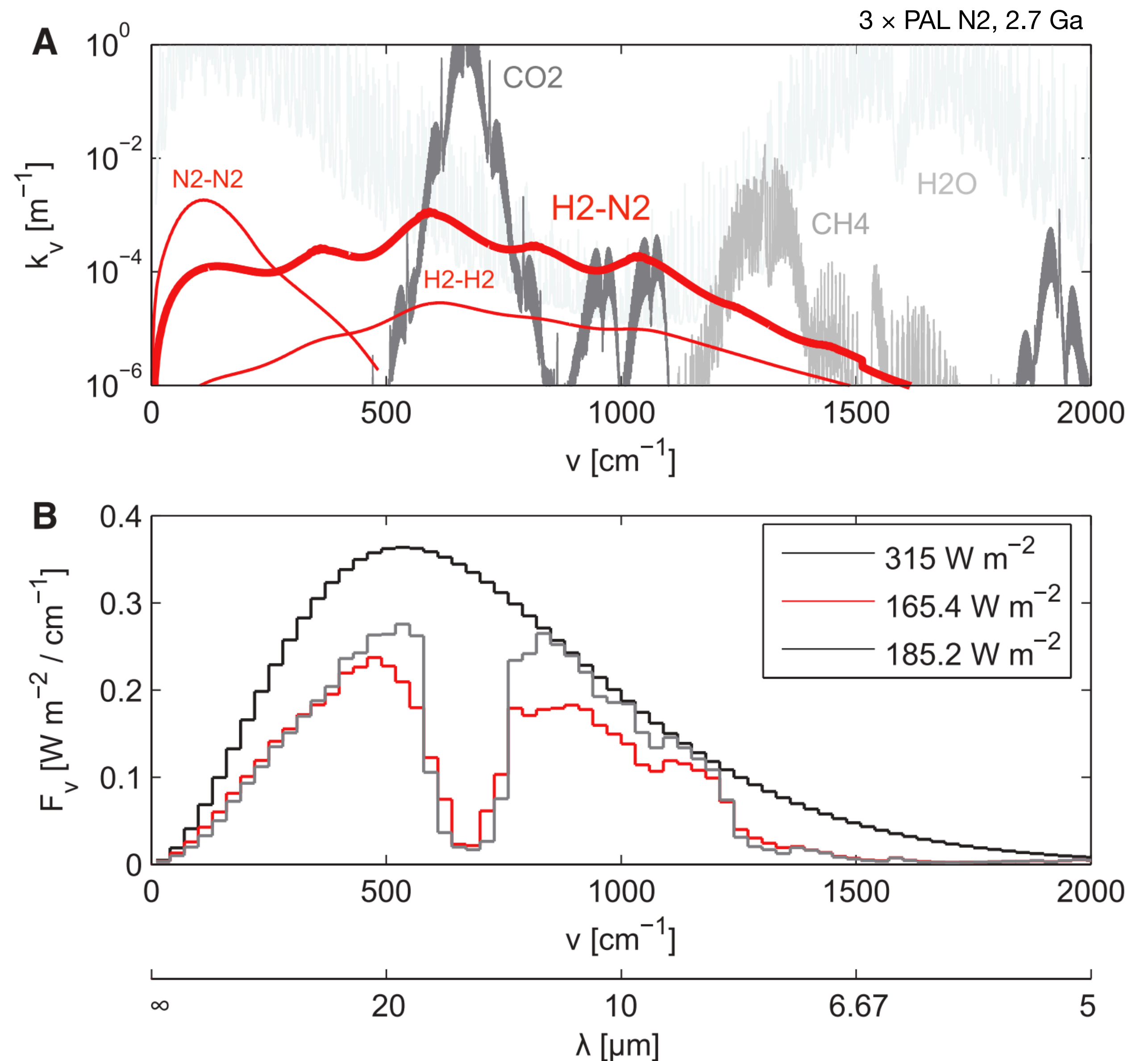
# Volatile partitioning and mantle stratification during late-stage magma ocean solidification

Tim Lichtenberg



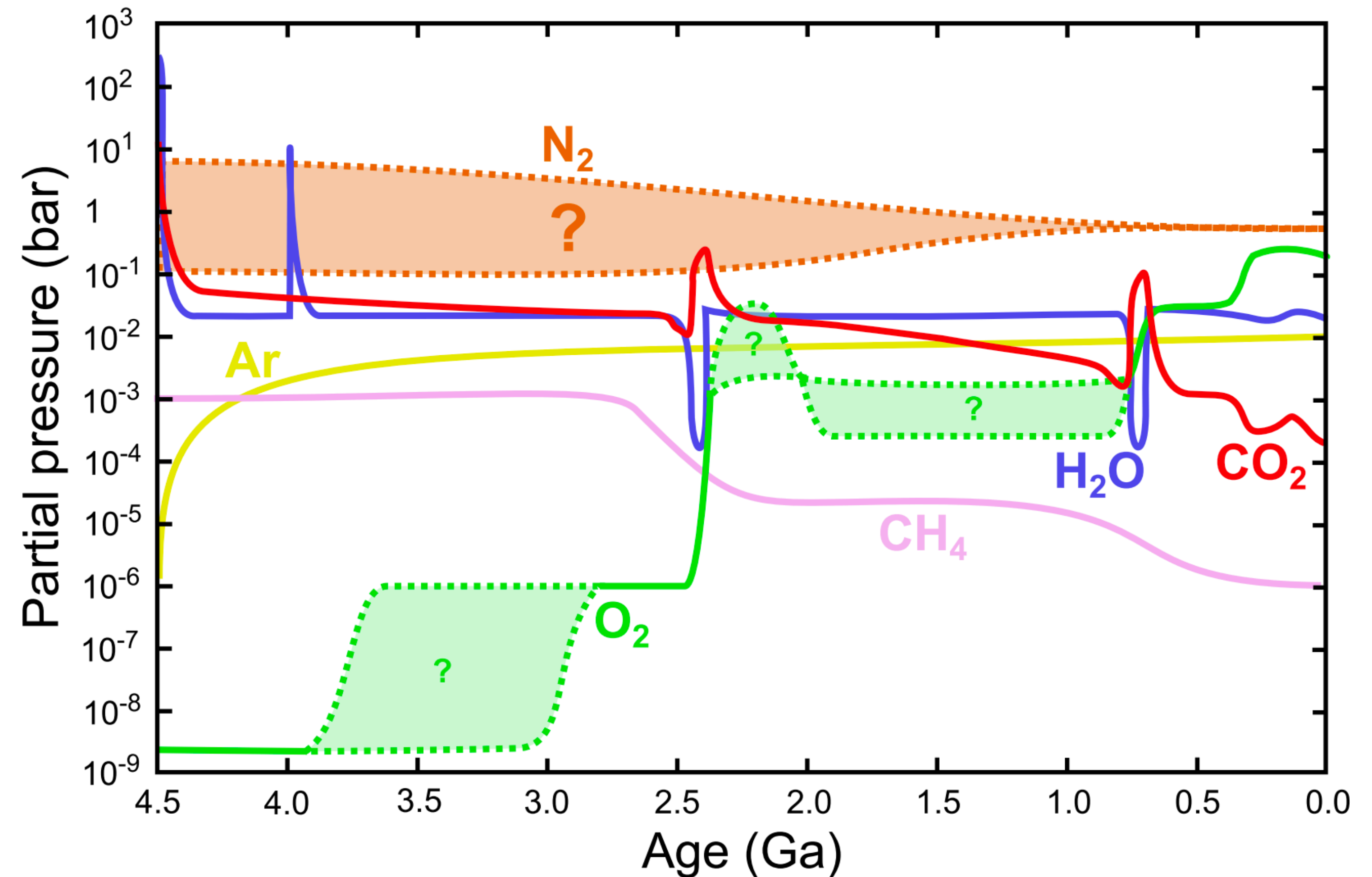
# Relevance

- Atmospheric composition
- Faint Young Sun paradox
- Mantle redox state
- Cessation of core formation
- Tectonic regime of early Earth
- Extrapolation to exoplanets
- Mars-Earth divergence
- Subaerial prebiotic chemistry



# Relevance

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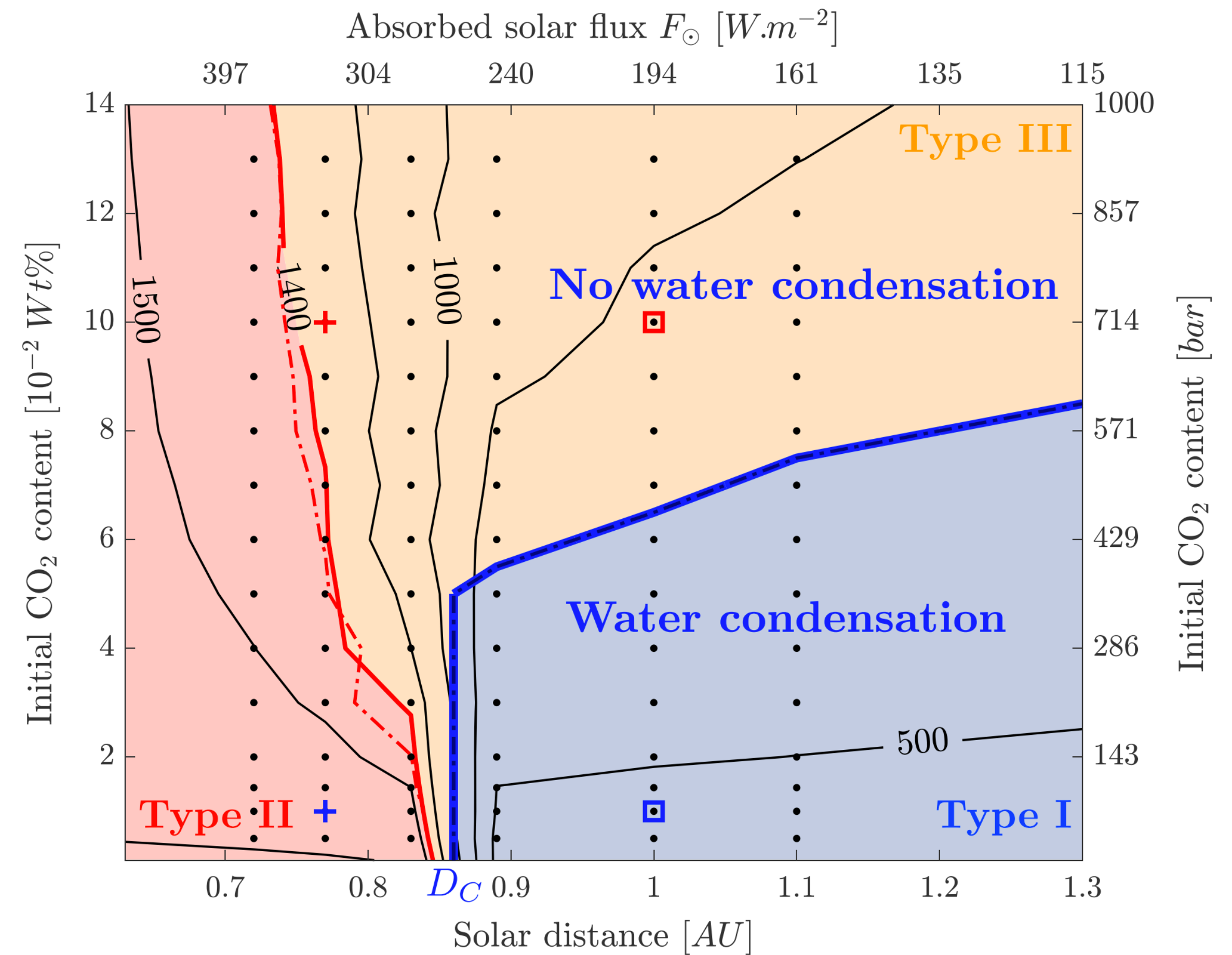
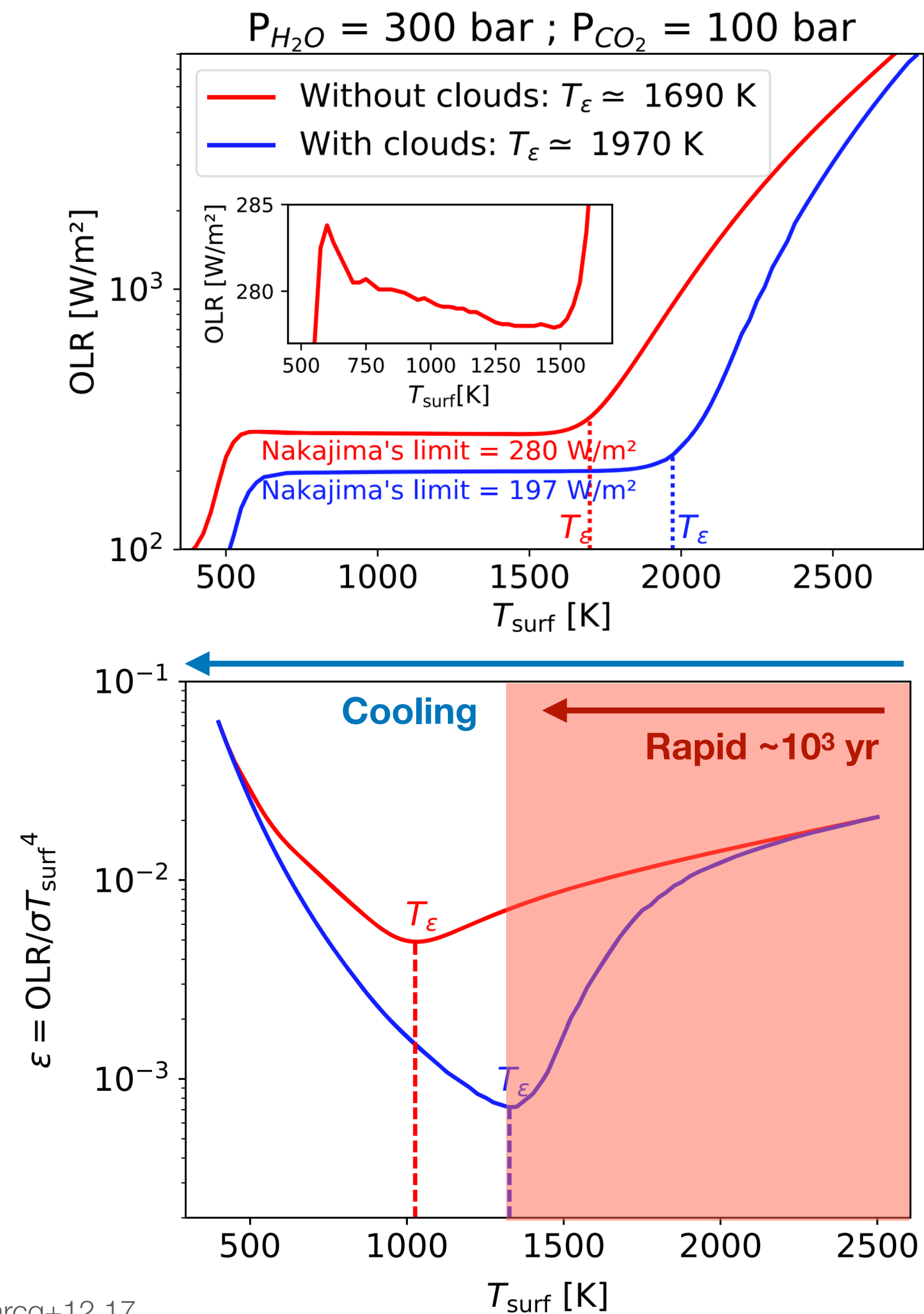


