High-dimensional stable isotope signatures:
Principle and applications in studying air, water, and soils

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南京 stable isotope ecology symposium; Oct. 15-18, 2017

稳定同位素的δ概念

We are looking at a very small difference, i.e. a normalized ratio or a ratio of two ratios.

$$\delta = (R/R_{ref}) -1$$

$$\delta' = \ln (R/R_{ref})$$

相对于化学反应的<u>浓度</u>等参数来说，δ已经是个高维度的概念了。

$$\delta^{18}O, \ \delta^{34}S, \ \delta^{15}N, \ \delta^{13}C, \ \delta^{37}Cl...$$

Traditional

$\delta^7\text{Li}, \delta^{57}\text{Fe}, \delta^{201}\text{Hg}, \delta^{65}\text{Cu}, \delta^{80}\text{Se}...$

Non-traditional

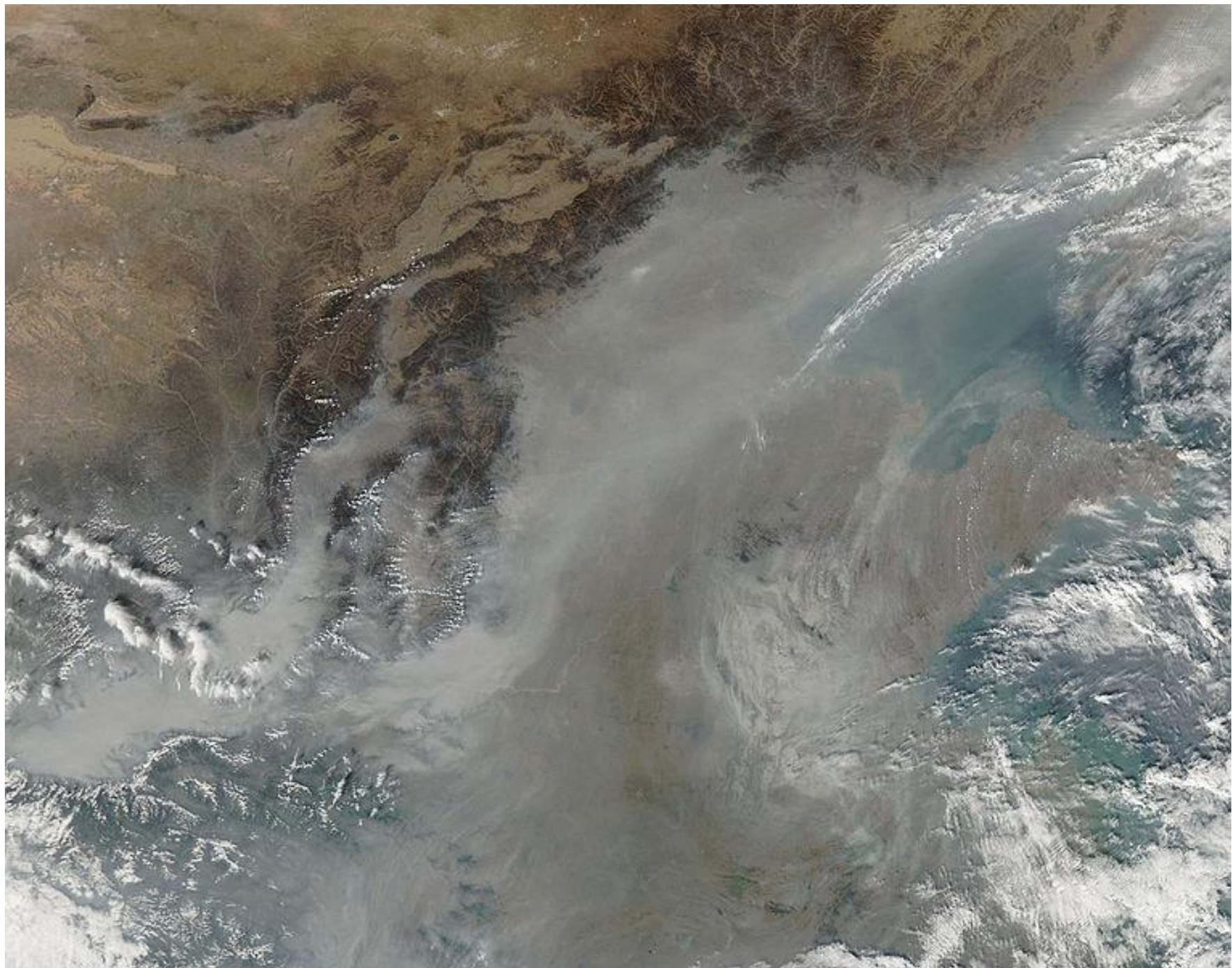$\Delta^{17}O$, $\Delta^{33}S$, $\Delta^{199}Hg$, $\Delta^{36}O$, Δ_{47}, $\Delta^{13}CDH_3$, $\Delta^{12}CH_2D_2$, SP (N, C, S), **Θ, Z, ...**
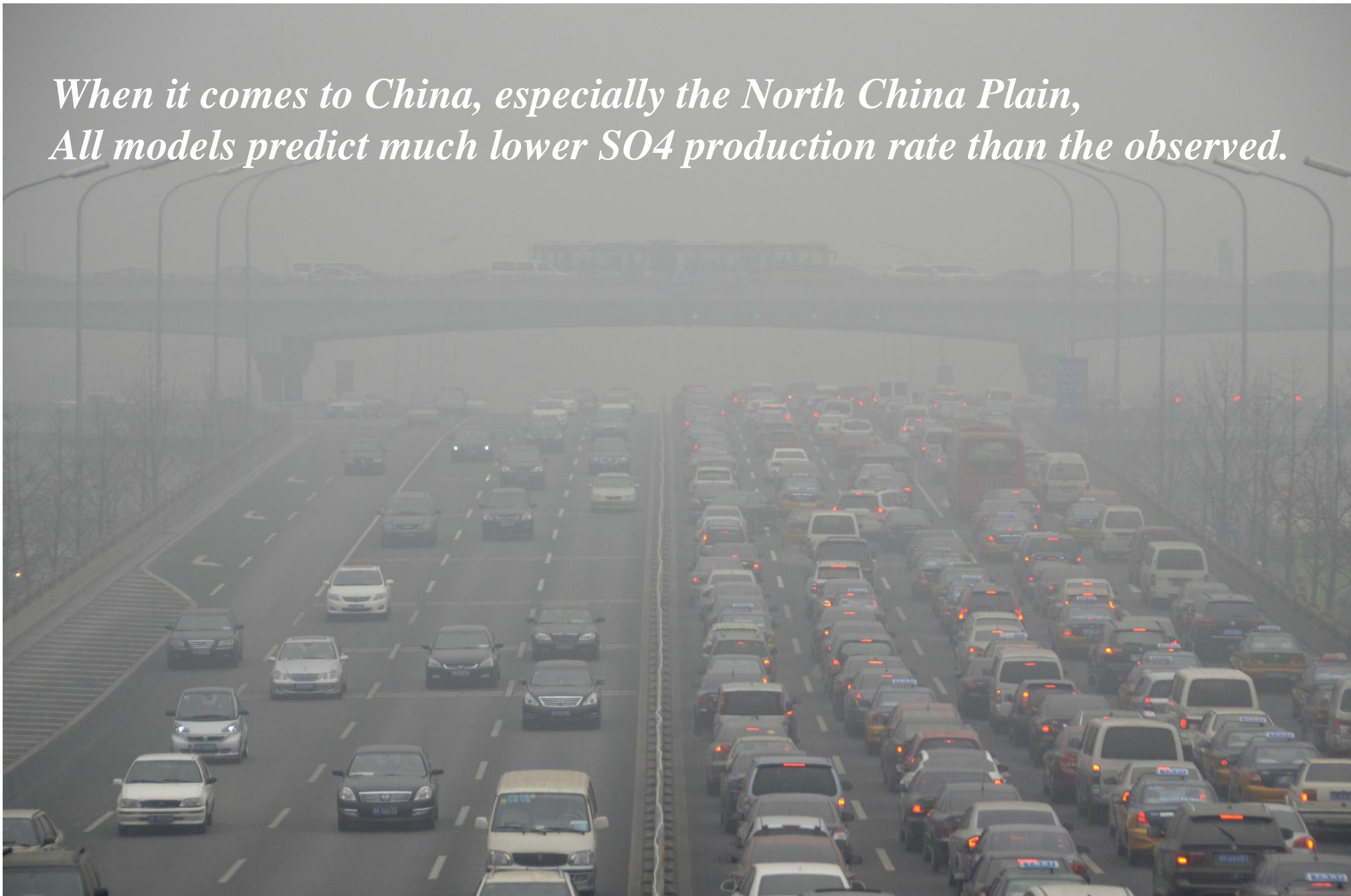
High-dimensional
(高维度)

