**1-D photochemical model to predict oxygen isotope anomalies in early Earth atmospheres**

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The goal of this project is to reduce uncertainties in the evolution of O\(_2\) levels over Earth history, using a 1-D photochemical model and triple oxygen isotope data.

### 1. The photochemical model, Atmos

**Fig. 1:** Schematic of model set-up. Adapted from Claire, personal communication.

We use and develop the 1-D coupled photochemical-climate model Atmos [e.g.\(1,2,3,4\)].

The model calculates production and loss of atmospheric species at each altitude layer, due to chemical reactions and vertical transport (Fig. 1).

Photolysis, lightning, particulate formation & deposition, rain, and influx of gases are included.

Outputs include species mixing ratio profiles.

### 2. Modelling of oxygen levels suggests two stable states

**Fig. 2** (above): \(O_2\) column density with \(O_2\) mixing ratio for 2024 model atmospheres [from Gregory et al., in review]. For Case 1, we varied \(O_2\) flux and kept \(CH_4:O_2\) flux ratio constant; for Case 2, we varied \(CH_4:O_2\) flux ratio at constant \(O_2\) flux; for Case 3, we included an oxidative weathering flux term for \(O_2\).

**Fig. 3** (right): Potential constraints on oxygen levels over Earth history, from the clustering of model solutions from this study with high-\(O_2\) or trace-\(O_2\) mixing ratios (purple regions)\(^16\). Adapted from \([9]\).

**Fig. 4:** Collecting samples from the Atacama Desert, Chile (Dec 2017). Credit: A. Zerkle.

### 3. Incorporating triple oxygen isotopes into Atmos in order to predict \(\Delta^{17}O\)

#### i) Background to atmospheric \(\Delta^{17}O\)

**O\(_2\) gains a large, positive \(\Delta^{17}O\) value...**

... which is propagated to \(O^{(1)}\), \(CO_2\), \(NO_2\), \(SO_2\), and \(H_2O_2\) via chemical reactions (e.g. \([10]\)).

**Due to mass balance, \(O_2\) has a small, negative \(\Delta^{17}O\) value, dependent on \(pCO_2\), \(O_2\), and primary productivity...**

... which can be incorporated into stable sulphate and preserved in the geological record.

\(\text{where } \Delta^{17}O = \delta^{17}O - 0.528 \delta^{18}O\)

#### ii) Developing Atmos

We have incorporated the three isotopes of oxygen in order to predict \(\Delta^{17}O\) profiles of atmospheric species and \(\Delta^{17}O\) values of species reaching the Earth’s surface through wet and dry deposition.

#### iii) Model validation and calibration...

... involves comparison with existing data (e.g. \([11, 12, 13]\)), existing model results (e.g. \([14, 15]\)), and recently-collected salt concentration and oxygen isotope data from Atacama nitrates and sulphates.

#### iv) Research in progress

- What is the minimum \(pO_2\) required for a non-zero \(\Delta^{17}O\) to be measurable in geological record sulphates?
- What kind of \(\Delta^{17}O_{O_2}\) values might be expected for the high-\(O_2\) and trace-\(O_2\) atmospheres from the flux-driven modelling results presented above (Fig. 3)?

**SUMMARY:** We are developing an oxygen isotope model to predict \(\Delta^{17}O\) in different species under different conditions, in order to explore our hypothesis of two stable states for oxygen concentrations.

**Fig. 5:** Maria Elena, Atacama Desert, Chile

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### References


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### Sharing

Geoscience Online, EGU, 5th May 2020

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