# Major challenges & opportunities

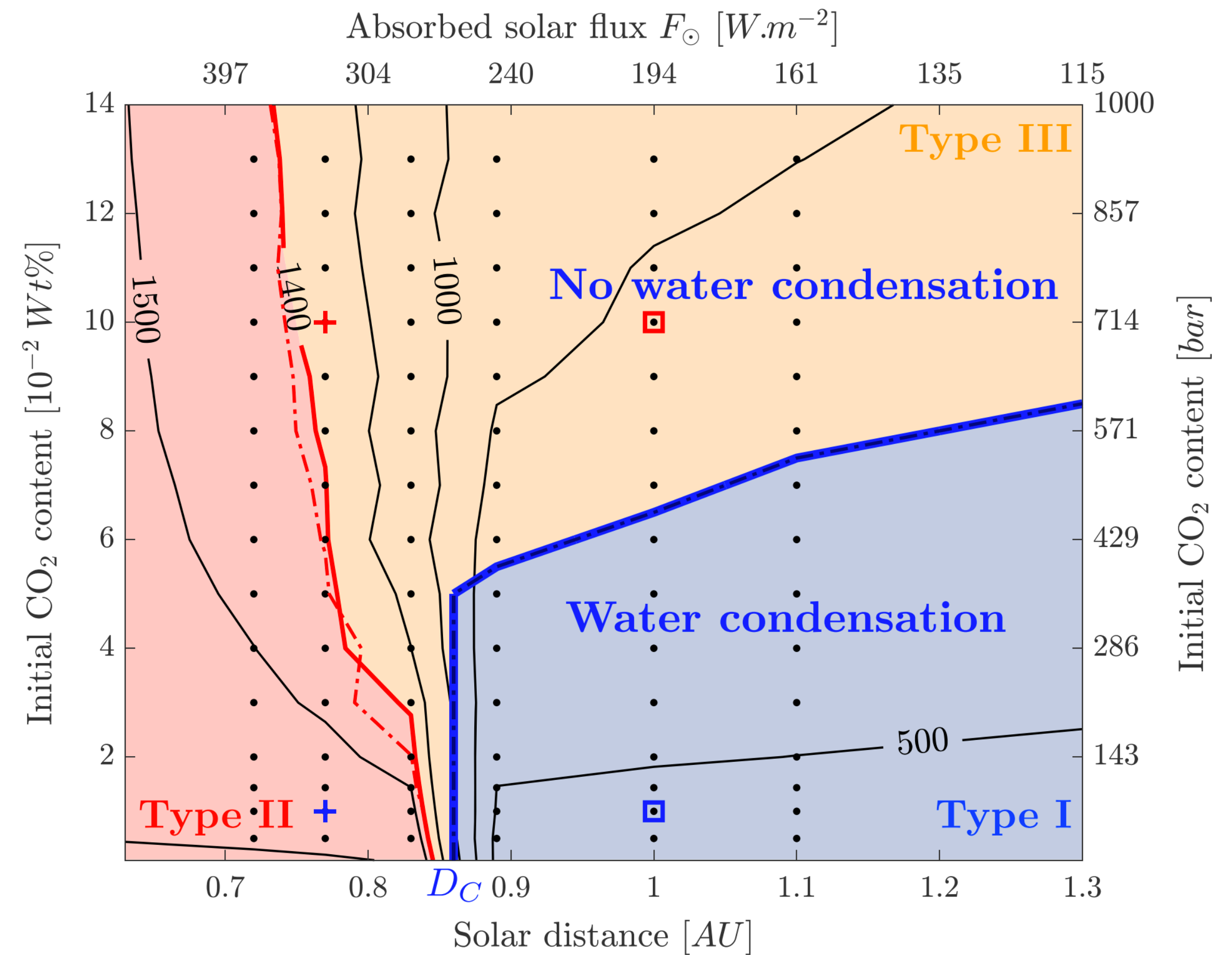
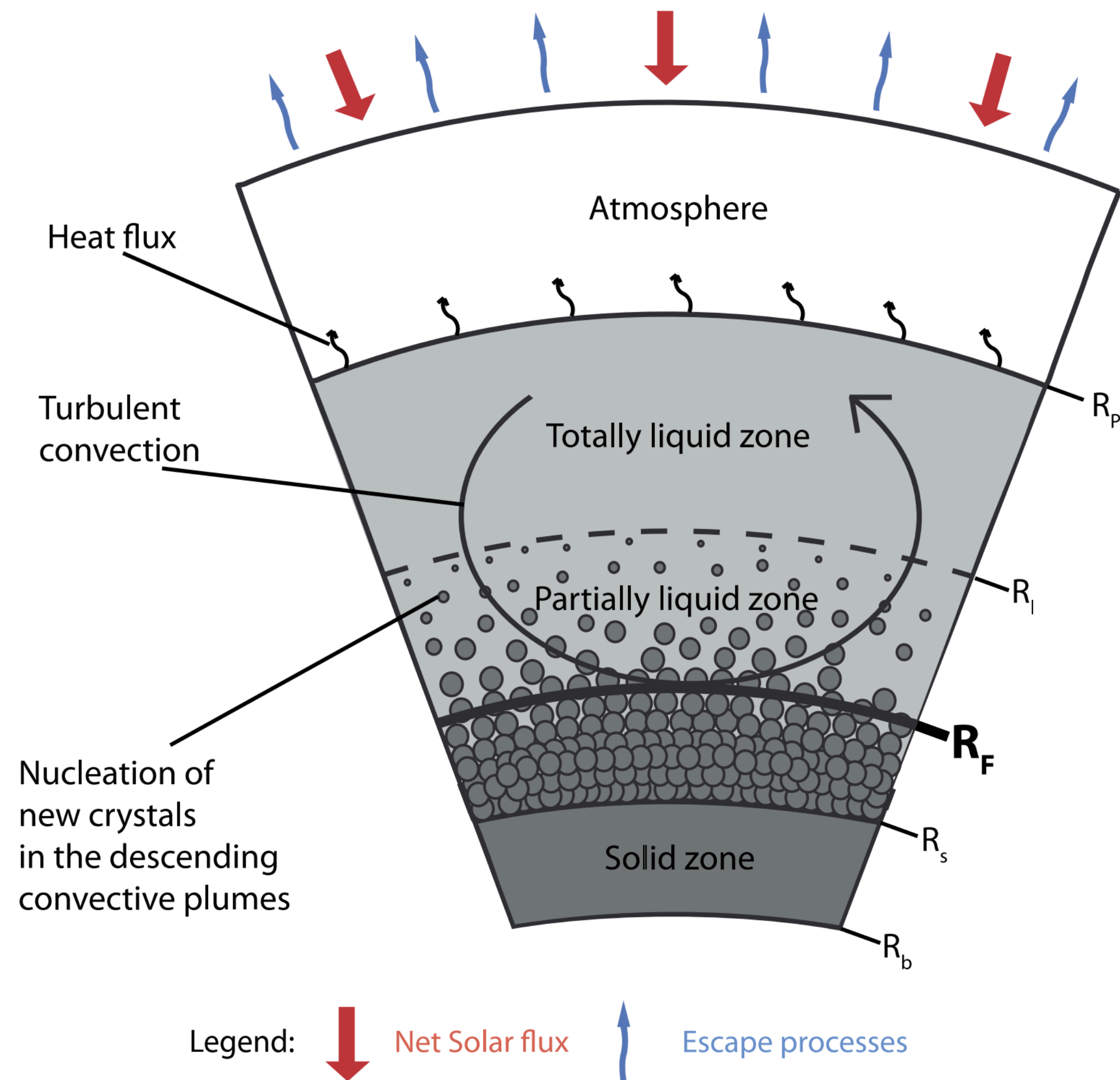
- Provide a bridge from planet formation to long-term planet evolution
- Constraints on early Earth geochemistry poor
- Magma ocean (MO) evolution complex: interplay between siderophile + atmophile partitioning, atmospheric chemistry/radiation, fluid dynamics
- Suspension flow regime (so far) inaccessible/too expensive for computational geodynamics
- Timing of volatile addition better constrained
- Majority of former results based on 0D to 1D approximations
- Former models neglect mantle fluid dynamics
- Only very few studies w/ two-phase flow approach
- Synergies of expertise in Katz + Pierrehumbert groups



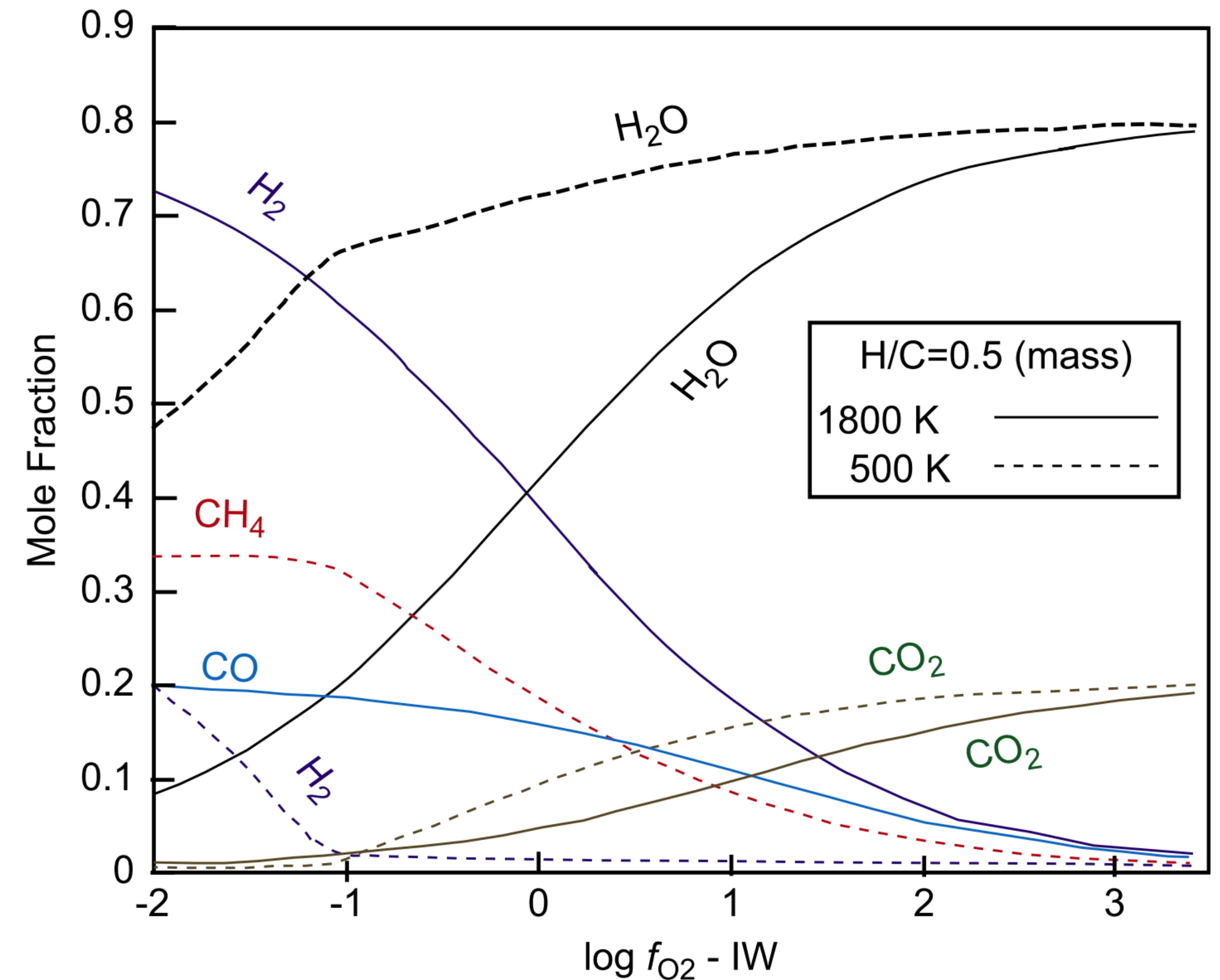
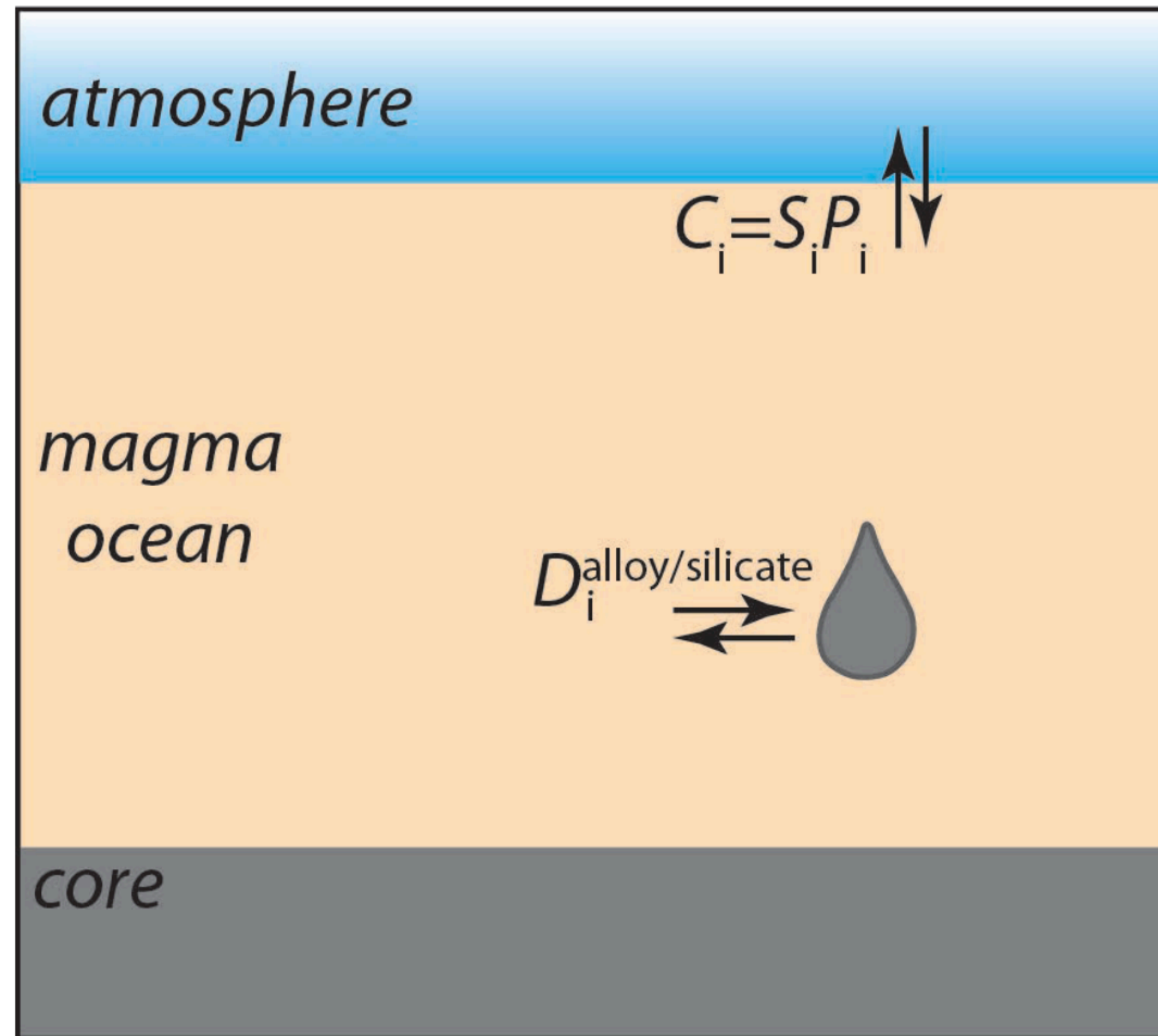
# Early Earth's surface environment



# Atmosphere – MO connection

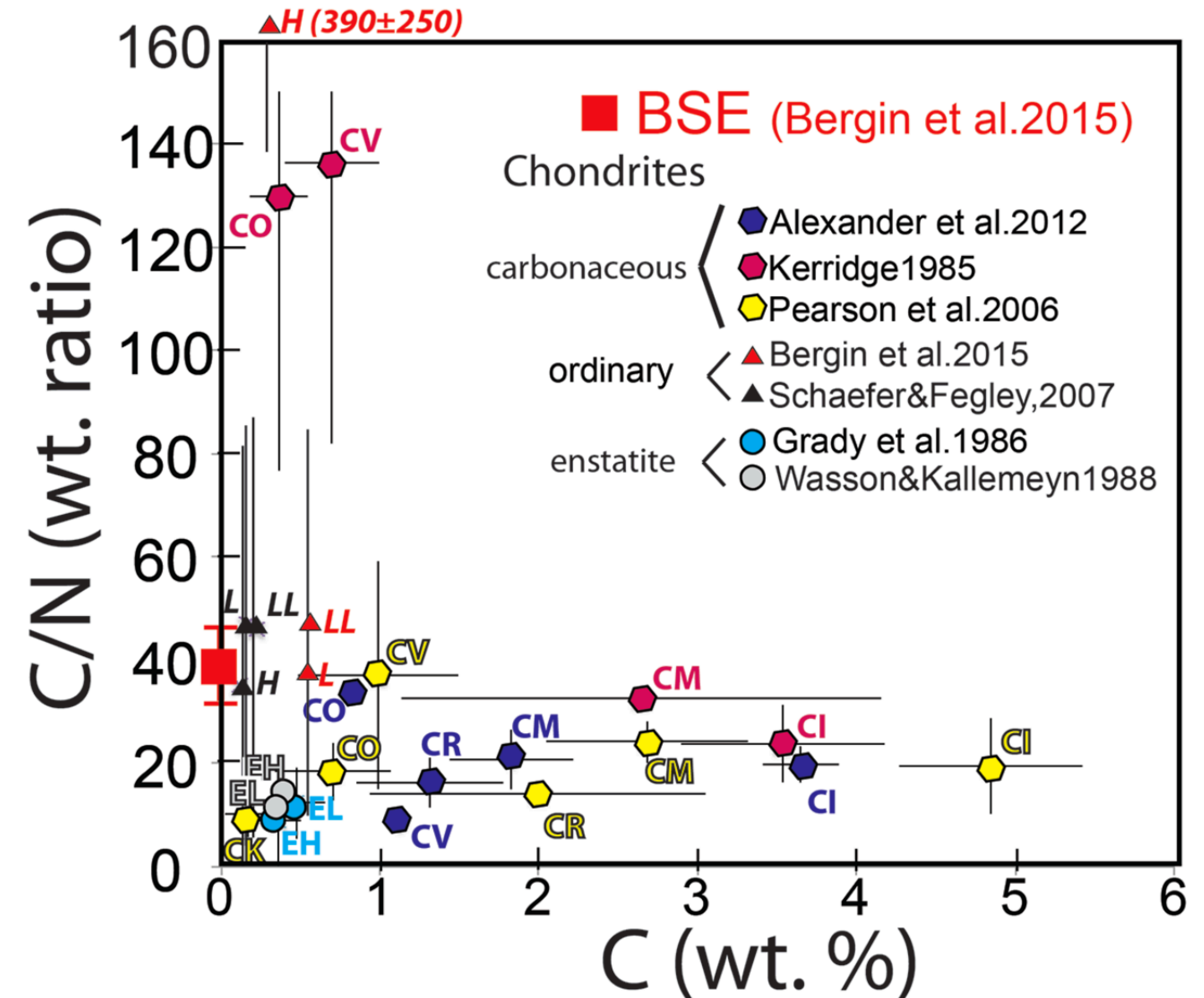
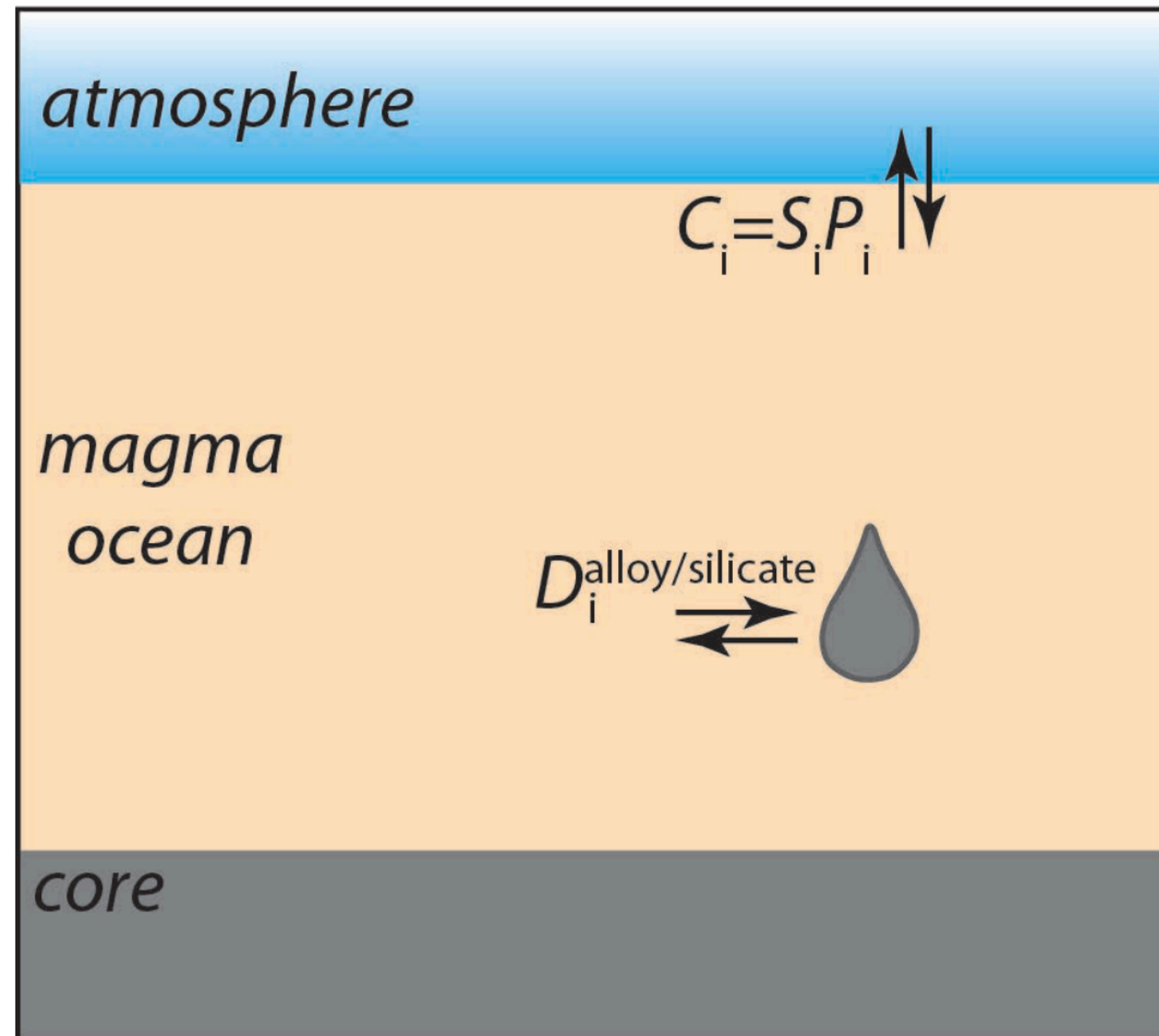