The third eye:
Perception beyond ordinary sight

Air

When it comes to China, especially the North China Plain,
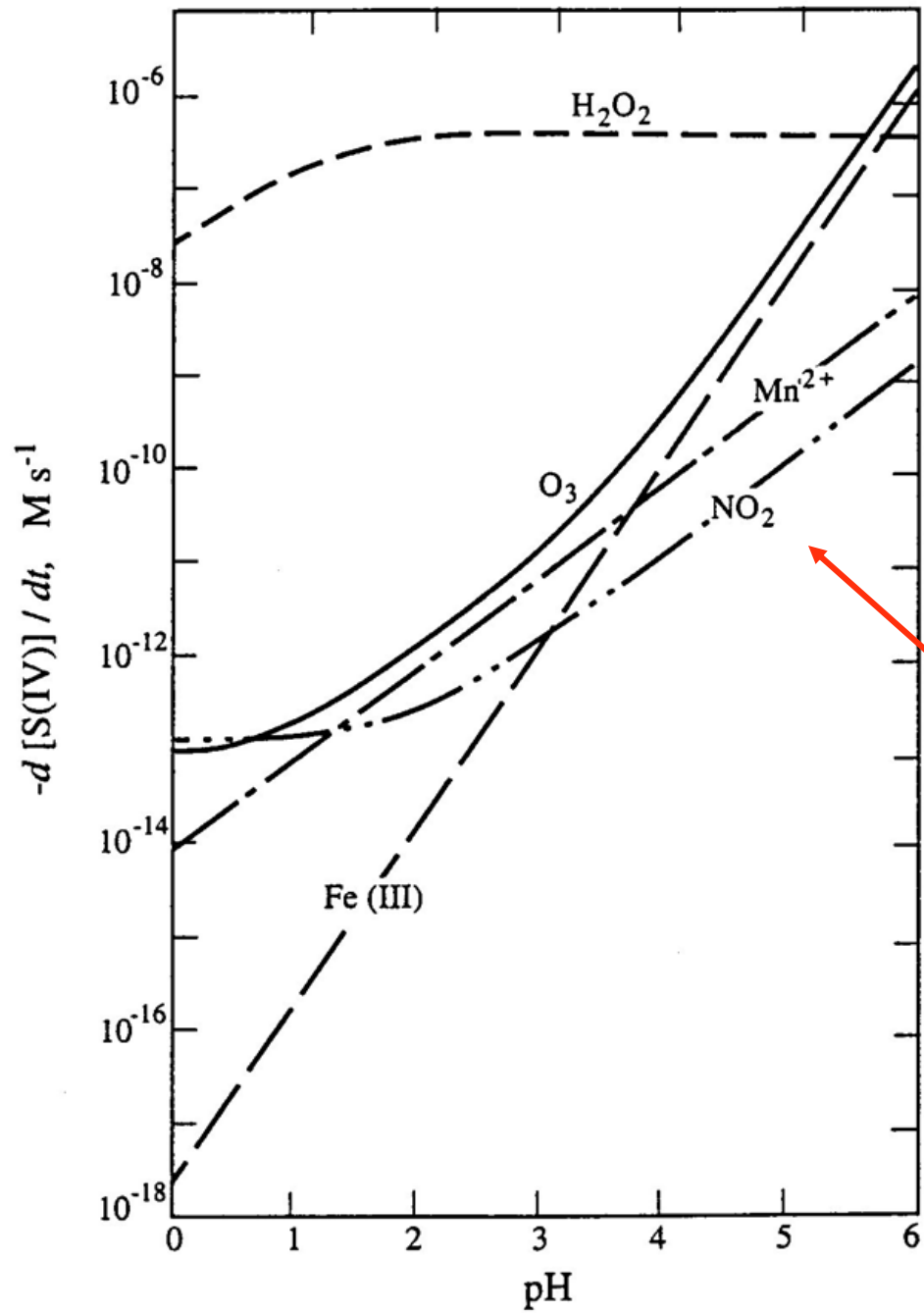All models predict much lower SO4 production rate than the observed.

$$H_2S, DMS, SO_2 \rightarrow SO_4^{2-}$$

Gas

Aqueous

Heterogeneous (surface)

Pathways and rates for aqueous-phase SO_2 oxidation in the atmosphere

Seinfeld & Pandis, 1998

Oxidation of Gas-Phase SO_2 on the Surfaces of Acidic Microdroplets: Implications for Sulfate and Sulfate Radical Anion Formation in the Atmospheric Liquid Phase

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ABSTRACT: The oxidation of $SO_2(g)$ on the interfacial layers of microdroplet surfaces was investigated using a spray-chamber reactor coupled to an electrospray ionization mass spectrometer. Four major ions, HSO_3^-, $SO_3^{\bullet-}$, $SO_4^{\bullet-}$ and HSO_4^-, were observed as the $SO_2(g)/N_2(g)$ gas-mixture was passed through a suspended microdroplet flow, where the residence time in the dynamic reaction zone was limited to a few hundred microseconds. The relatively high signal intensities of $SO_3^{\bullet-}$, $SO_4^{\bullet-}$, and HSO_4^- compared to those of HSO_3^- as observed at pH < 3 without addition of oxidants other than oxygen suggests an efficient oxidation pathway via sulfite and sulfate radical anions on droplets possibly via the direct interfacial electron transfer from HSO_3^- to O_2. The concentrations of HSO_3^- in the aqueous aerosol as a function of pH were controlled by the deprotonation of hydrated sulfur dioxide, $SO_2 \cdot H_2O$, which is also affected by the pH dependent uptake coefficient. When $H_2O_2(g)$ was introduced into the spray chamber simultaneously with $SO_2(g)$, HSO_3^- is rapidly oxidized to form bisulfate in the pH range of 3 to 5. Conversion to sulfate was less at pH < 3 due to relatively low HSO_3^- concentration caused by the fast interfacial reactions. The rapid oxidation of $SO_2(g)$ on the acidic microdroplets was estimated as