# Simplistic equilibrium partitioning models



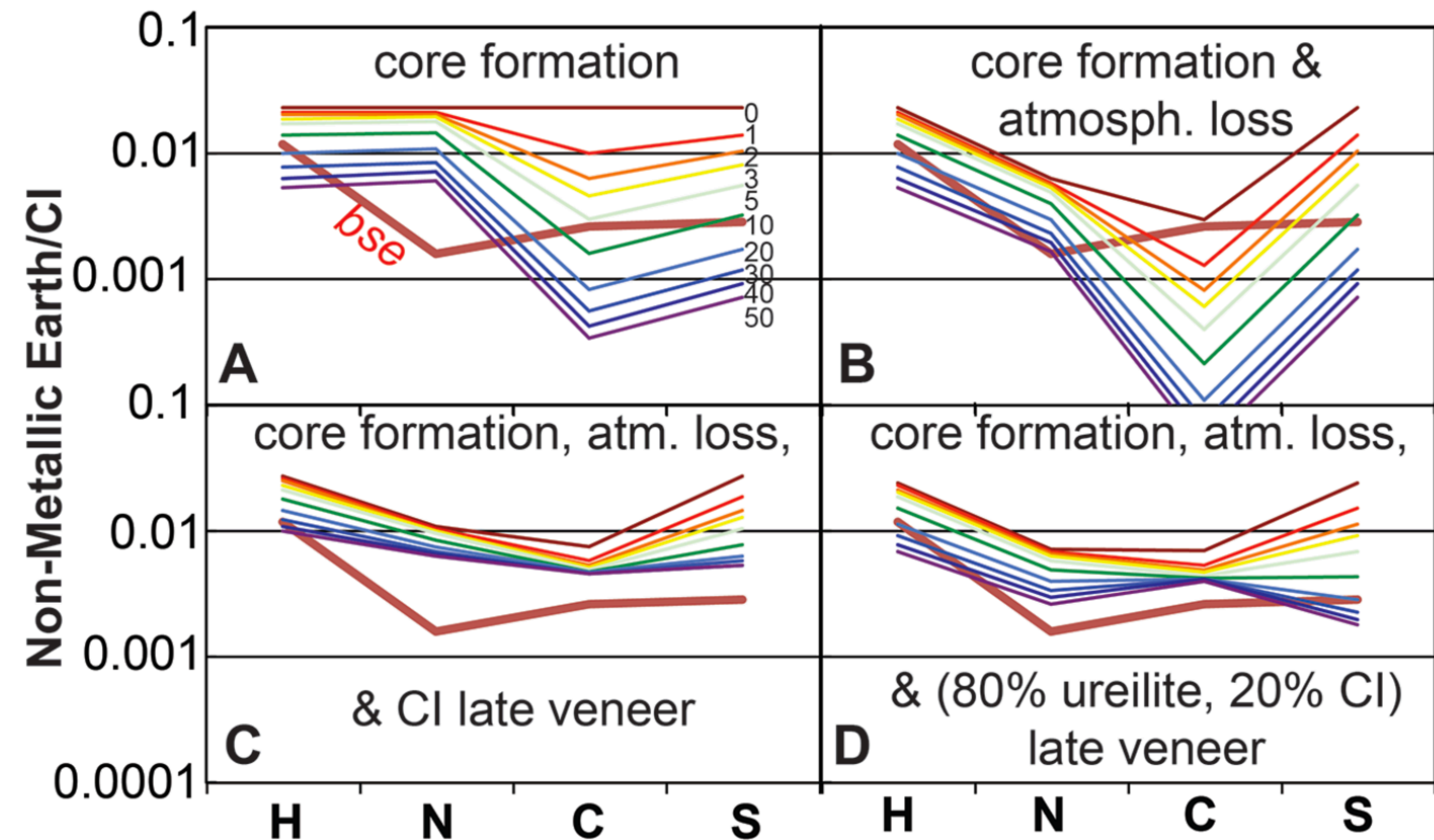
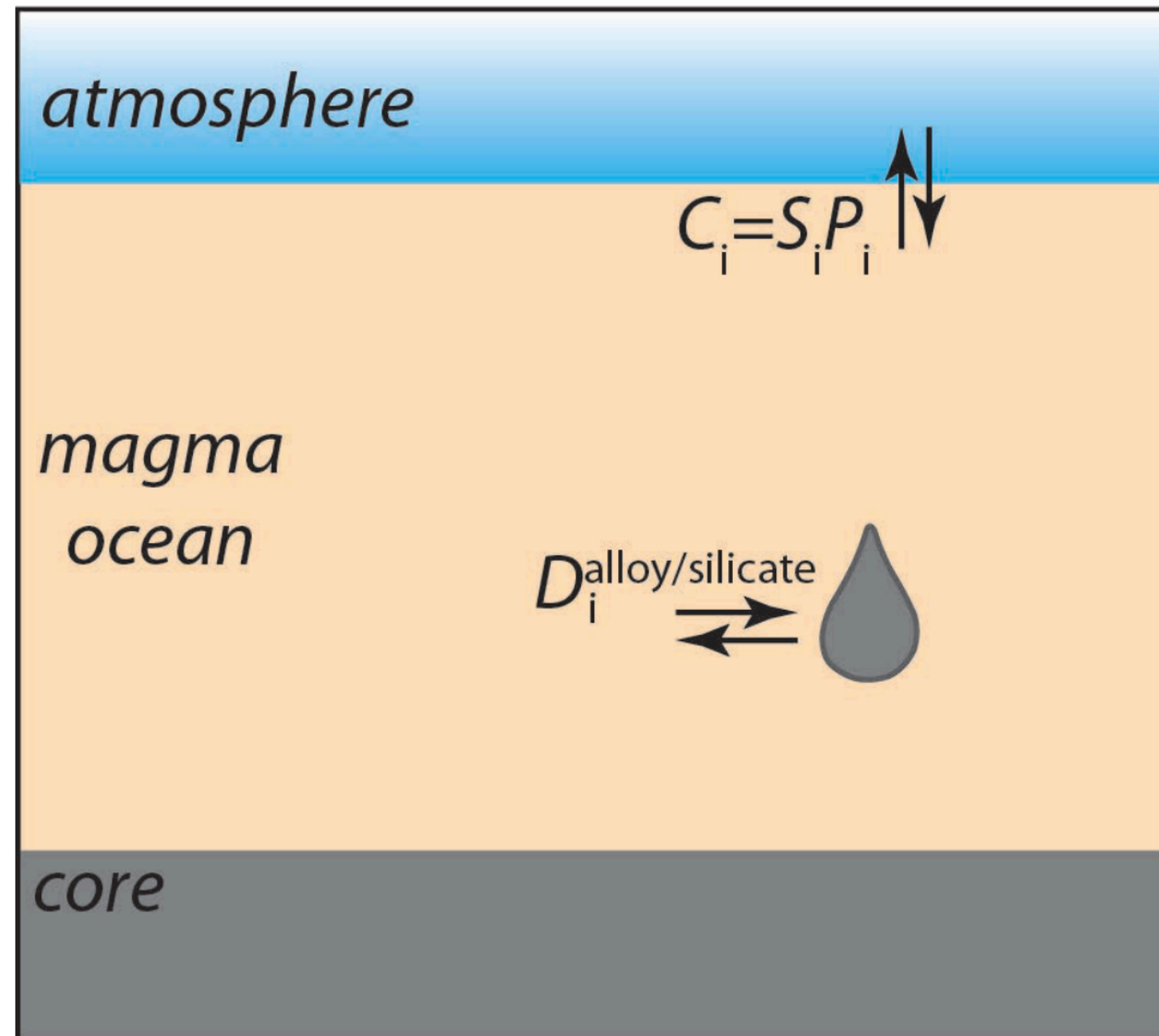


# Simplistic equilibrium partitioning models

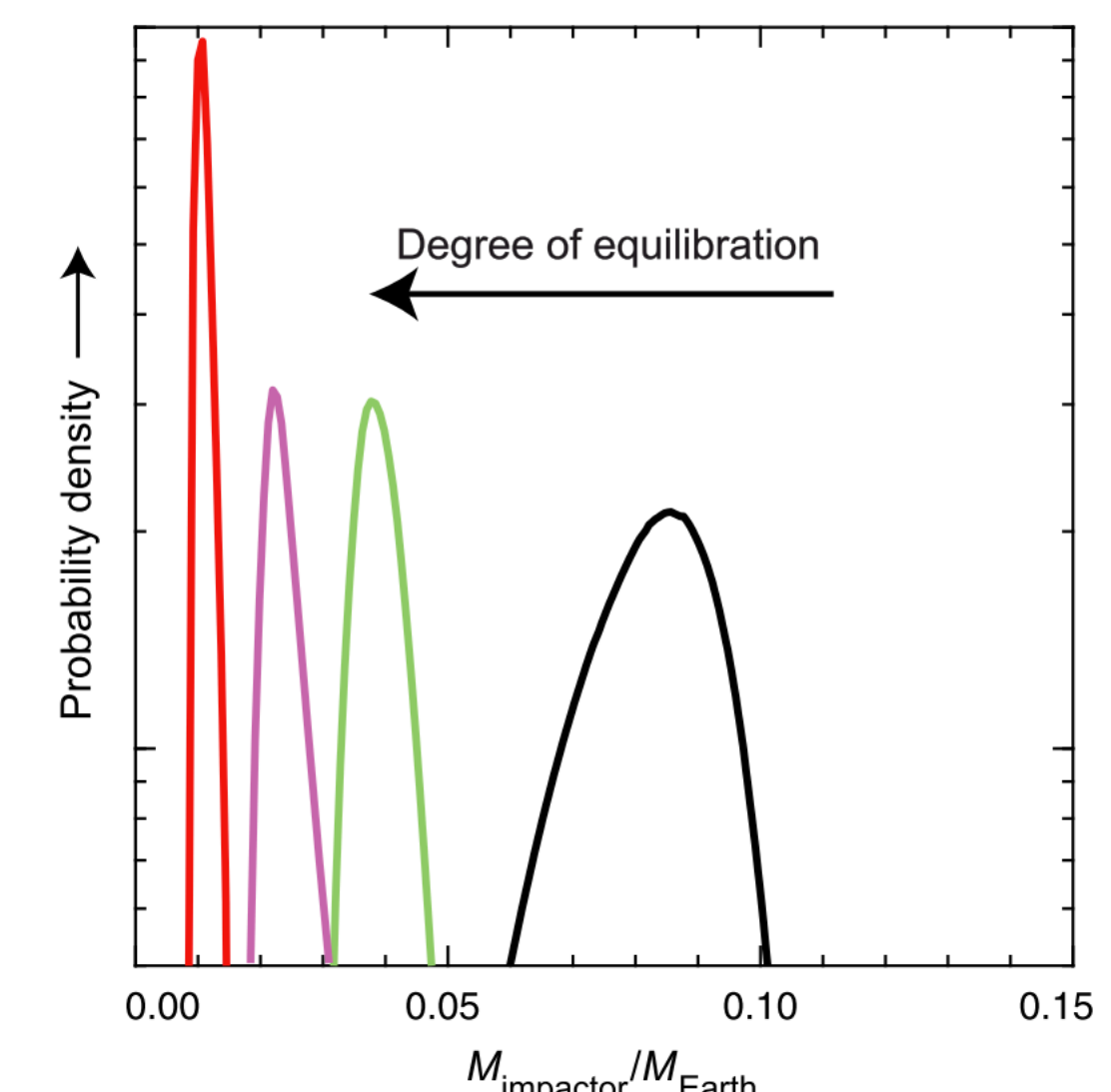
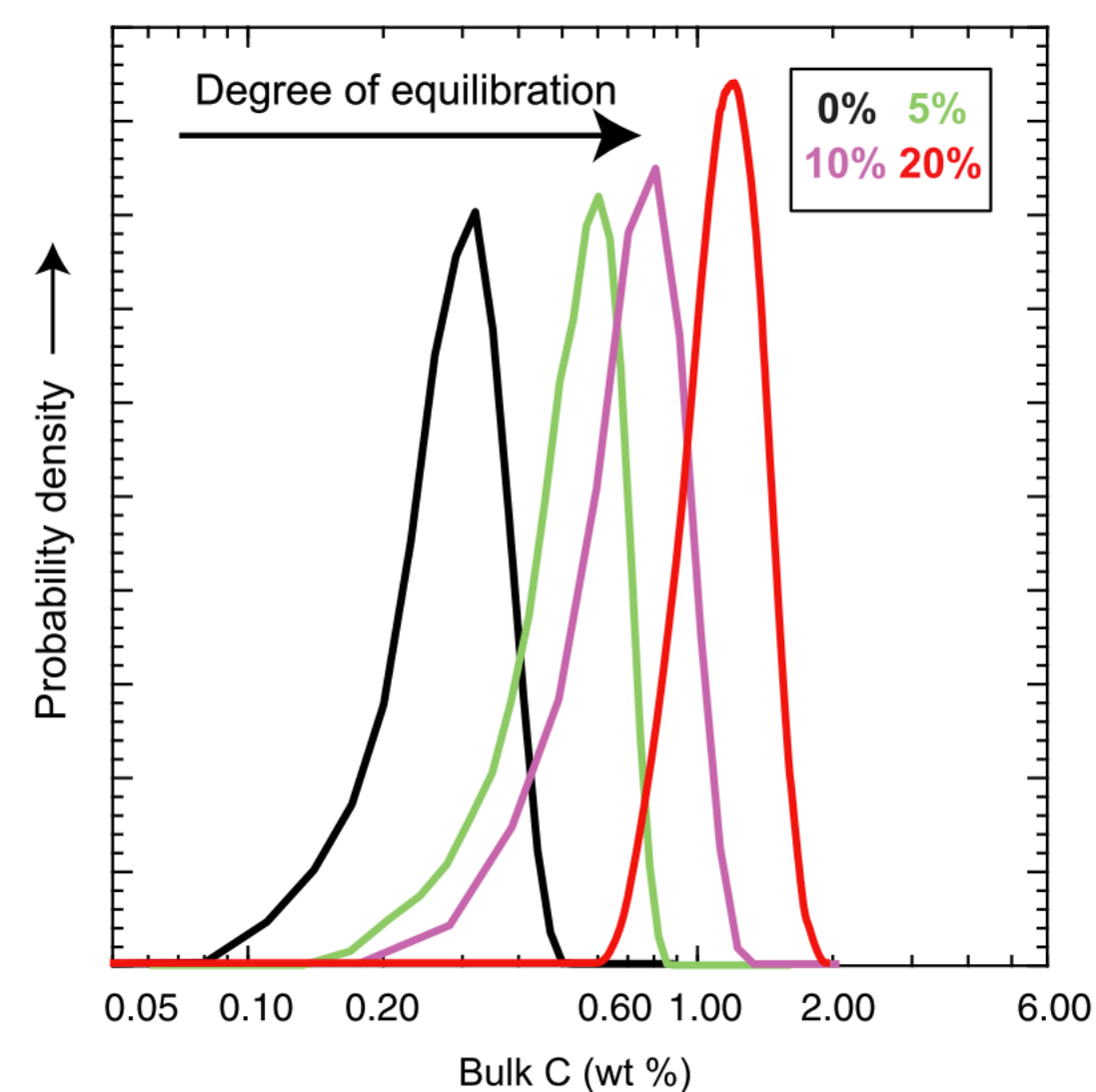
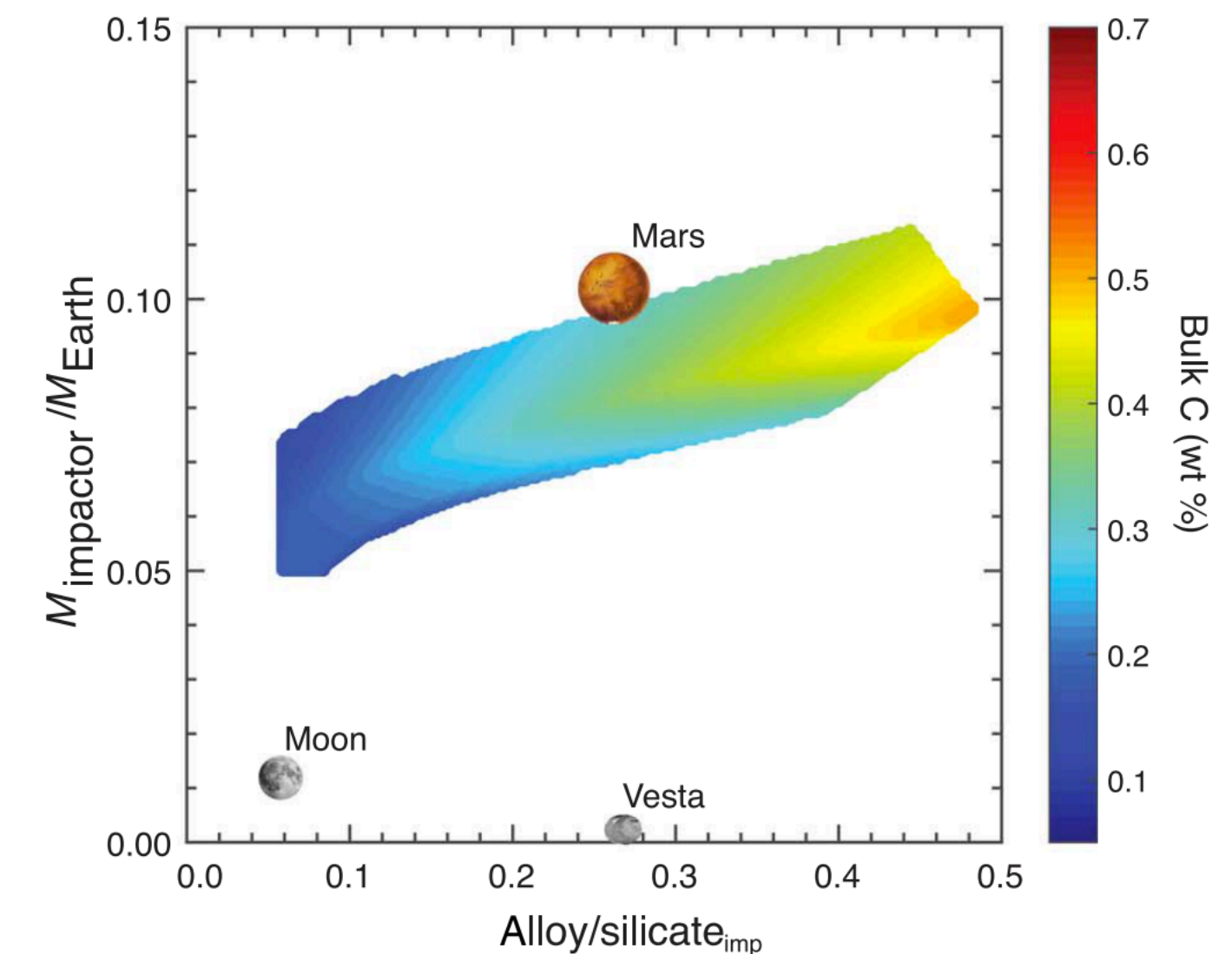
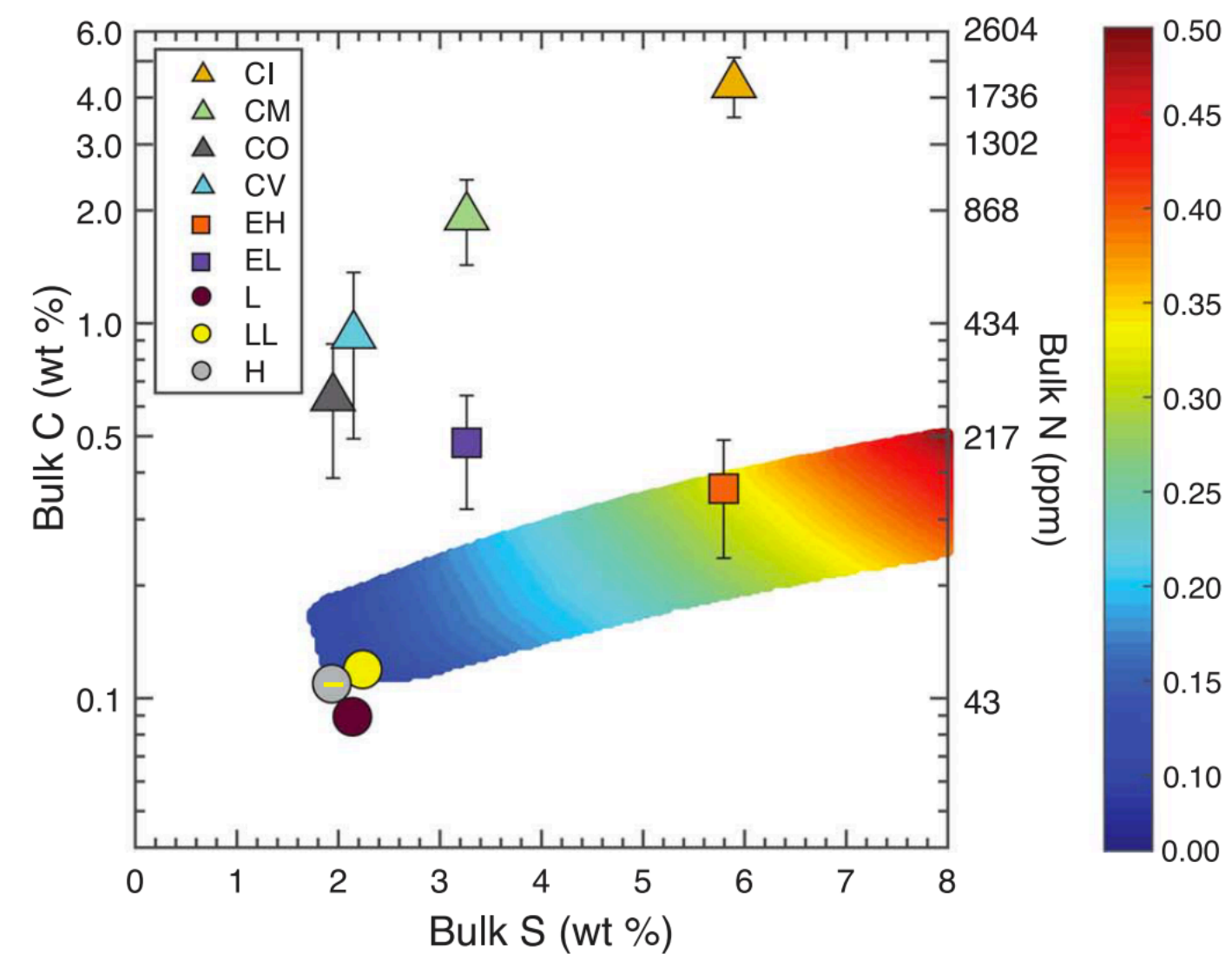
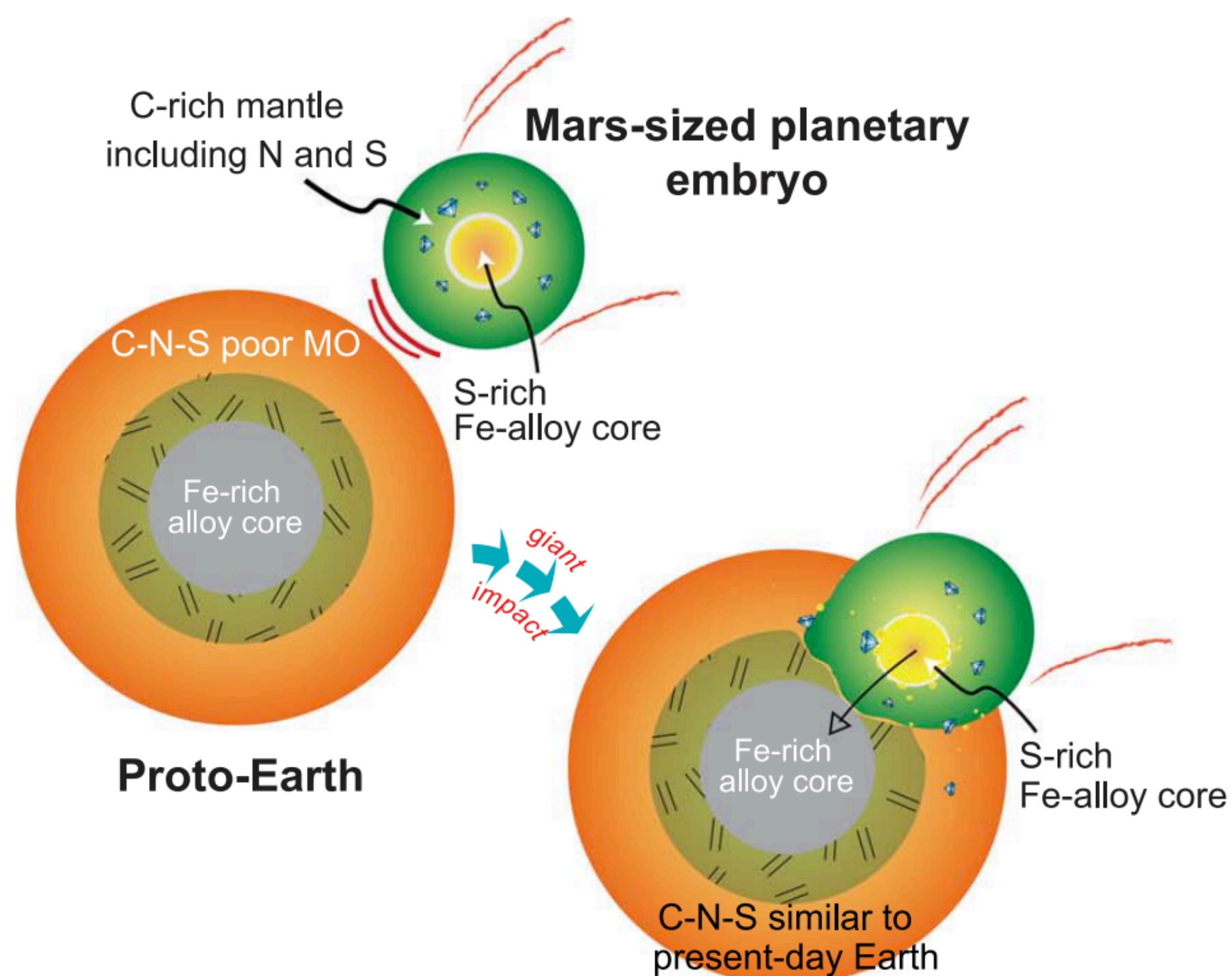




# Equilibrium partitioning + *some* evolution

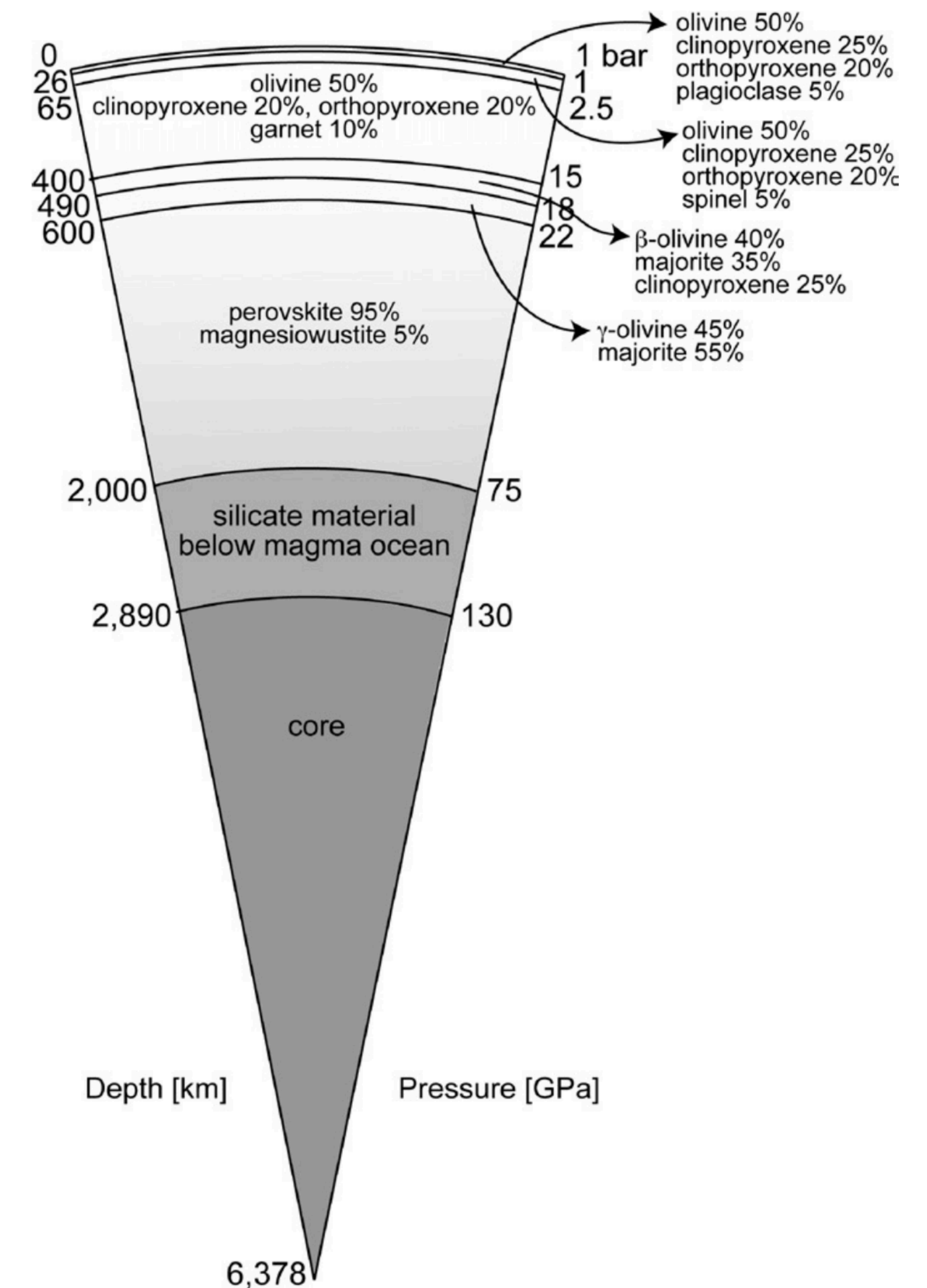
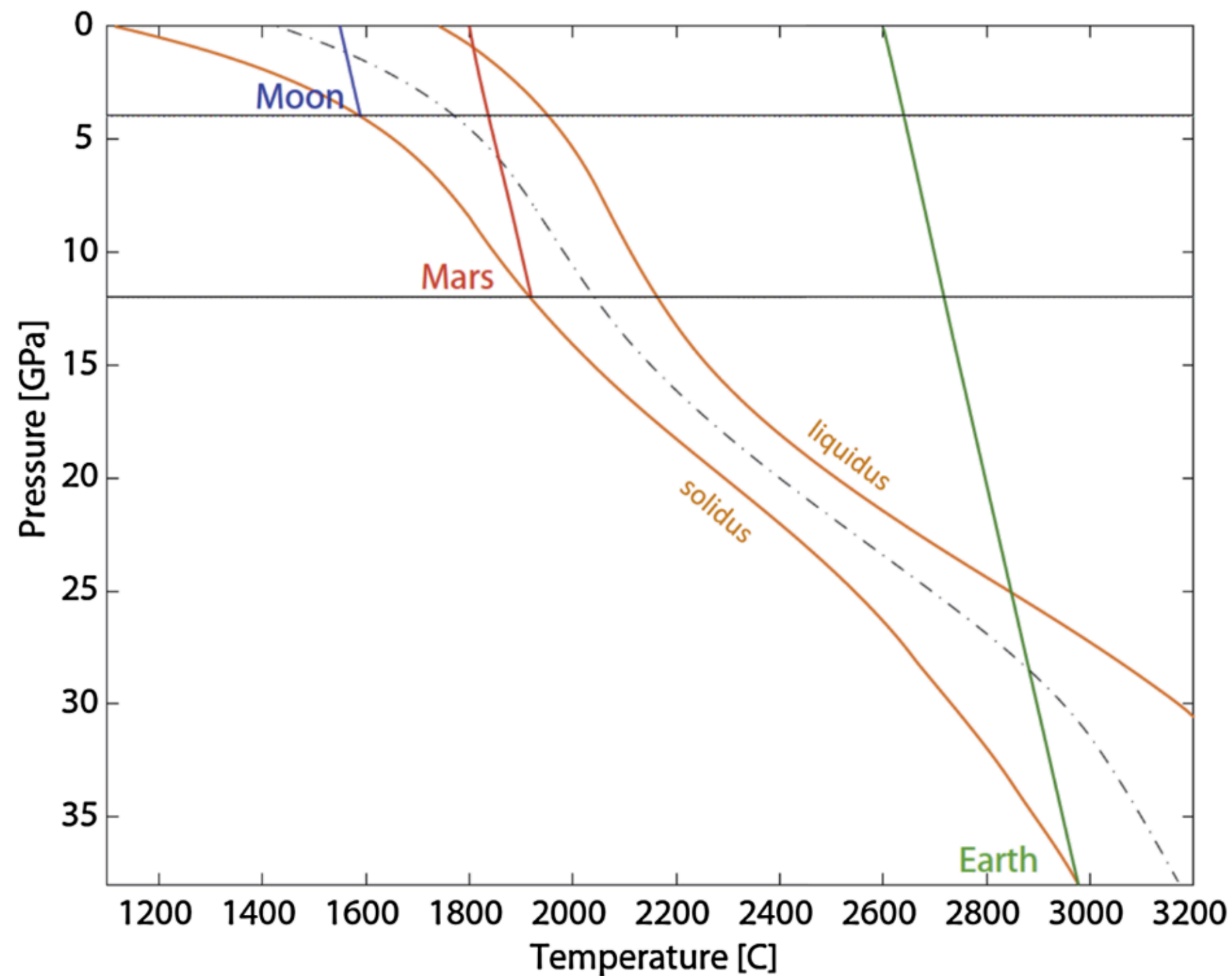


# The Moon-forming impact to the rescue

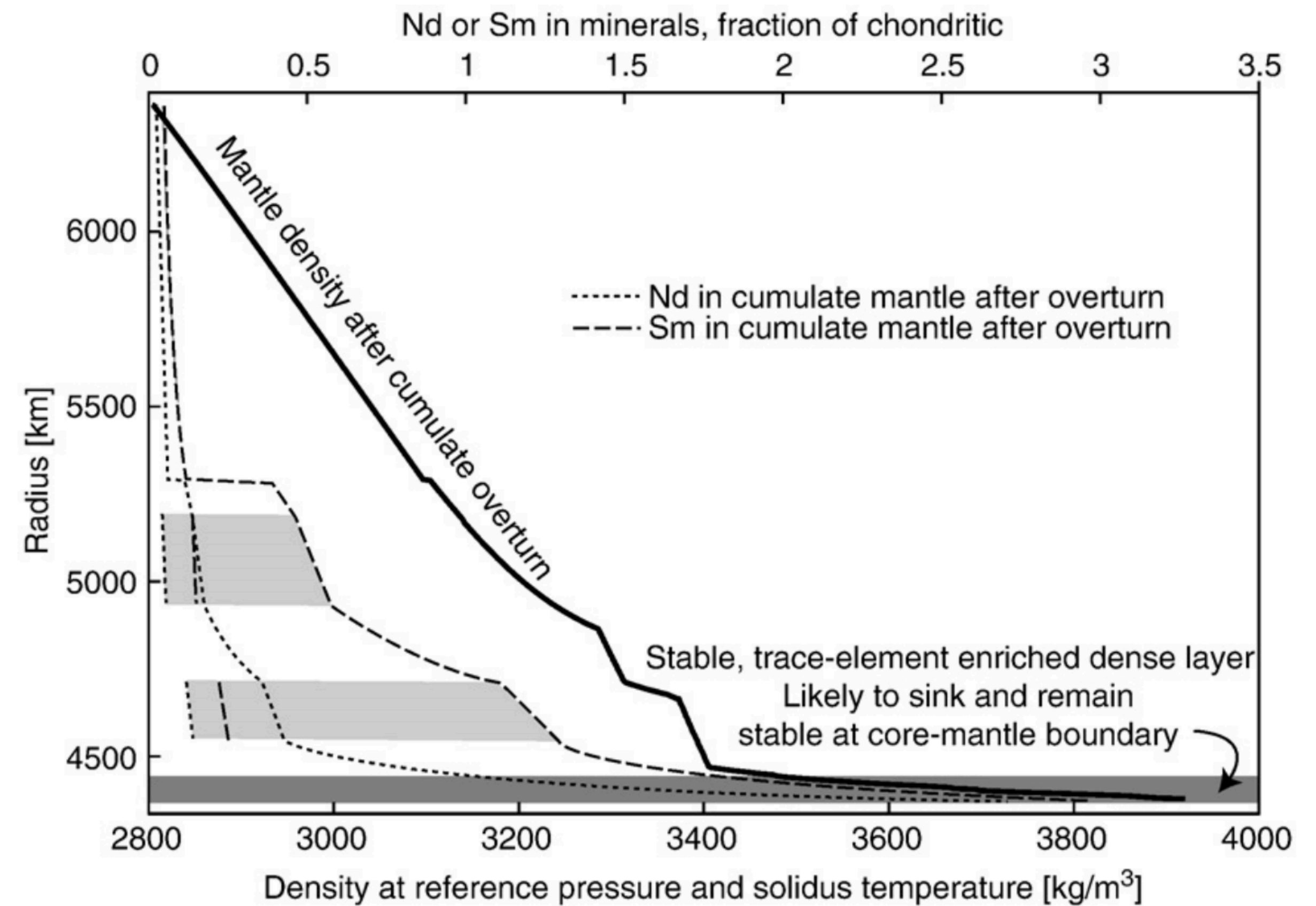
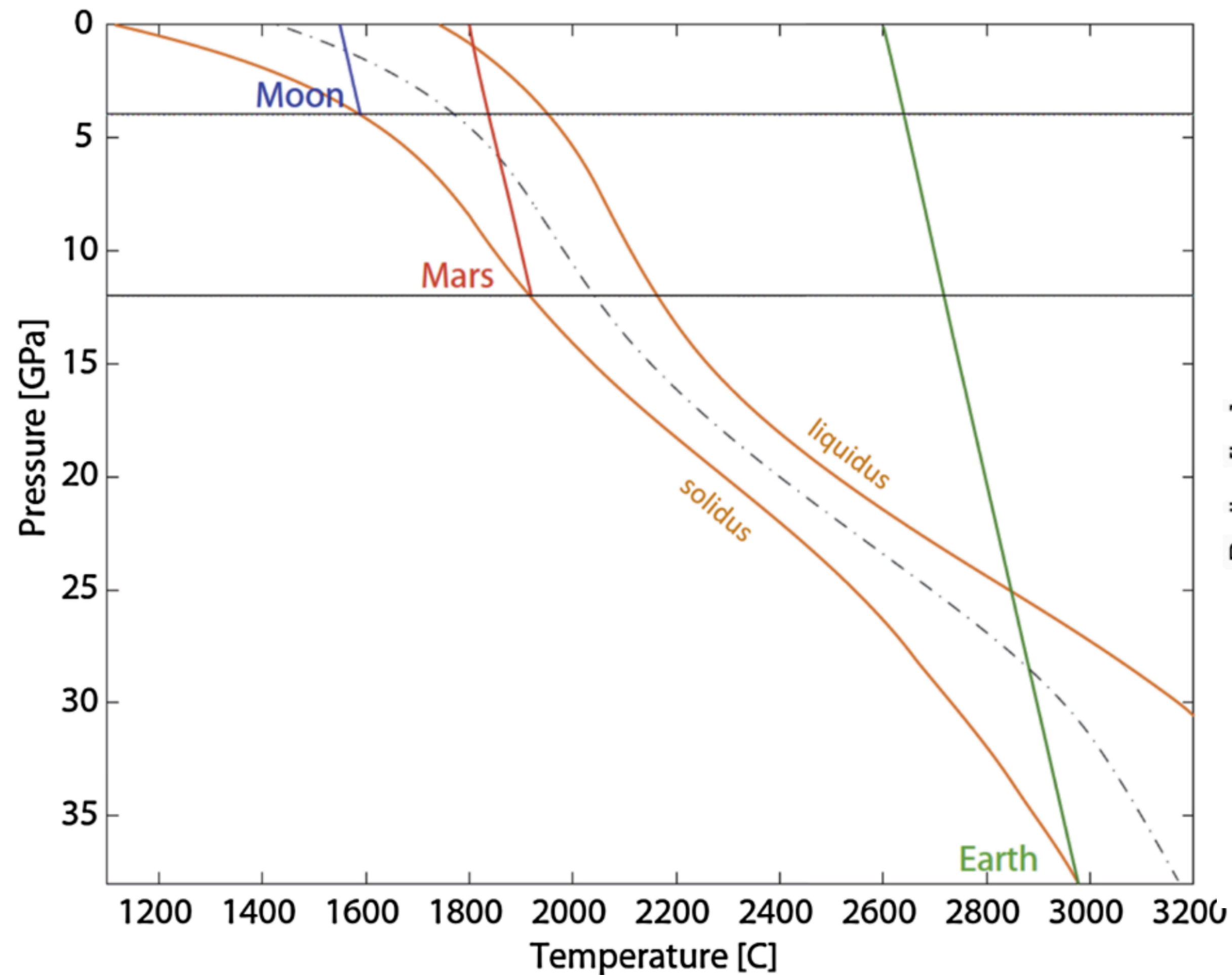