SO_2
H^+
H^+
H^+
H^+
H^+
O_2
SO_3^-, HSO_3^-
SO_4^-, HSO_4^-

2016

SCIENCE ADVANCES | RESEARCH ARTICLE
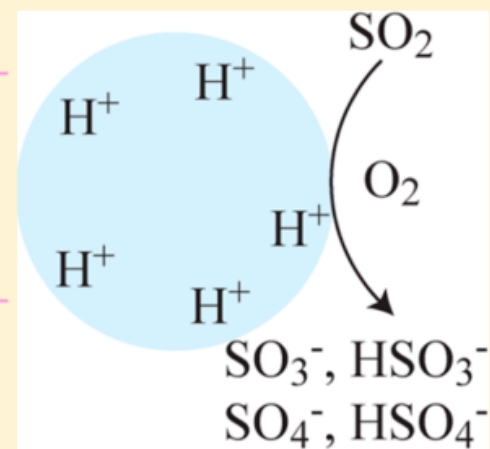
ENVIRONMENTAL SCIENCE

Reactive nitrogen chemistry in aerosol water as a source of sulfate during haze events in China

Yafang Cheng,[1]*[†] Guangjie Zheng,[1,2]* Chao Wei,[1] Qing Mu,[1] Bo Zheng,[2] Zhibin Wang,[1] Meng Gao,[3,4] Qiang Zhang,[5] Kebin He,[2†] Gregory Carmichael,[3,4] Ulrich Pöschl,[1†] Hang Su[6,1†]

Fine-particle pollution associated with winter haze threatens the health of more than 400 million people in the North China Plain. Sulfate is a major component of fine haze particles. Record sulfate concentrations of up to ~300 $\mu g\ m^{-3}$ were observed during the January 2013 winter haze event in Beijing. State-of-the-art air quality models that rely on sulfate production mechanisms requiring photochemical oxidants cannot predict these high levels because of the weak photochemistry activity during haze events. We find that the missing source of sulfate and particulate matter can be explained by reactive nitrogen chemistry in aerosol water. The aerosol water serves as a reactor, where the alkaline aerosol components trap SO_2, which is oxidized by NO_2 to form sulfate, whereby high reaction rates are sustained by the high neutralizing capacity of the atmosphere in northern China. This mechanism is self-amplifying because higher aerosol mass concentration corresponds to higher aerosol water content, leading to faster sulfate production and more severe haze pollution.

INTRODUCTION

Persistent haze shrouding Beijing and the North China Plain (NCP) during cold winter periods threatens the health of ~400 million people living in a region of ~300,000 km². Characteristic features of the winter haze in

ering the gas phase and cloud/fog chemistry, there is still a large gap between modeled and observed sulfate (Fig. 1C). Adding an apparent heterogeneous process with sulfate production rates that scale with aerosol surface area and RH can greatly improve model predictions

Persistent sulfate formation from London Fog to Chinese haze

Gehui Wang[a,b,c,d,e,1], Renyi Zhang[c,d,f,2], Mario E. Gomez[c,d,g], Lingxiao Yang[c,h], Misti Levy Zamora[c], Min Hu[f], Yun Lin[c], Jianfei Peng[c,f], Song Guo[c,f], Jingjing Meng[a,b,i], Jianjun Li[a,b], Chunlei Cheng[a,b,i], Tafeng Hu[a,b], Yanqin Ren[a,b,i], Yuesi Wang[j], Jian Gao[k], Junji Cao[a,b], Zhisheng An[a,b,l], Weijian Zhou[a,b,m], Guohui Li[a,b], Jiayuan Wang[a,b,i], Pengfei Tian[c,n], Wilmarie Marrero-Ortiz[c,d], Jeremiah Secrest[c,d], Zhuofei Du[f], Jing Zheng[f], Dongjie Shang[f], Limin Zeng[f], Min Shao[f], Weigang Wang[c,o,p], Yao Huang[a,b,i], Yuan Wang[q], Yujiao Zhu[c,r], Yixin Li[c], Jiaxi Hu[c], Bowen Pan[c], Li Cai[c,s], Yuting Cheng[a,b,i], Yuemeng Ji[c,t], Fang Zhang[c,l], Daniel Rosenfeld[c,u], Peter S. Liss[c,v], Robert A. Duce[c], Charles E. Kolb[c,w], and Mario J. Molina[x,2]

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Sulfate aerosols exert profound impacts on human and ecosystem   and there have been high SO₂ emissions from combustion of coal

SCIENTIFIC REPORTS

OPEN

High levels of ammonia do not raise fine particle pH sufficiently to yield nitrogen oxide-dominated sulfate production

Hongyu Guo [1], Rodney J. Weber[1] & Athanasios Nenes[1,2,3,4]

High levels of ammonia (NH_3) have been suggested to elevate ambient particle pH levels to near neutral acidity (pH = 7), a condition that promotes rapid SO_2 oxidation by NO_2 to form aerosol sulfate concentration consistent with "London fog" levels. This postulation is tested using aerosol data from representative sites around the world to conduct a thorough thermodynamic analysis of aerosol pH and its sensitivity to NH_3 levels. We find that particle pH, regardless of ammonia levels, is always acidic even for the unusually high NH_3 levels found in Beijing (pH = 4.5) and Xi'an (pH = 5), locations where sulfate production from NO_x is proposed. Therefore, major sulfate oxidation through a NO_2-mediated pathway is not likely in China, or any other region of the world (e.g., US, Mediterranean) where the aerosol is consistently more acidic. The limited alkalinity from the carbonate buffer in dust and seasalt can provide the only likely set of conditions where NO_2-mediated oxidation of SO_2 outcompetes with other well-established pathways. The mildly acidic levels associated with excessive amounts of ammonia can promote high rates of SO_2 oxidation through transition metal chemistry, this may be an alternative important aerosol chemical contributor to the extreme pollution events.

However, these attempts are probably one of the many possible solutions to the discrepancies.

Model revision:
Too many knobs (adjustable parameters)

Independent tests of the atmospheric sulfate chemistry models are imperative.