# Fractional crystallisation during freezing

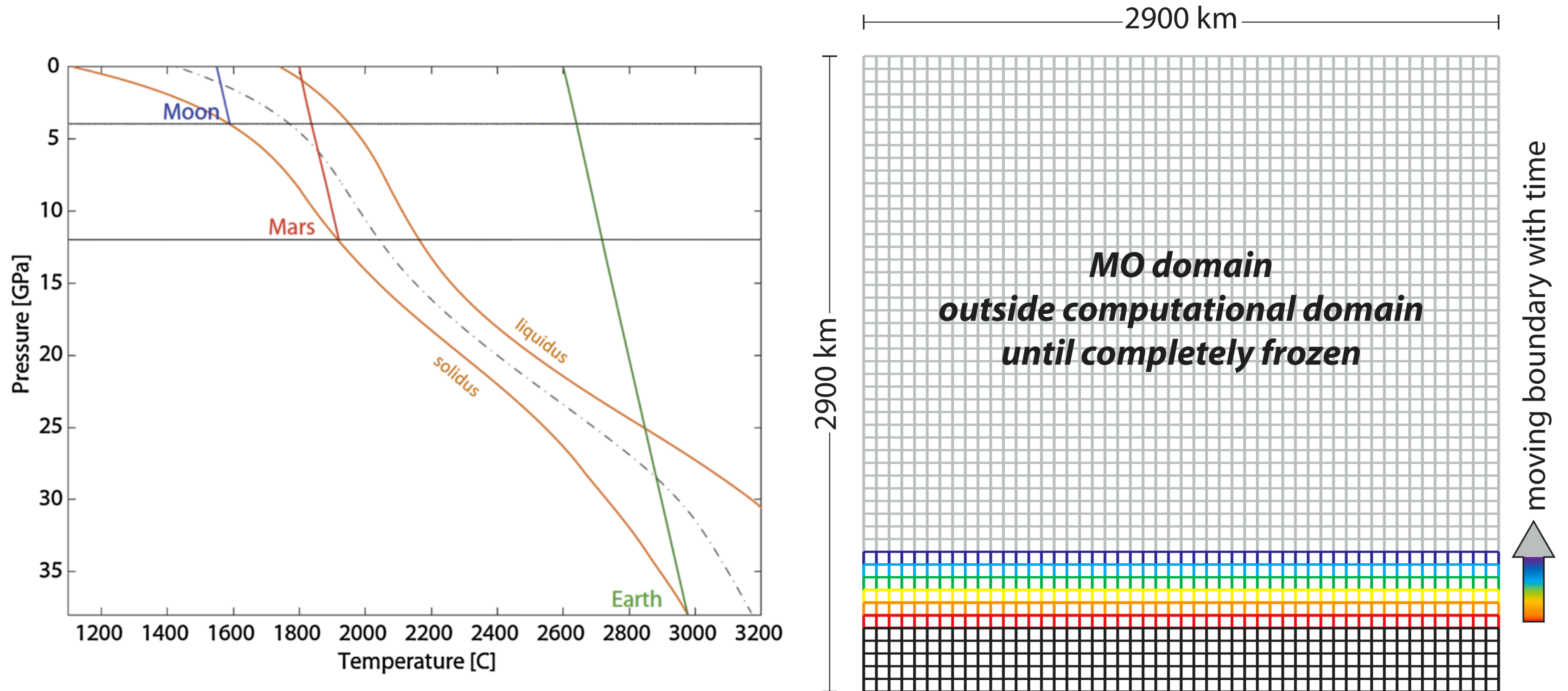


# Fractional crystallisation during freezing

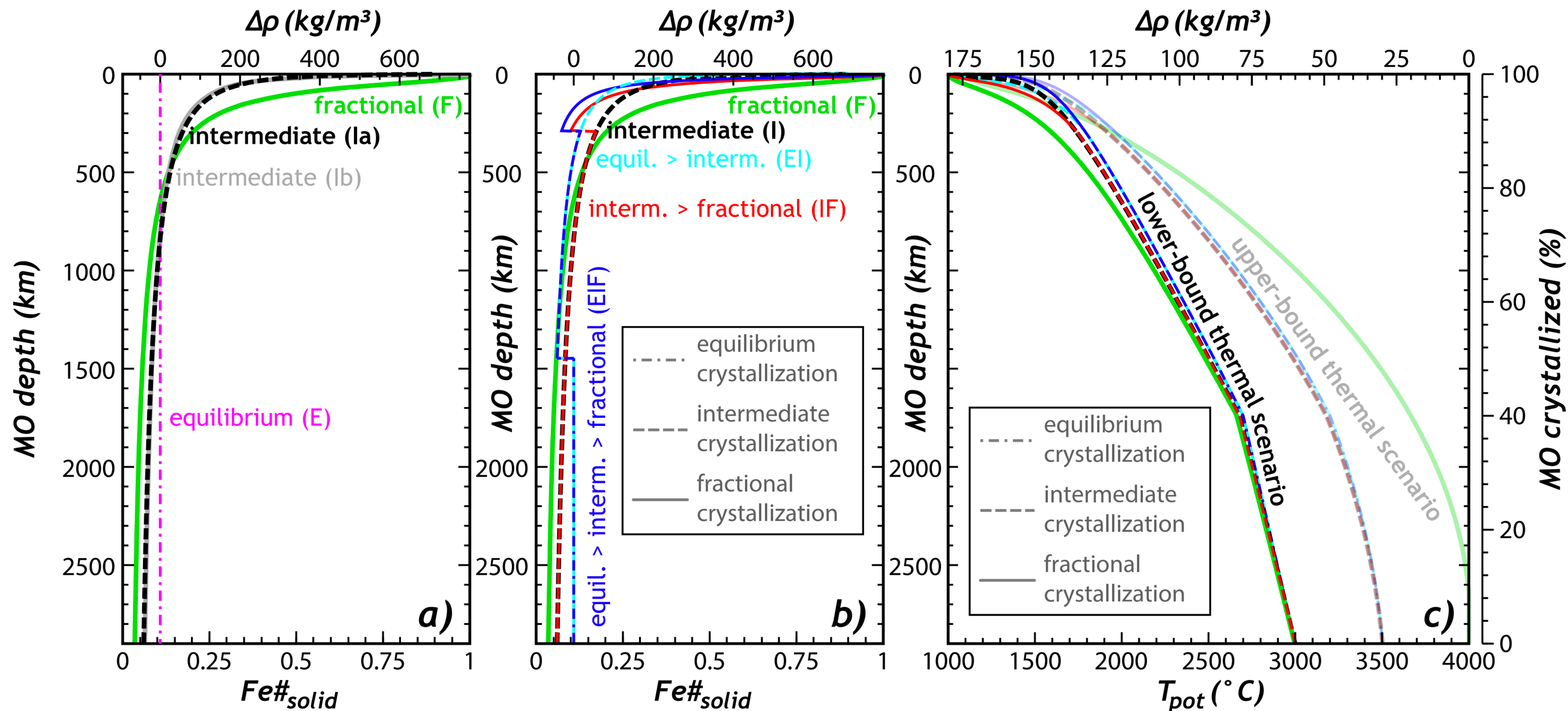




# Fractional crystallisation during freezing

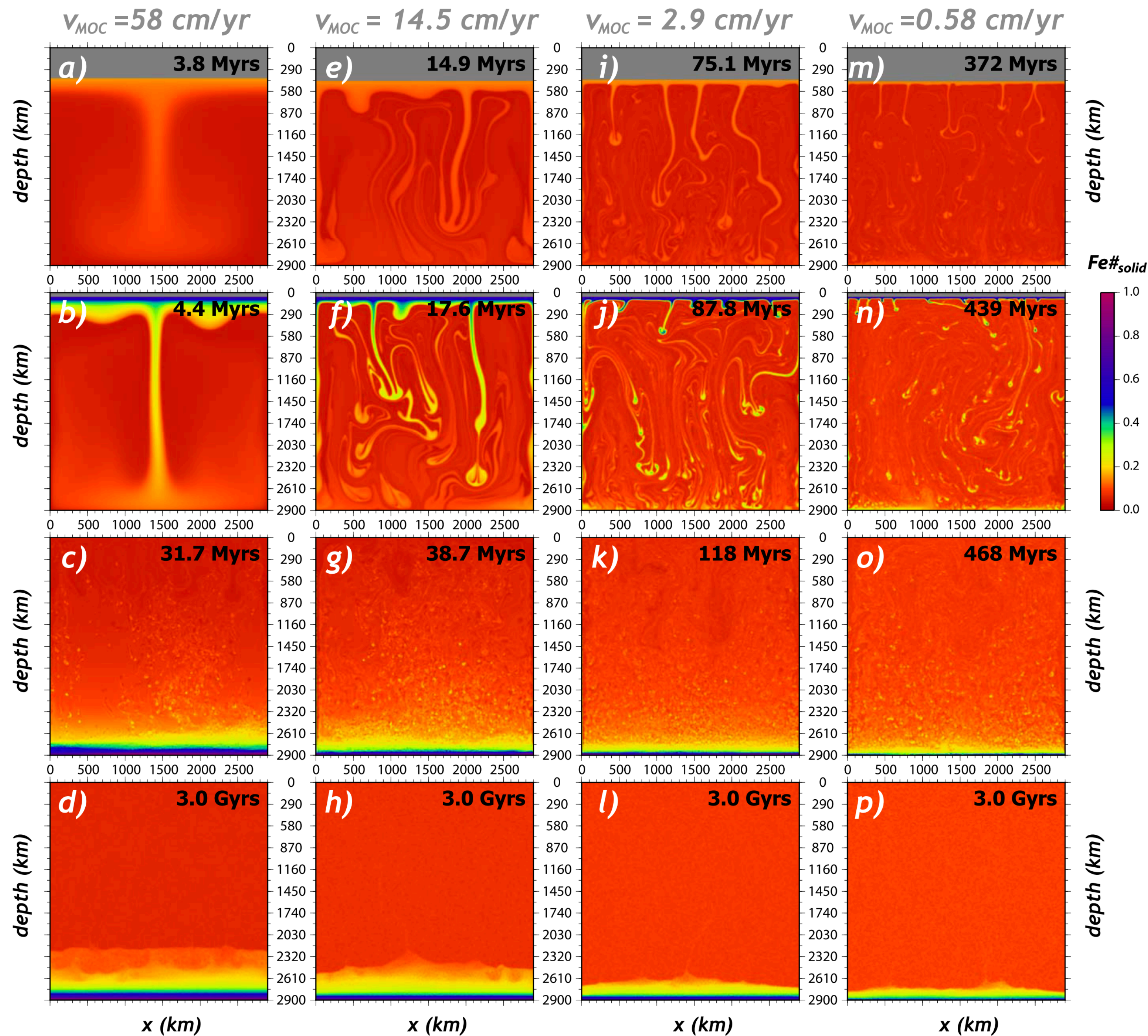
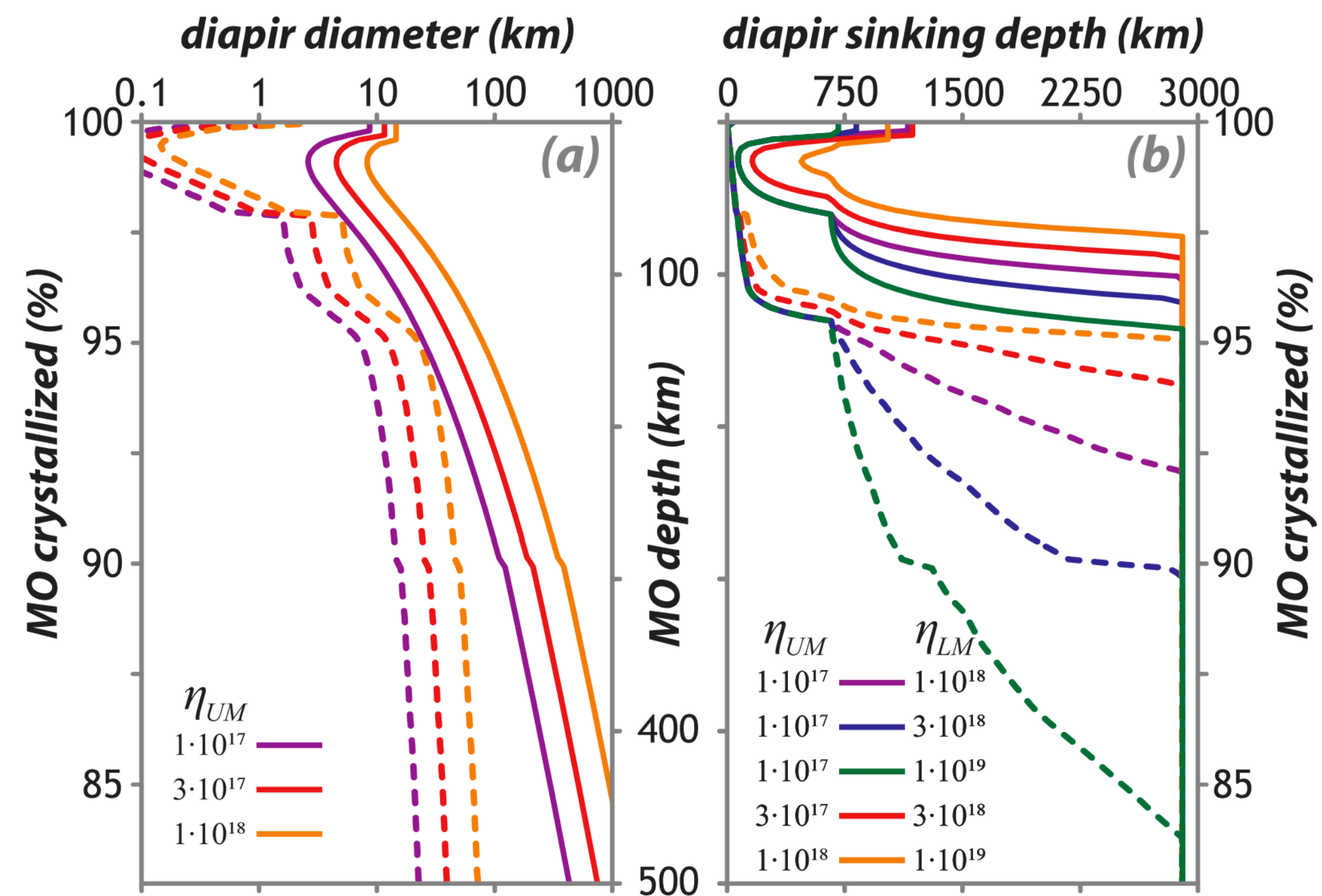


# MO thermal structure bracketed





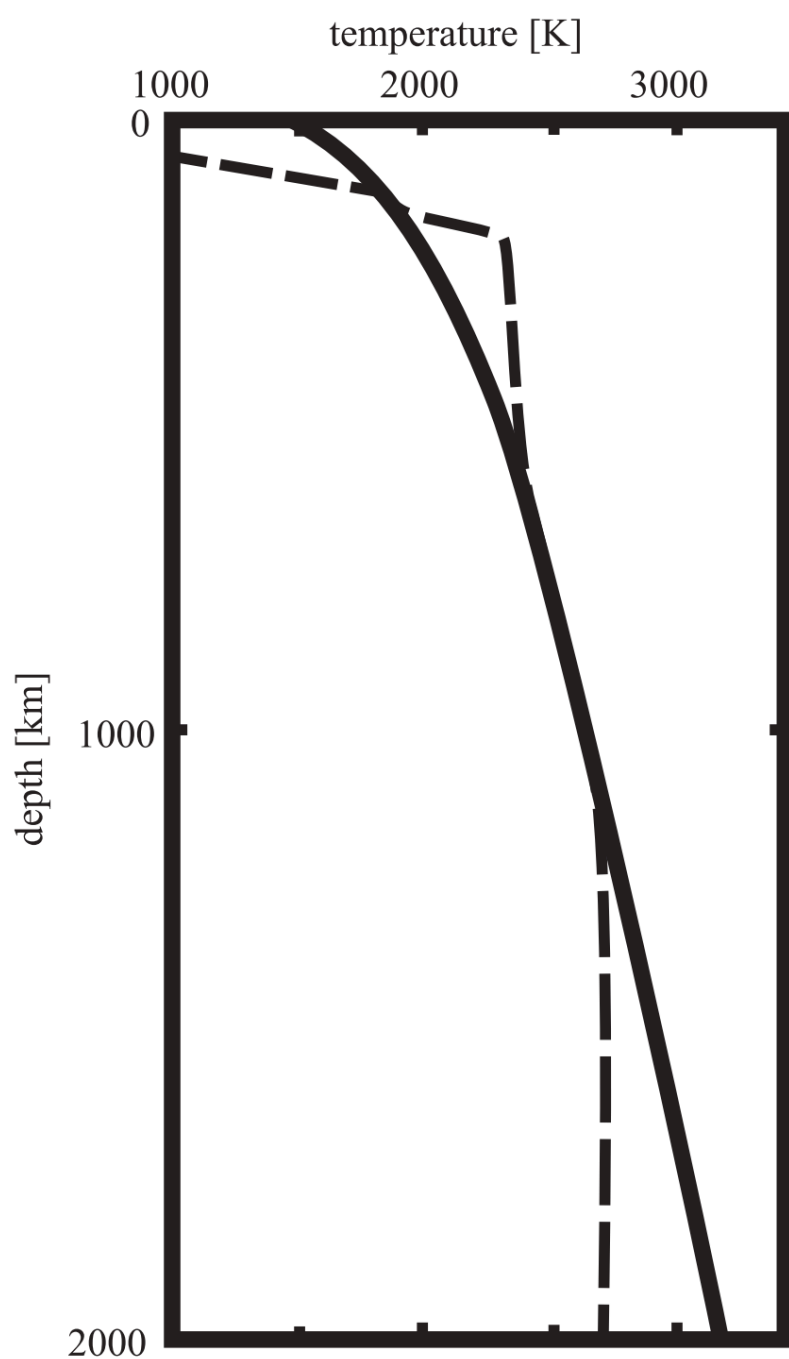
# Incremental overturns?