Atmospheric sulfate	Oxidants	Sulfate $\Delta^{17}O$
SO_2 oxidation (secondary)	O_3 (aq)	~ +10
	H_2O_2 (aq)	~ +0.9
	·OH, ·HO_2 (gas or aq)	~0
	O_2 + metal ions	~0
	organic peroxides	?
	NO_2	?
Primary sulfate	O_2	~0
Physical removal of SO_2 + surface oxidation	probably H_2O, O_2	~0
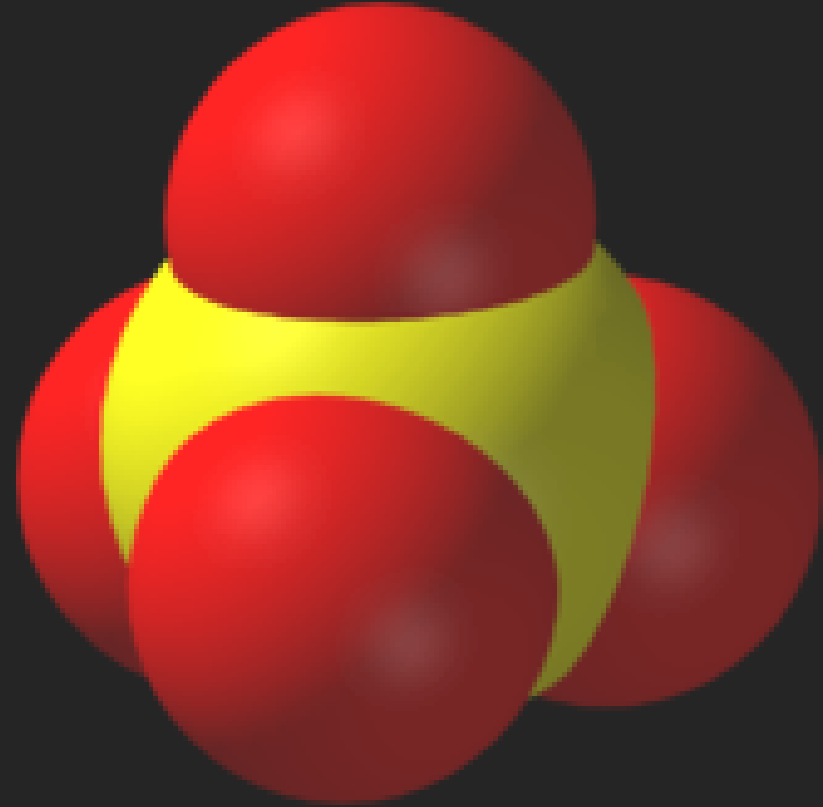
High-dimensional S and O isotope signatures in atmospheric sulfate

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Water

-55‰

0‰

$\delta^{18}O$

+5‰

wallpapercave.com

http://i.imgur.com/kVfJUOD.jpg

www.travelswithtwo.com

Evariston et al., 2015

Surface Water Samples - Washington State

http://www.pitt.edu/~mabbott1/climate/mark/Current_Research/NOCA/noca.html

Water on Earth

$$\delta'^{17}O = 0.528 \ (\pm 0.0001) \ \delta'^{18}O - 0.033 \ (\pm 0.003)$$
$$R^2 = 0.99999$$

A

Luz & Barkan, 2010, GCA
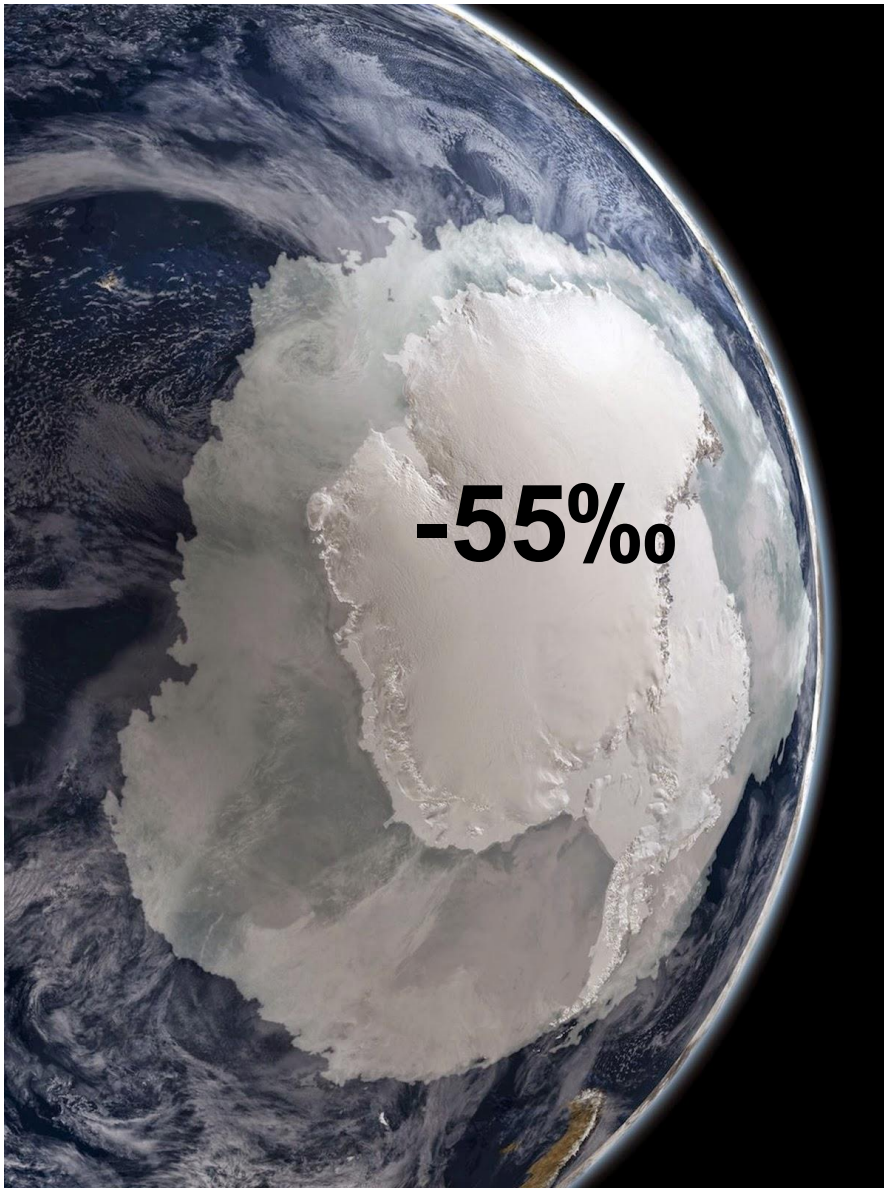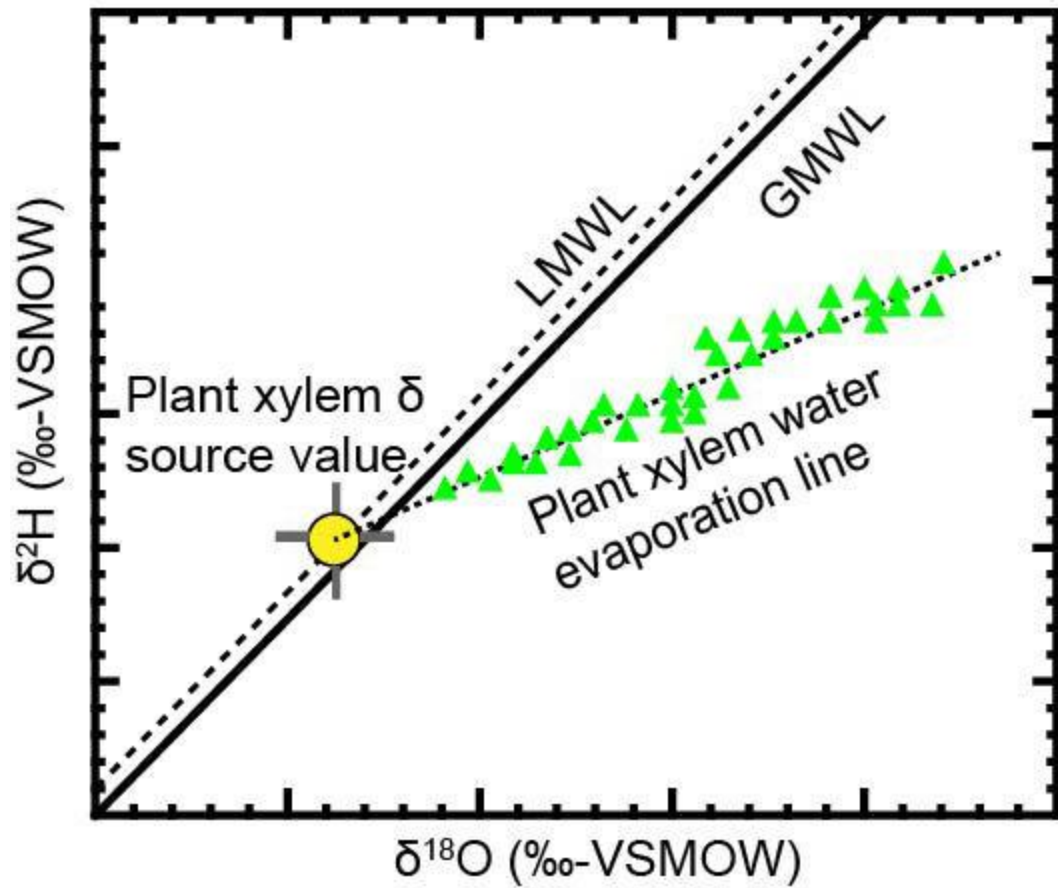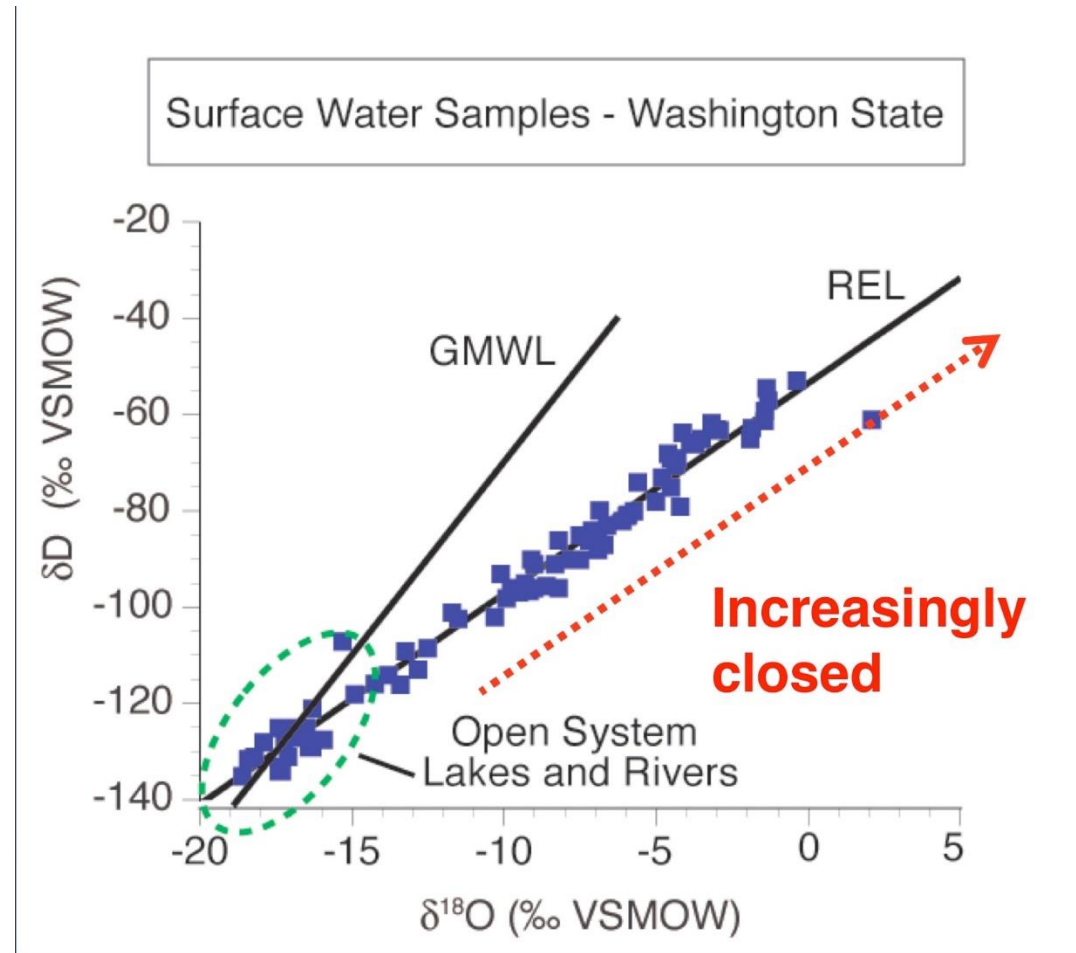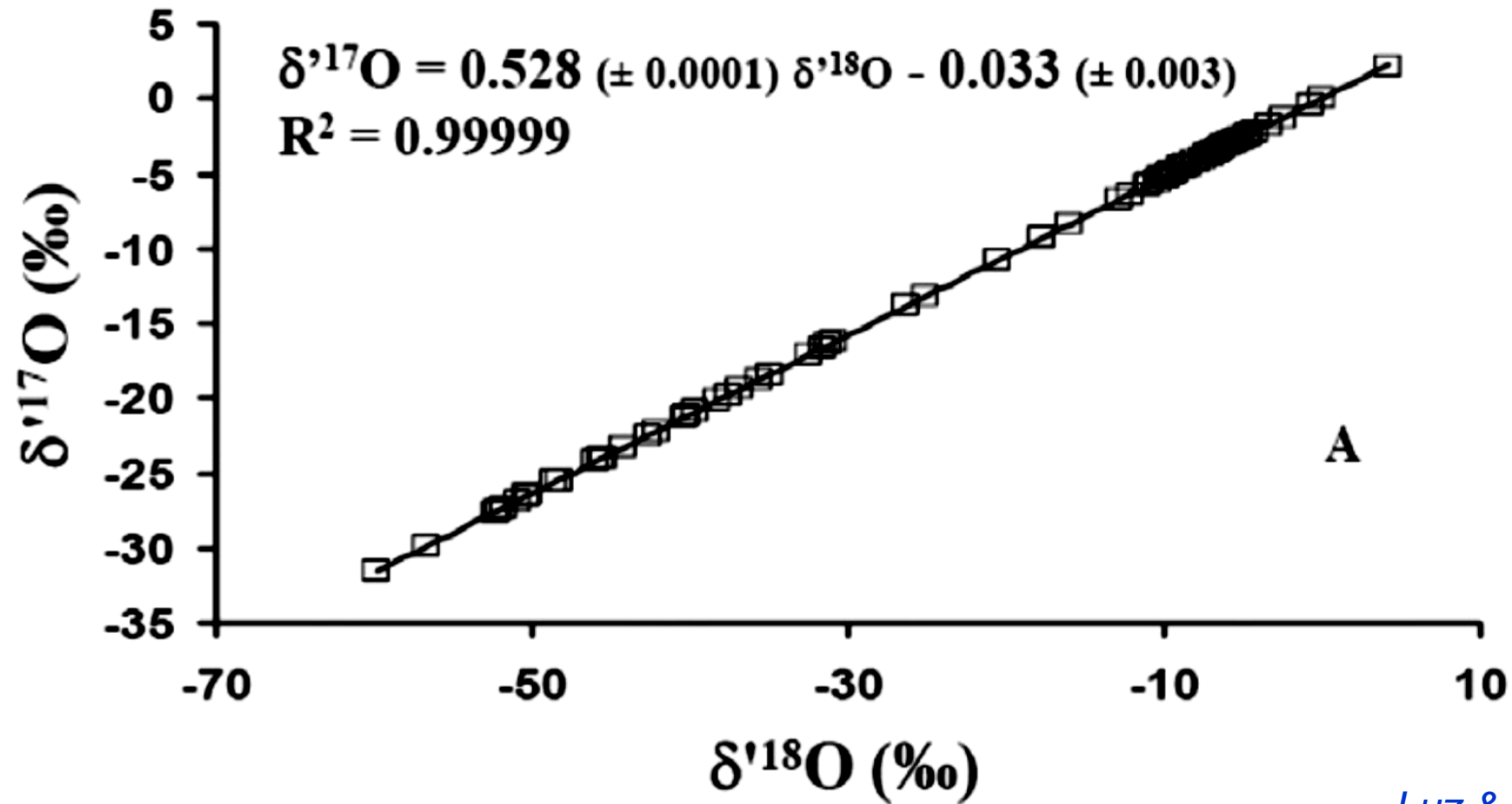
The triple oxygen isotope exponent for different <u>mass-dependent</u> processes is <u>measurably</u> different.