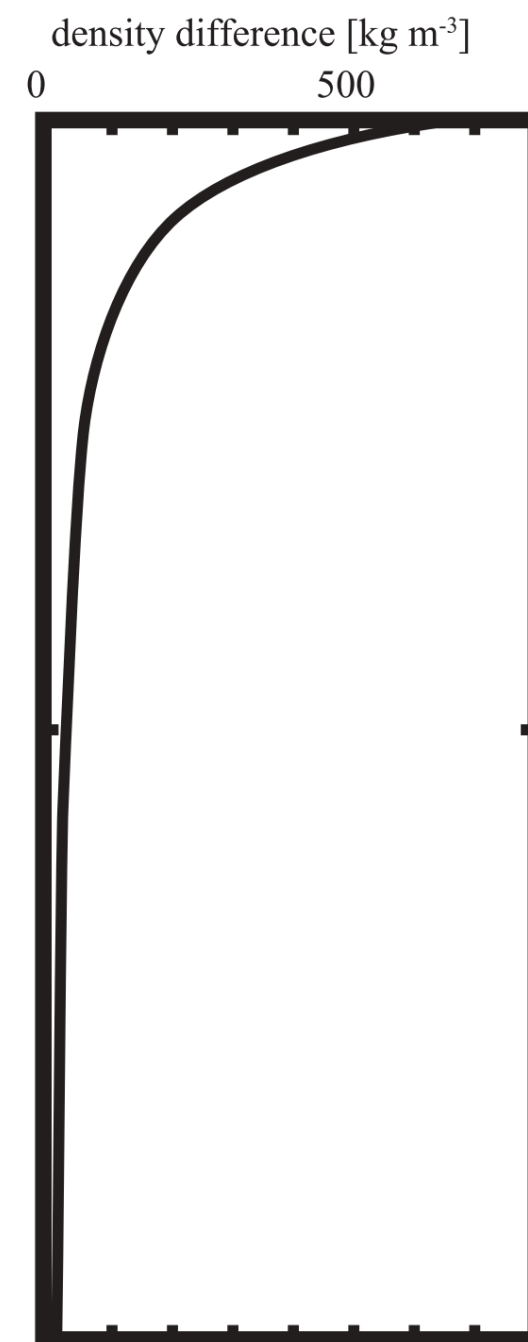


# Two-phase flow to remix stratified mantle?

(a) the melting or solidus curve & the initial temperature



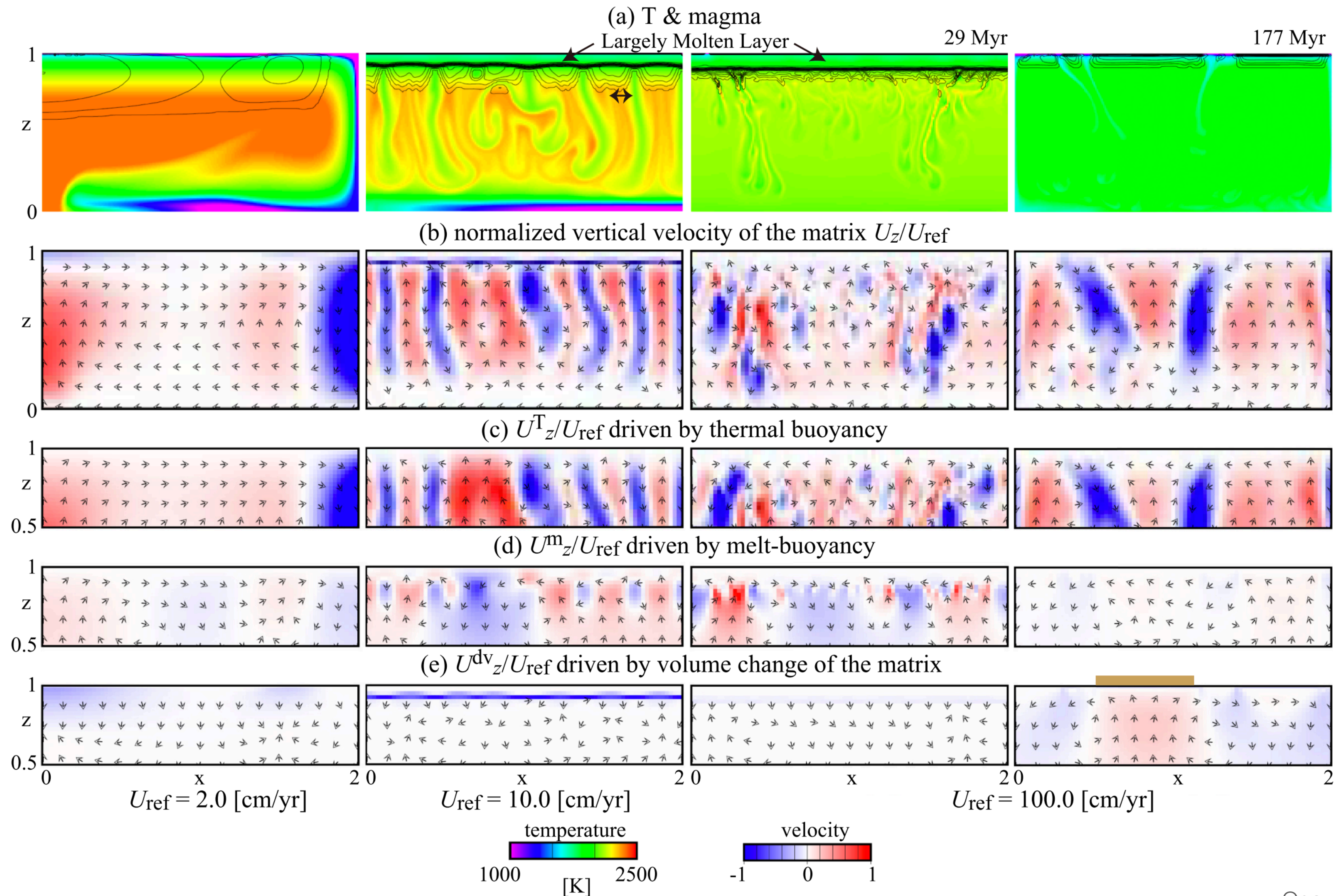
(b) the density difference between magma and matrix



Case C1:  $Ra = 2 \times 10^5$

Case C2:  $Ra = 2 \times 10^7$

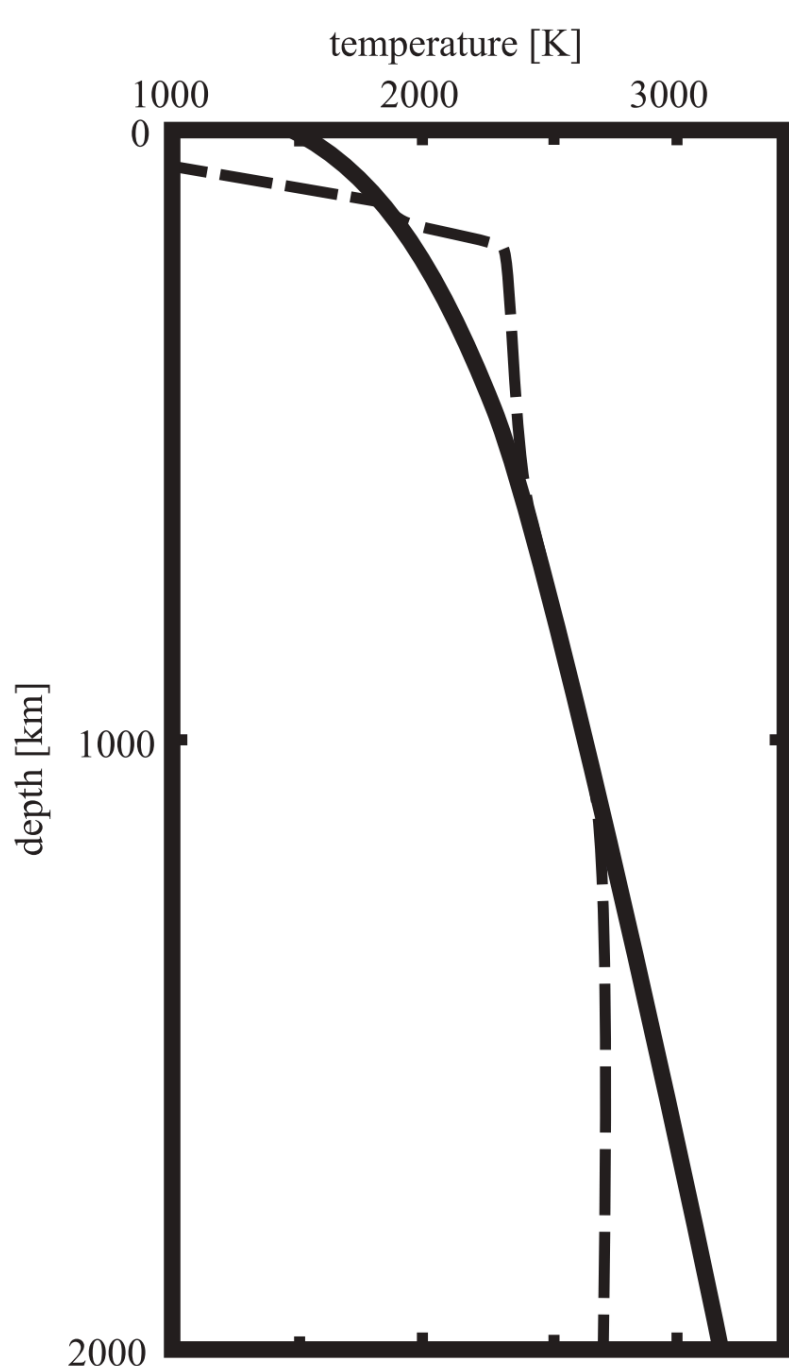
Case V:  $Ra = 2 \times 10^7$ ; variable  $\eta$



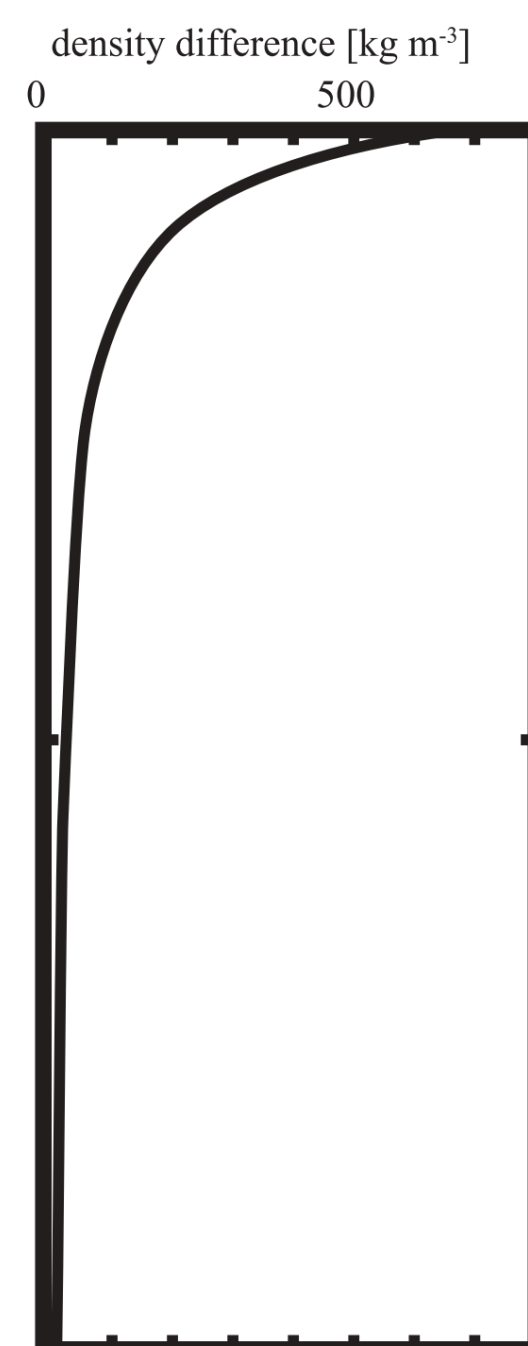


# Two-phase flow to remix stratified mantle?

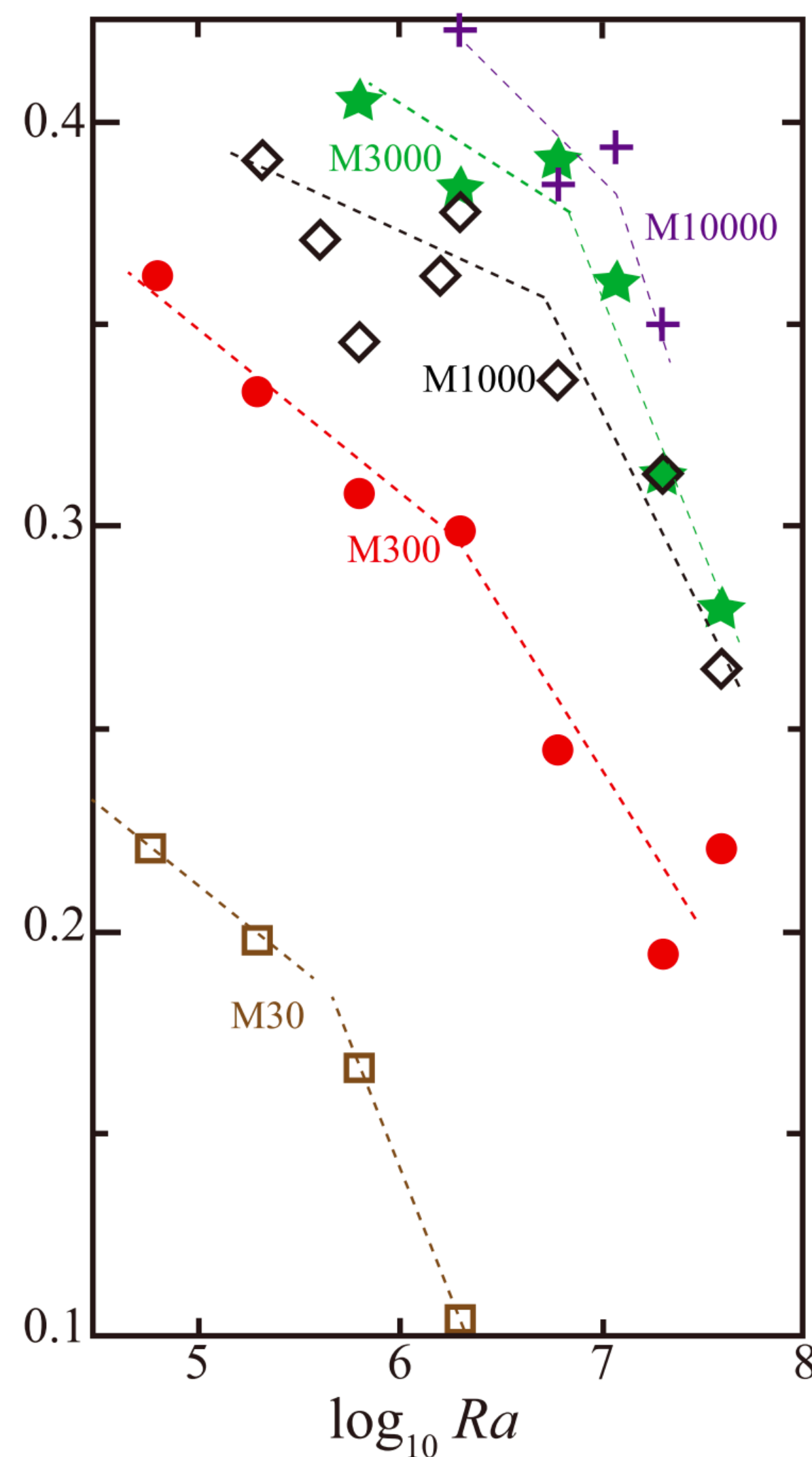
(a) the melting or solidus curve & the initial temperature



(b) the density difference between magma and matrix

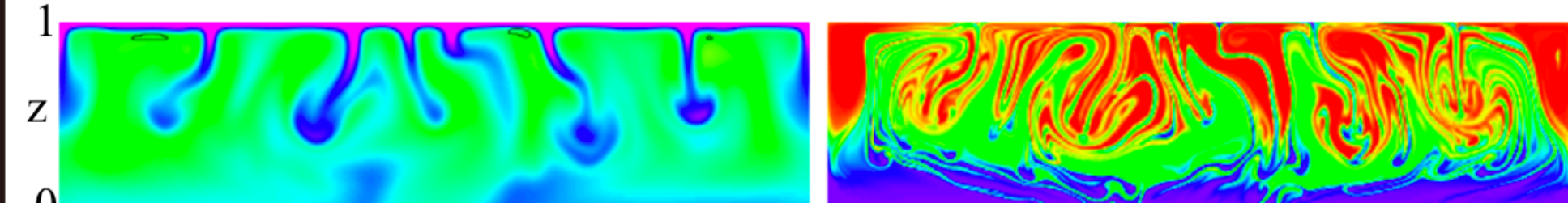


(a) rms-average of  $(\xi - \xi_{\text{init}})$  at depths

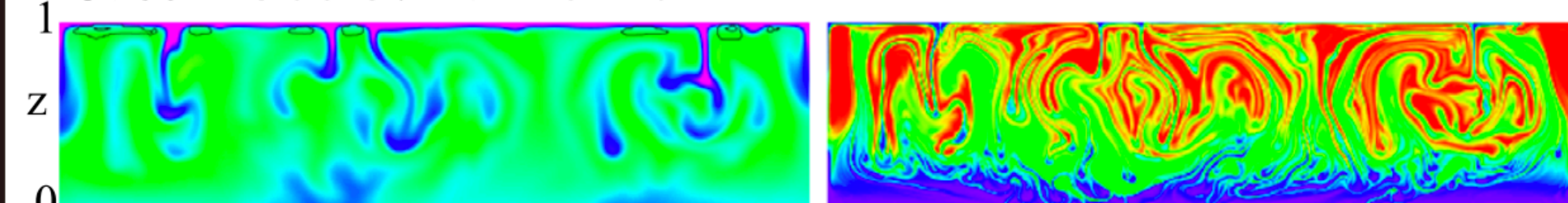


(b) temperature & magma

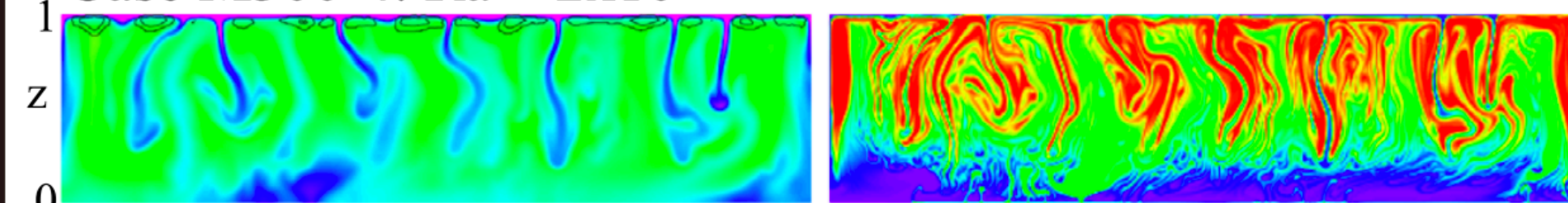
Case M300-2:  $Ra = 2 \times 10^5$



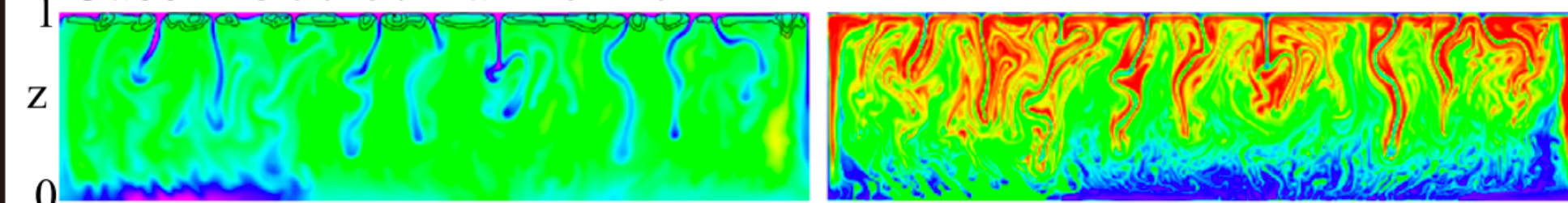
Case M300-3:  $Ra = 6 \times 10^5$



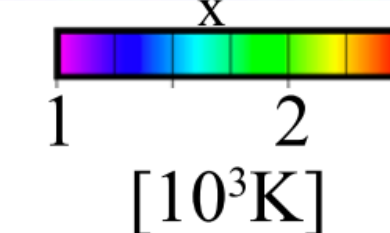
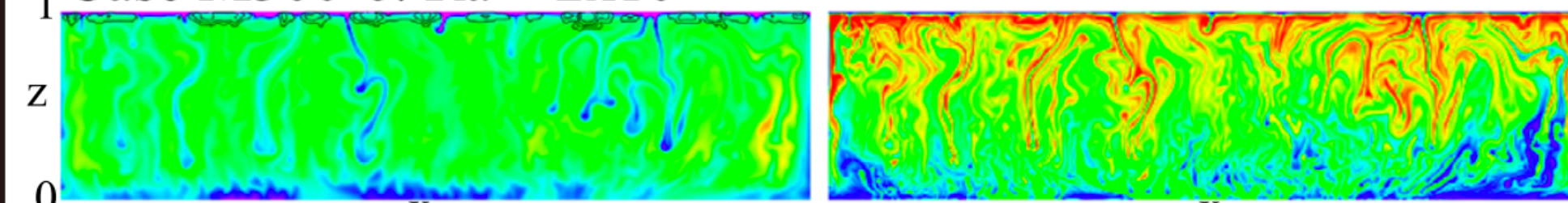
Case M300-4:  $Ra = 2 \times 10^6$



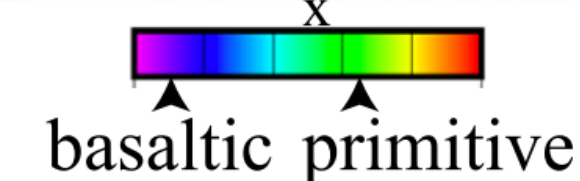
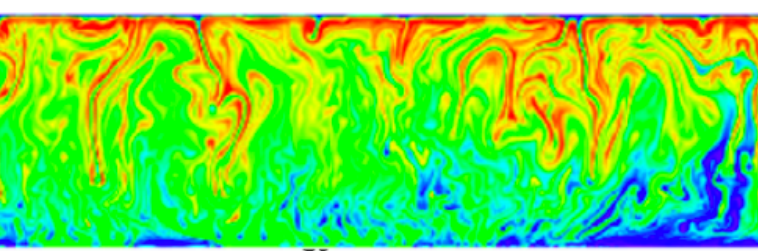
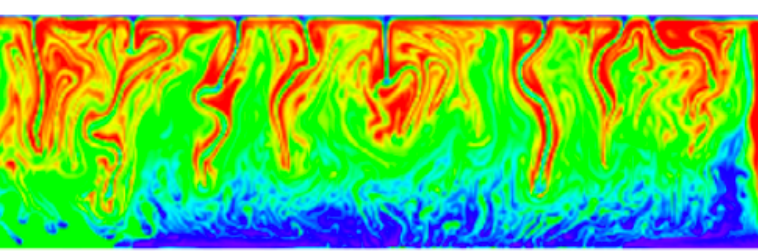
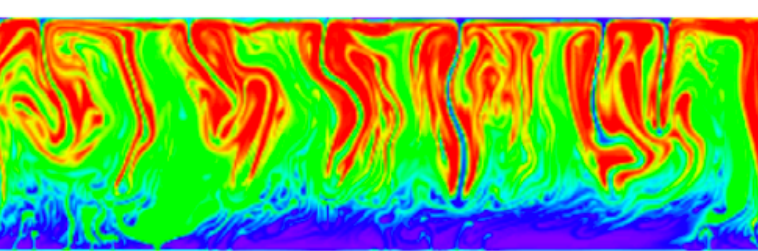
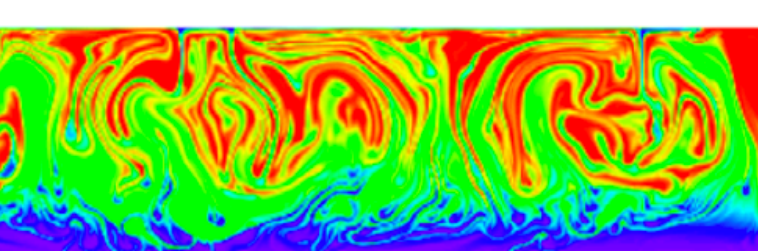
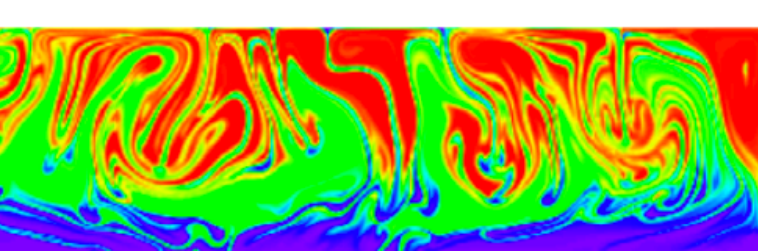
Case M300-5:  $Ra = 6 \times 10^6$



Case M300-6:  $Ra = 2 \times 10^7$



(c) composition



# What to do / project goals

- Quantify impact of incremental overturns
  - ▶ Mantle compositional stratification
    - ➡ Mantle redox gradient
    - ➡ Layering stability
  - ▶ BSE C-H-N-S ratio/total budget
  - ▶ Uppermost mantle/plume chemistry?
- Earliest atmospheric composition
- Avoid bracketing of thermal evolution(?)
- Self-consistent atmospheric treatment
  - ▶ Pre-computed flux for various atmospheric compositions (+ solar insolation) as boundary condition
- Melt-solid compositional distribution
  - ▶ Composition tracking
- Computational feasibility
- Starting conditions



# What to do / project goals

- Quantify impact of incremental overturns

- ▶ Mantle compositional stratification

- ➡ Mantle redox gradient

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- ▶ BSE C-H-N-S ratio/total budget

- ▶ Uppermost mantle/plume chemistry?

- Earliest atmospheric composition

- Avoid bracketing of thermal evolution(?)

## 1. Whole-mantle MO

- ▶ Density-inverted incremental overturns

## 2. After overturn

- ▶ Bracket overturn stratification

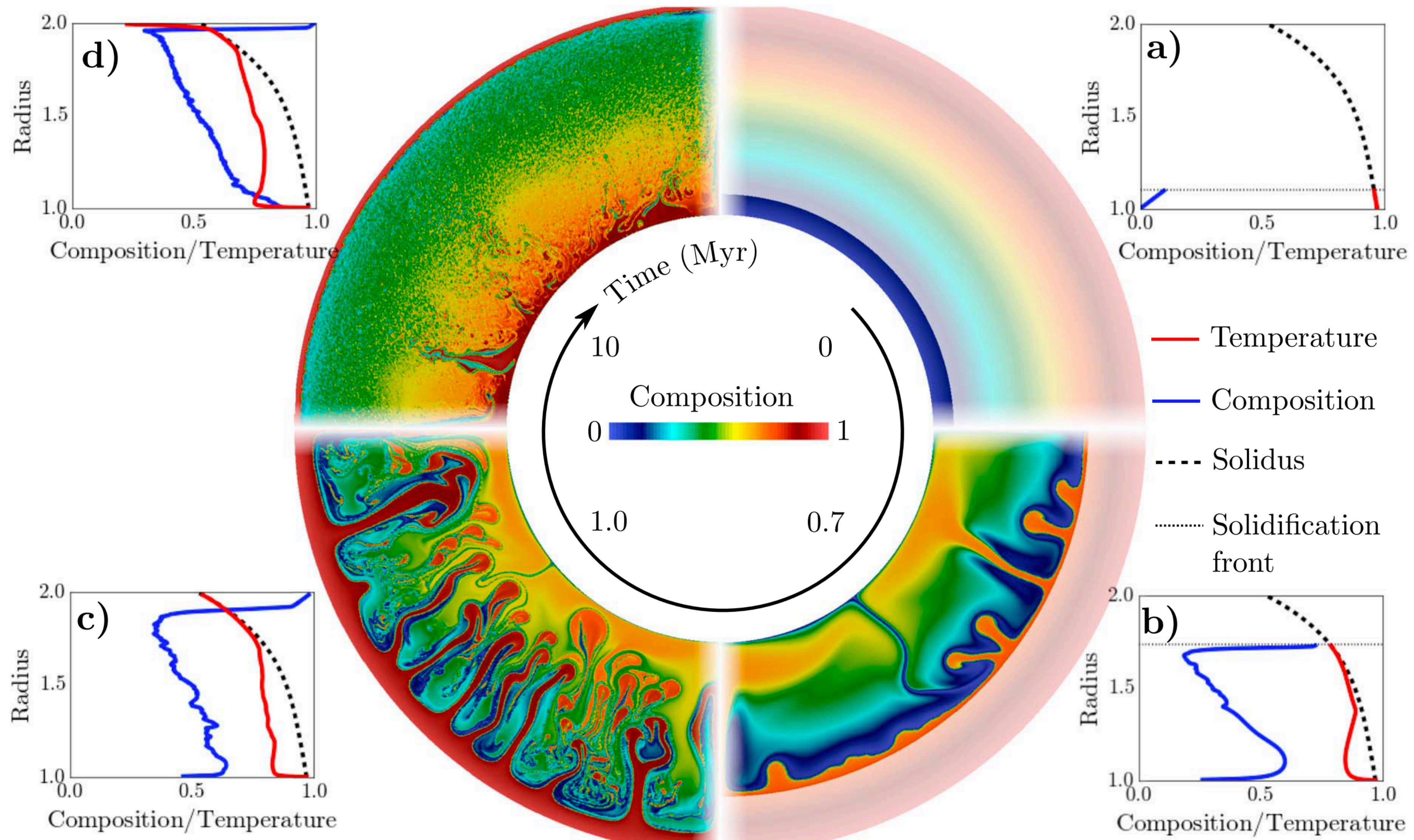
- ▶ Compute remixing of stratification + volatile partitioning

## 3. Intermediate (late-stage) MO

- ▶ Bracket early thermal evolution, assume end-member late-stage thermal-compositional profile



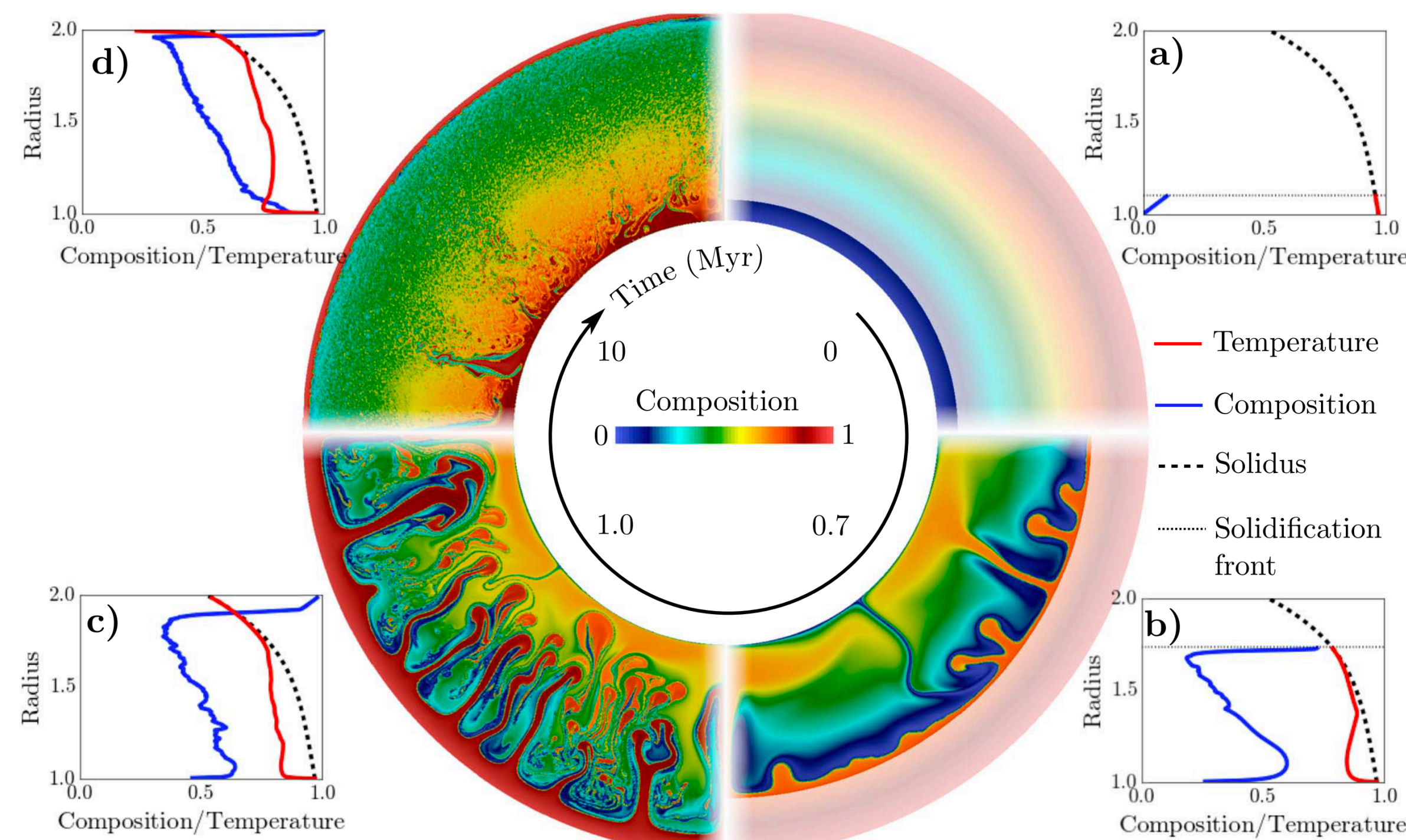
# 1. Whole-mantle MO $\rightarrow$ global volatile budget





# 1. Whole-mantle MO $\rightarrow$ global volatile budget

- Whole mantle completely molten
- Initial temperature profile following adiabat when bottom intersects with liquids
- Employ partition coefficients for alloy/O + CHNS ratios
  - ▶ Track composition/mixing + density inversion
  - ▶ Oversaturated volatiles released to atmosphere
- MO heat flux through eddy diffusivity



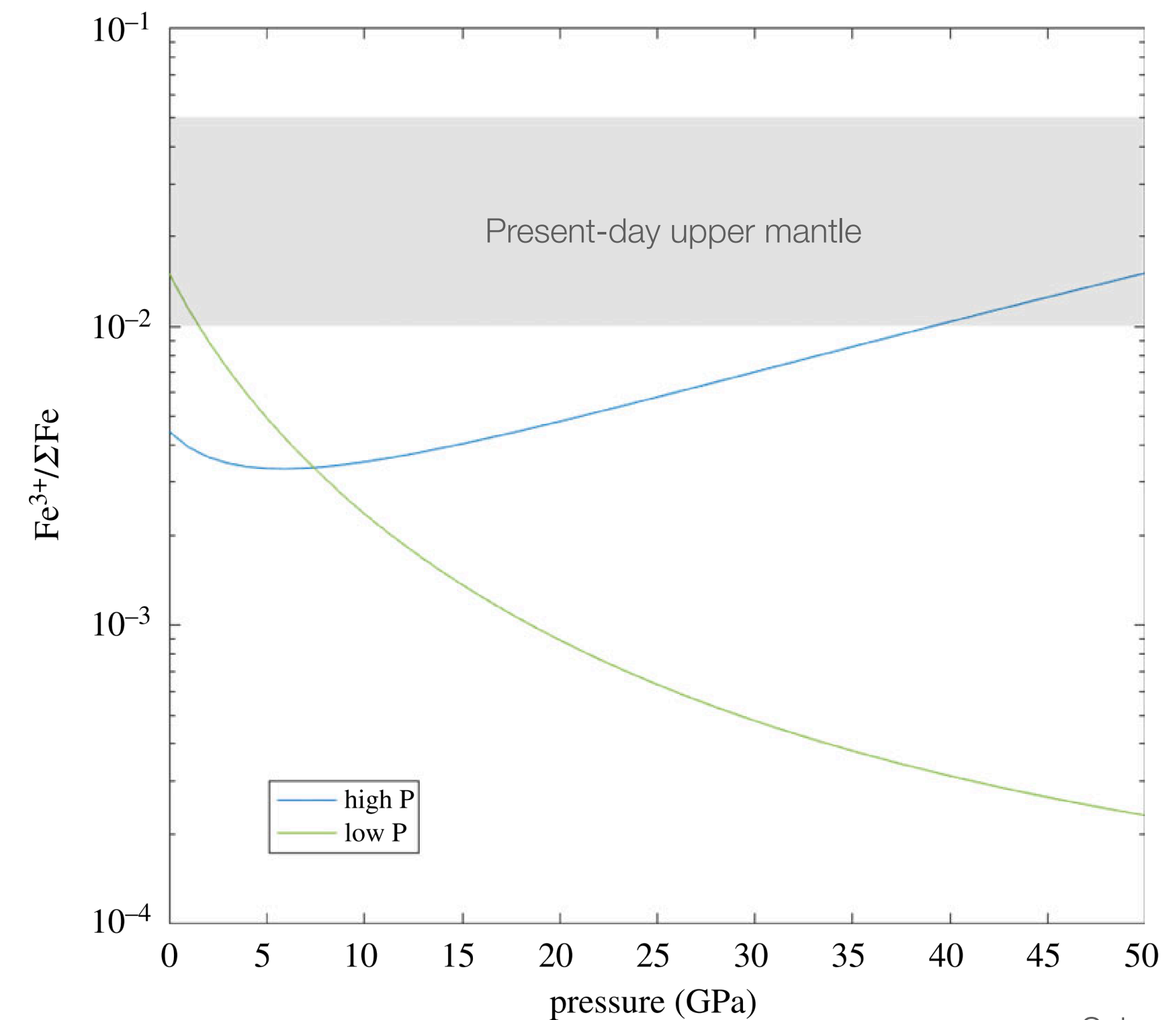
# 1. Whole-mantle MO

- Whole mantle completely molten
- Initial temperature profile following mantle liquidus
- **Employ partition coefficients for alloy/O + CHNS ratios**
  - ▶ Track composition/mixing + density inversion
  - ▶ Oversaturated volatiles released to atmosphere
- MO heat flux through eddy diffusivity