$$\theta \equiv \ln^{17}\alpha/\ln^{18}\alpha$$

(θ varies mostly in the range of 0.51 to 0.53)

B. Luz, A. Angert, E. Young, R. Tanaka, A. Pack, N. Levin, B. Passey, Z. Sharp, S. Assonov, J. Kaiser, D. Rumble, M. Miller ……
E. Young, E. Schauble, Y. Liu

δ'¹⁸O

Seawater

Diffusion
$\theta_{diff} = 0.518$

Equilibrium
$\theta_{eq} = 0.529$

Vapor transport and
precipitation in closed
Rayleigh Distillation style
$S = 0.528$

Equilibrated vapor

Initial vapor due to
degrees of relative humidity
in source regions

δ'¹⁷O

Bao et al., 2016, AREPS

Fig. 9. Variation of measured $^{17}O_{excess}$ with d-excess for the squall line study (grey) and the seasonal variability (black). Variations of $^{17}O_{excess}$ vs. d-excess calculated with the 2D squall line model for domain 2 (orange). The two blue lines display the slope of $^{17}O_{excess}$ vs. d-excess predicted by the simple reevaporation model providing a constant isotopic composition of the water vapor.

"The influence of large-scale processes on the isotopic composition of water vapor (conditions at the evaporative source, convection and recycling along trajectories) can explain the second order difference between the two proxies. "

Landais et al., 2010

Africa Monsoon precipitation

Soils

McMurdo Dry Valleys, Antarctica
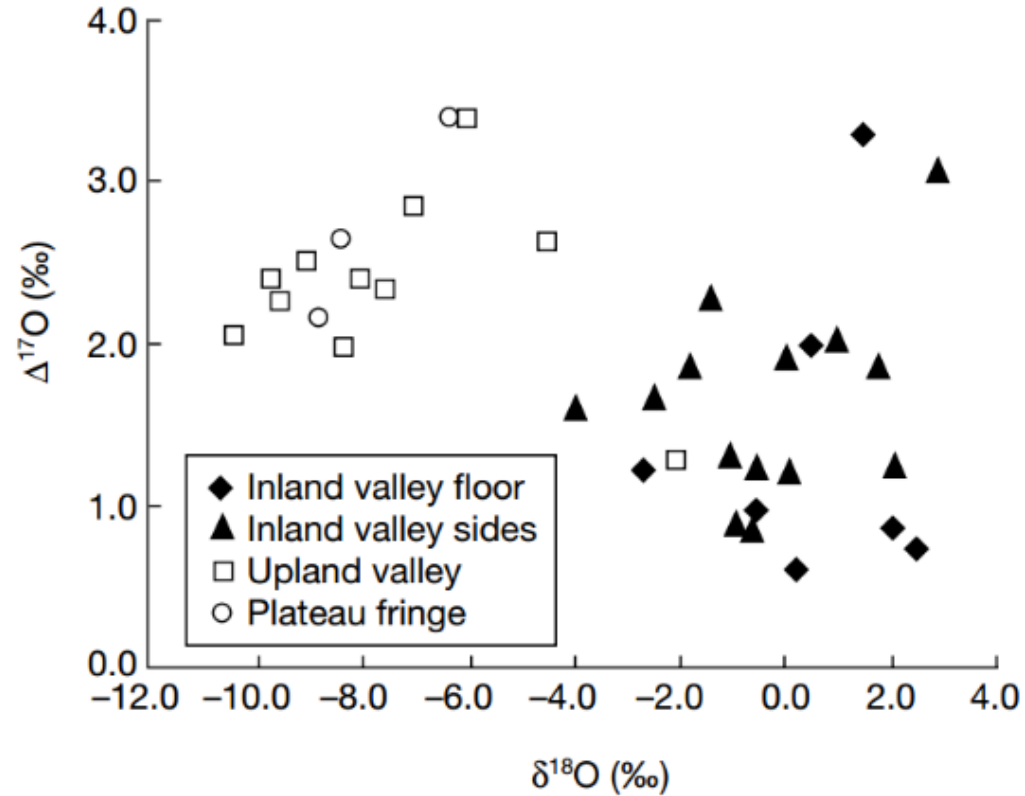
Figure 1 Sulphate $\delta^{18}O$ and $\Delta^{17}O$ values for soils from different climatic regions in Antarctic dry valleys. The error bar for $\delta^{18}O$ value can be as large as ± 0.8 (not shown); it is, however, only ± 0.05 for the $\Delta^{17}O$ value, owing to the covariations of $\delta^{18}O$ and $\delta^{17}O$ during measurement[12].
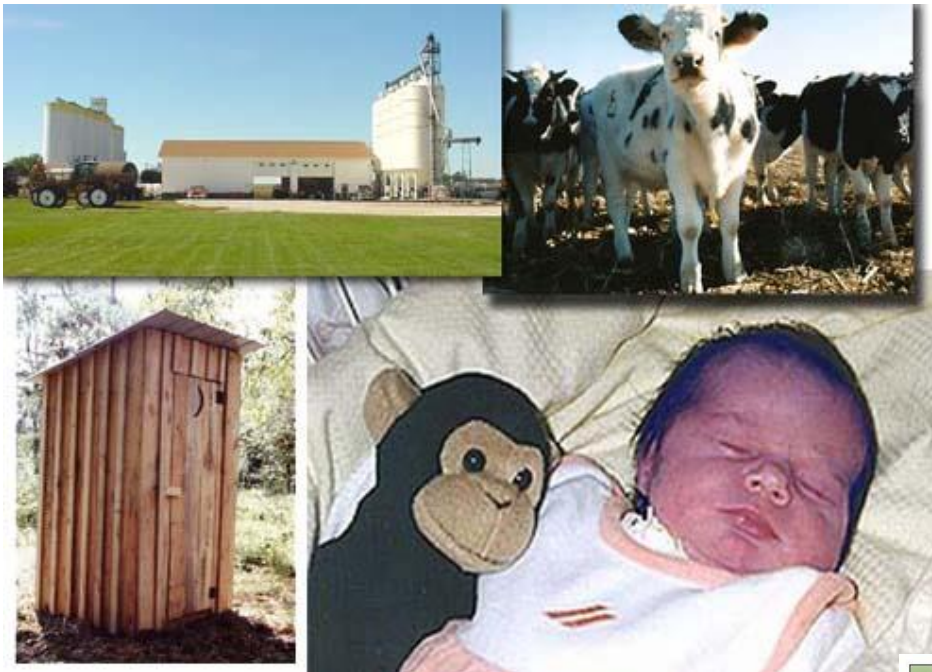
Origins of sulphate in Antarctic dry-valley soils as deduced from anomalous [17]O compositions

Huiming Bao*, Douglas A. Campbell*, James G. Bockheim†
& Mark H. Thiemens*

* Department of Chemistry & Biochemistry, Mail Code 0356, University of California San Diego, 9500 Gilman Drive, La Jolla, California 92093-0356, USA
† Department of Soil Science, University of Wisconsin, 1525 Observatory Drive, Madison, Wisconsin 53706-1299, USA

The dry valleys of Antarctica are some of the oldest terrestrial surfaces on the Earth. Despite much study of soil weathering and development, ecosystem dynamics and the occurrence of life in these extreme environments[1–3], the reasons behind the exceptionally high salt content of the dry-valley soils[4–6] have remained uncertain. In particular, the origins of sulphate are still controversial; proposed sources include wind-blown sea salt[5,7], chemical weathering[8], marine incursion[9], hydrothermal processes[10] and oxidation of biogenic sulphur in the atmosphere[1]. Here we report measurements of $\delta^{18}O$ and $\delta^{17}O$ values of sulphates from
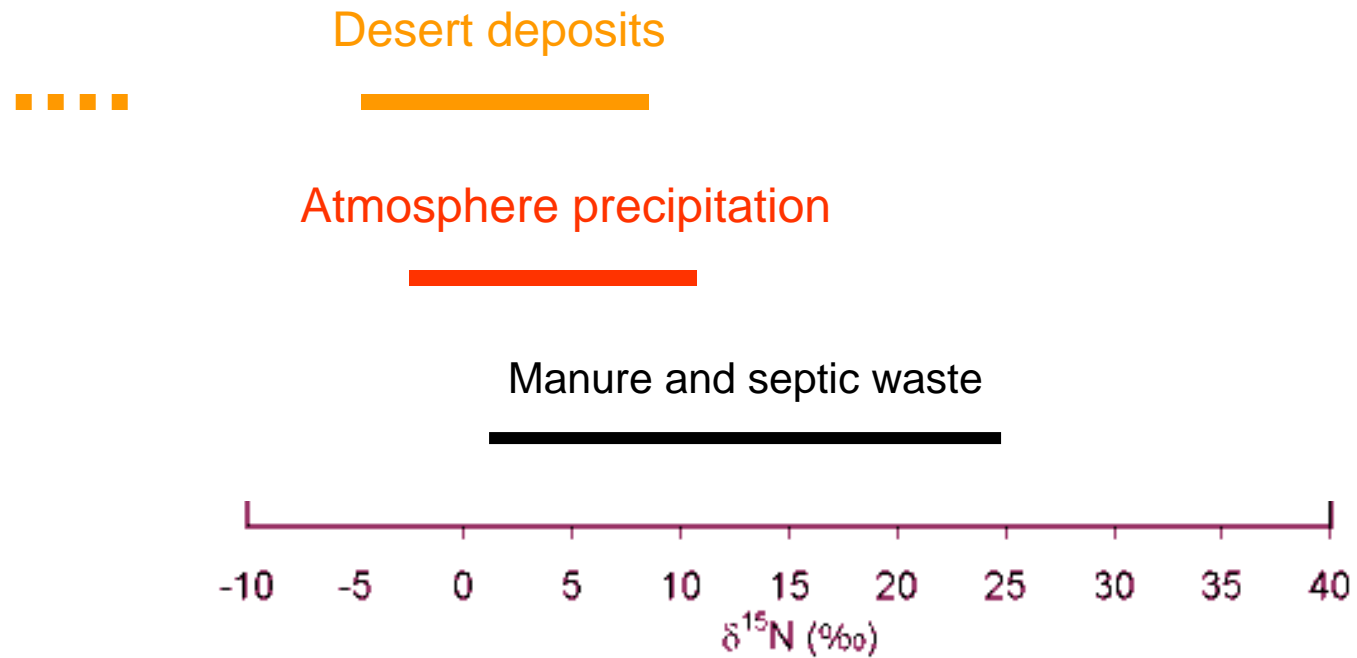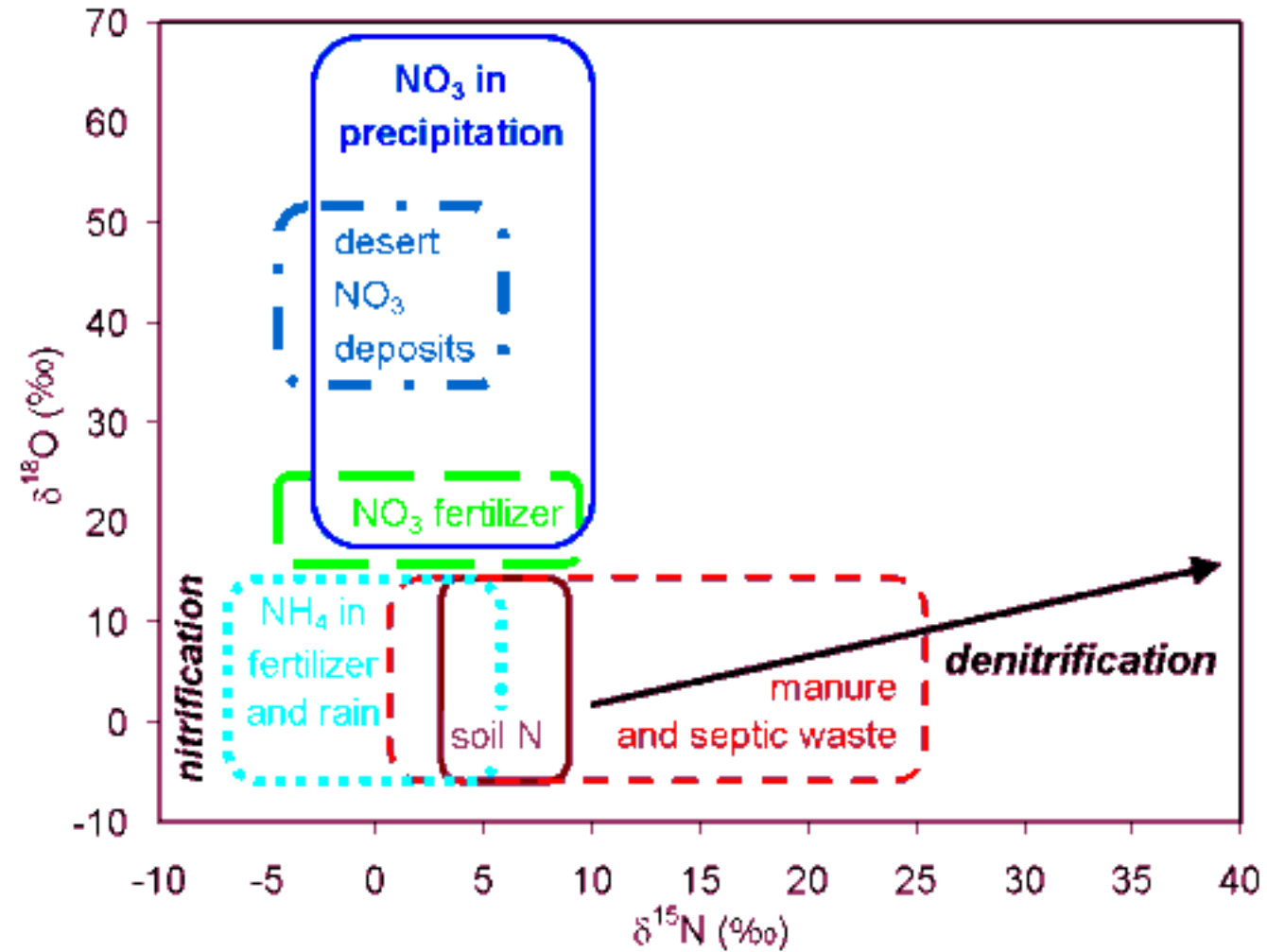
The nitrate problem