**TABLE 2.** Volatile solubilities and partition coefficients used for model calculations

|   |              | Solubility constants<br>$S_i$ (Eq. 6) (ppm/MPa) | Partition coefficients<br>$D_i^{\text{alloy/silicate}}$ |
|---|--------------|---|---|
| C | oxidized     | 1.6   | 500   |
|   | reduced      | 0.55  | 1000  |
|   | very reduced | 0.22  | 3000  |
| H | oxidized     | <sup>a</sup>                                    | 6.5   |
|   | reduced      | <sup>a</sup>                                    | 6.5   |
|   | very reduced | 5   | 6.5   |
| N | oxidized     | 1   | 20  |
|   | reduced      | 5   | 20  |
|   | very reduced | 50  | 20  |
| S | oxidized     | 5000  | 60  |
|   | reduced      | 5000  | 60  |
|   | very reduced | 5000  | 60  |

Hirschmann 16

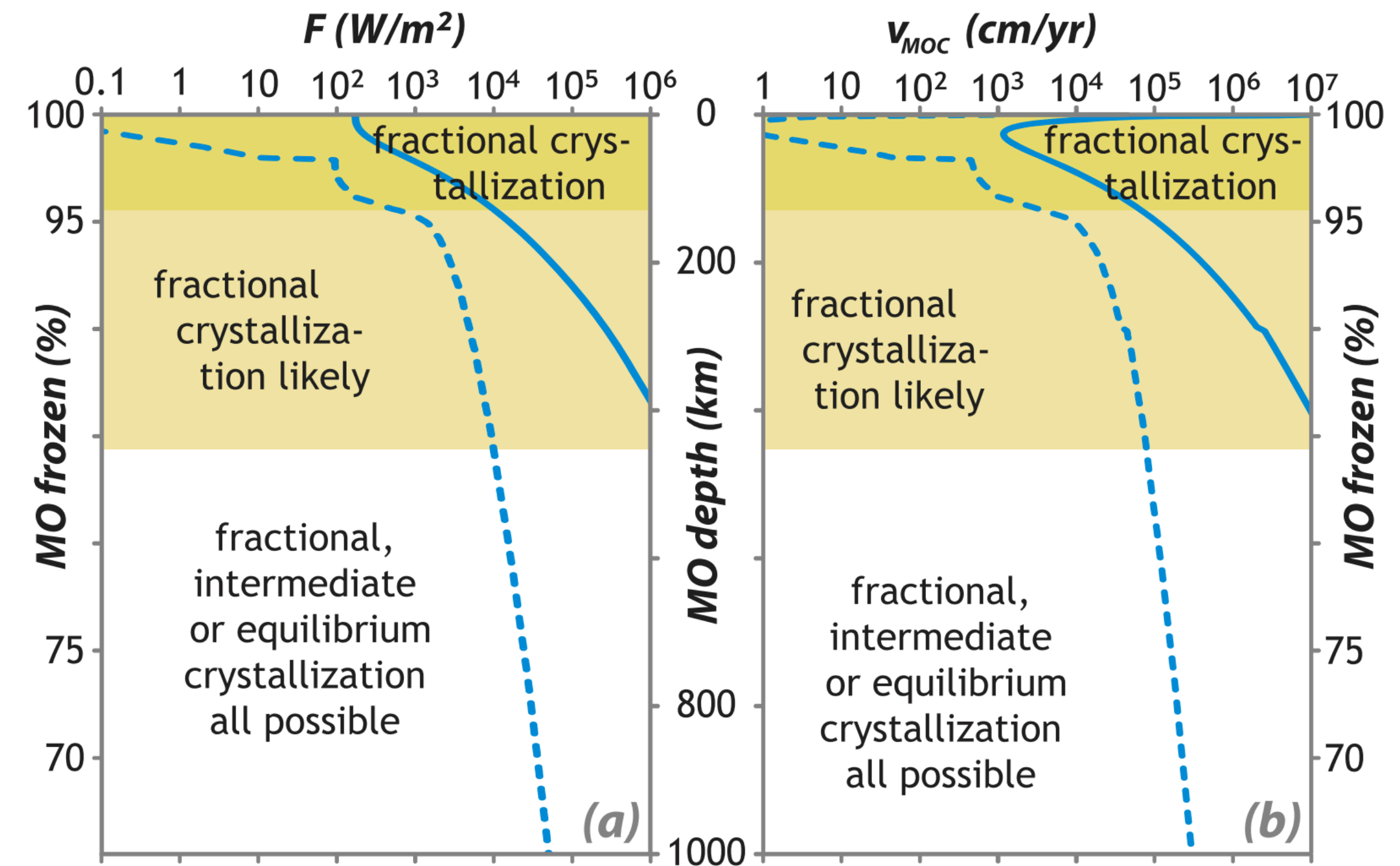


Schaefer & Elkins-Tanton 18



# 1. Whole-mantle MO $\rightarrow$ global volatile budget

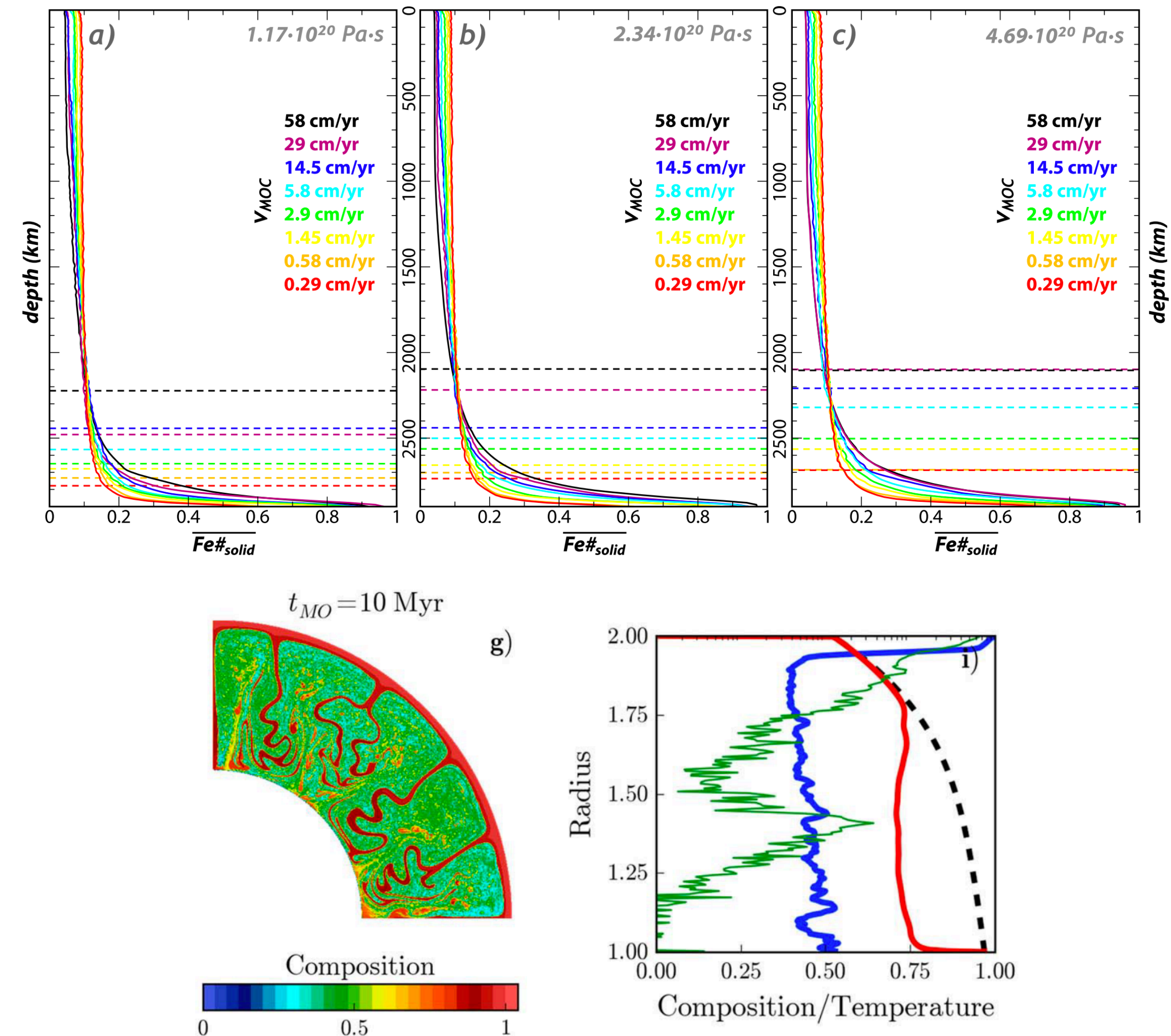
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- Employ partition coefficients for alloy/O + CHNS ratios
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  - ▶ Oversaturated volatiles released to atmosphere
- **MO heat flux through eddy diffusivity**



## 2. After overturn: remixing of stratified mantle

- Overturn is bracketed, primary late-stage result of overturn must be assumed
  - ▶ Mixing scenarios predicted differ
  - ▶ Some constraints can be taken from average mantle convection time + LLSVP compositions
- Density inversions are reduced to variations due to mantle composition
- Remixing from MMU feedback + enhanced plutonism?
  - ▶ Radiogenic heat-source partitioning

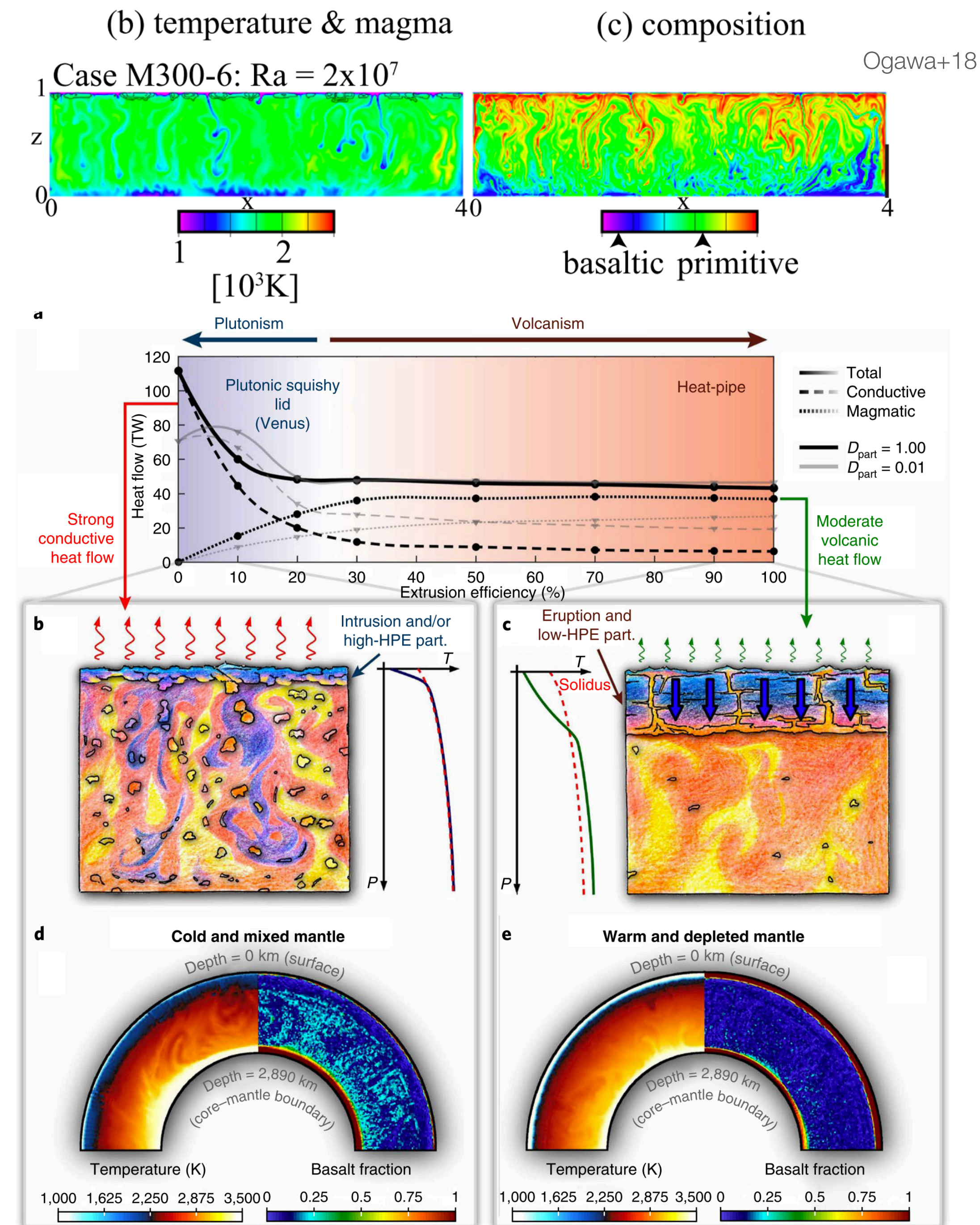
Ballmer+17





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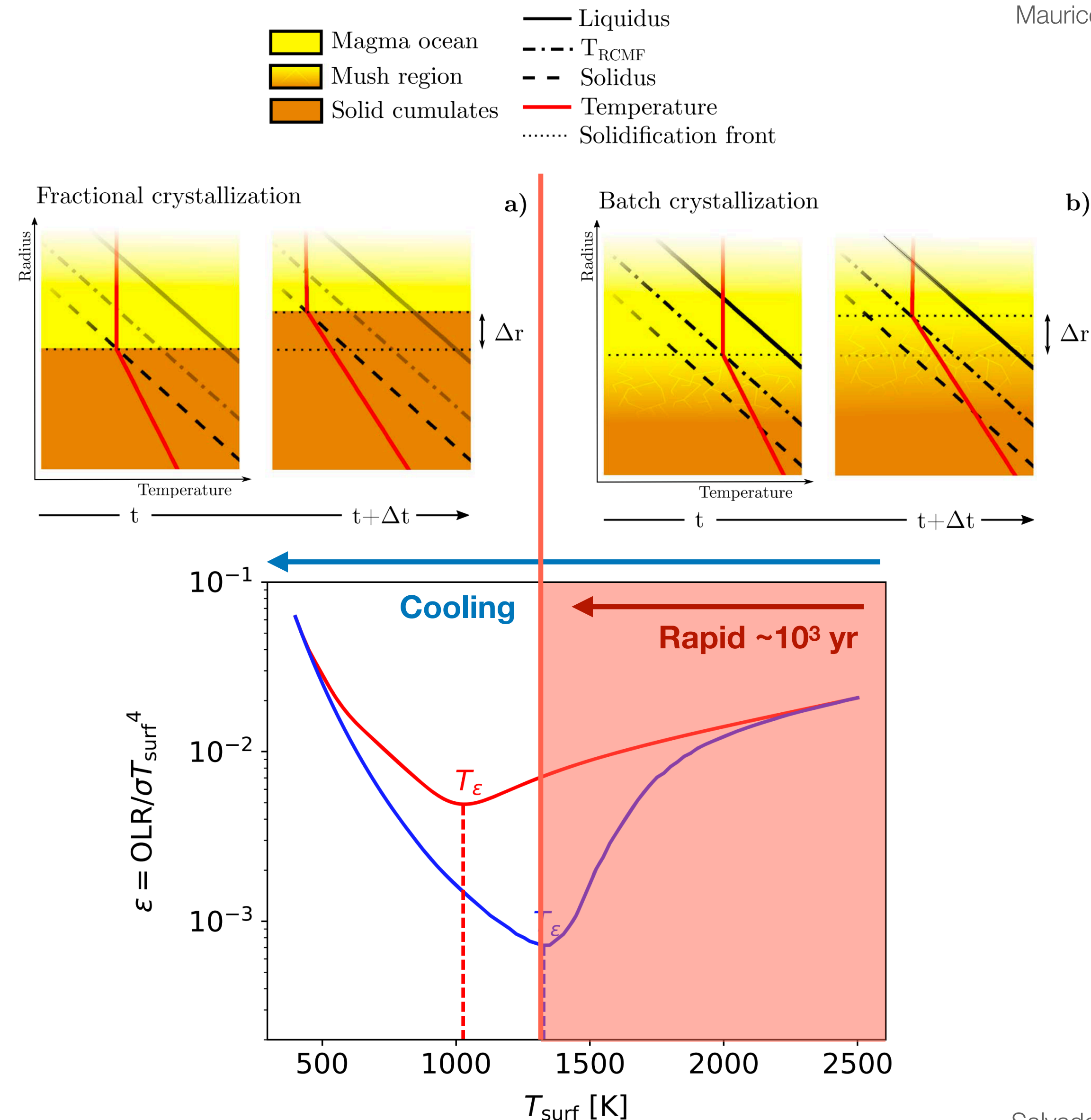




# 3. Intermediate (late-stage) MO

Maurice+17

- Bracketing rapid early MO evolution
  - ▶ Initial atmospheres dominated by either H<sub>2</sub>O/CO<sub>2</sub> (oxidised) or H<sub>2</sub>/CO (reduced)
  - ▶ Initial rapid cooling phase dominated by batch crystallisation
- Cannot avoid largely molten regions, but reduces uncertainties related to Fe partitioning
  - ▶ Fe-related density inversions
  - ▶ + MMU feedback (Ogawa+18)
  - ▶ + Intrusion feedback (Lourenco+18)
- Computationally a compromise



Salvador+17



# Summary & open questions

- 2D global or quarter-shell model
- Two-phase separation between melt and solid
- ◉ *Chemical partitioning of iron phases (or mantle chemical evolution) between silicate melt and rock?*
  - ▶ *Feedback between density inversions, MMU effect + plutonism?*
- ◉ *Volatiles continually released + fed to uppermost mantle vs. parameterised using Salvador+17 scaling relations?*
  - ▶ *Atmospheric phase space?*
- ◉ *Partitioning/chemical evolution?*
  - ▶ *Constants derived from geochemical experiments?*
  - ▶ *Parameterisation à la Rees Jones+?*
  - ▶ *Mixture of both w/ regards to Fe vs. H<sub>2</sub>O/CO<sub>2</sub>/volatiles and high/low melt regions?*
- ◉ *Eddy diffusivity?*
- ◉ *Numerical feasibility?*