http://news.jongo.com/articles/07/0821/30781/

NO$_3^-$ in one dimension: δ^{15}N

Desert deposits

Atmosphere precipitation

Manure and septic waste

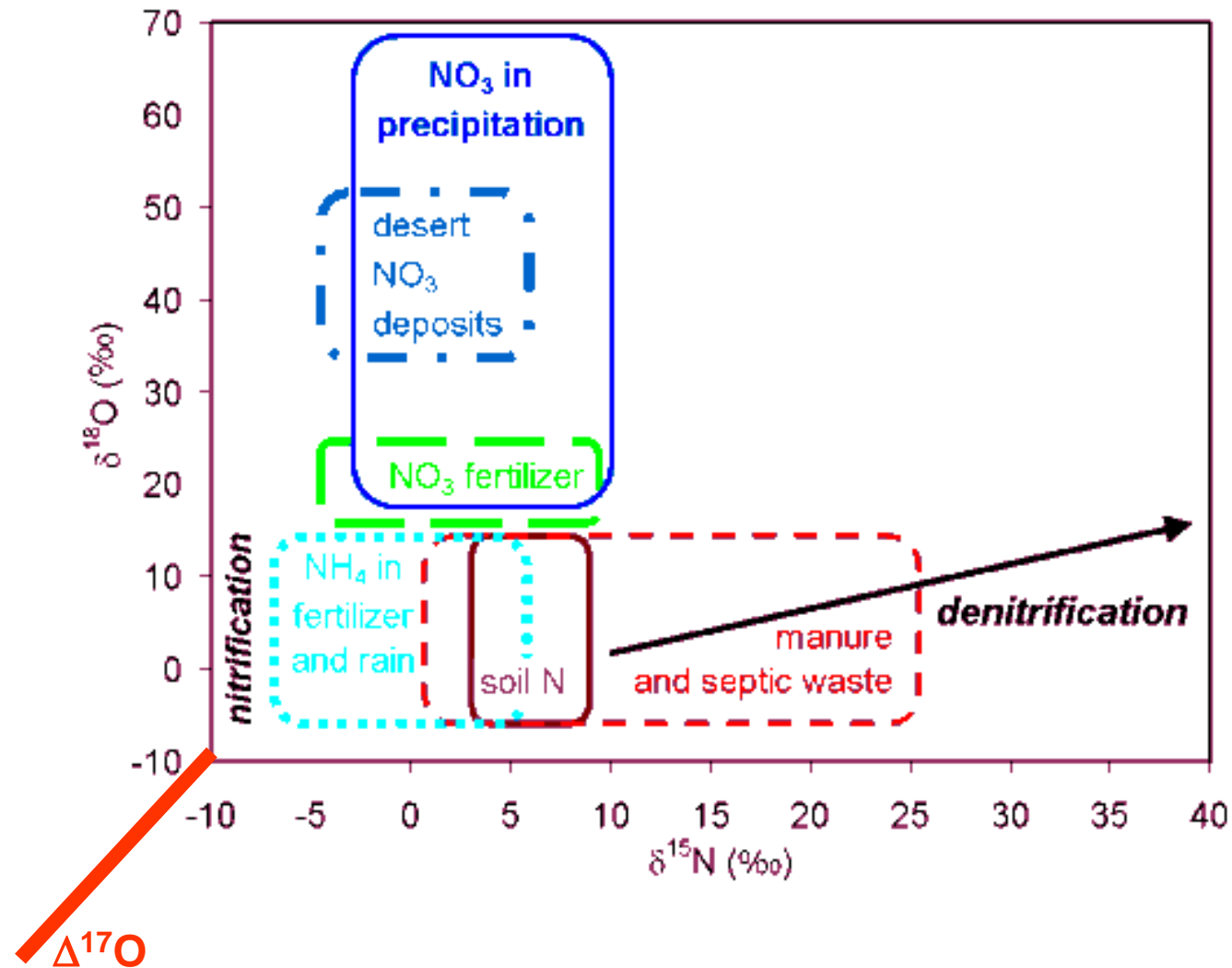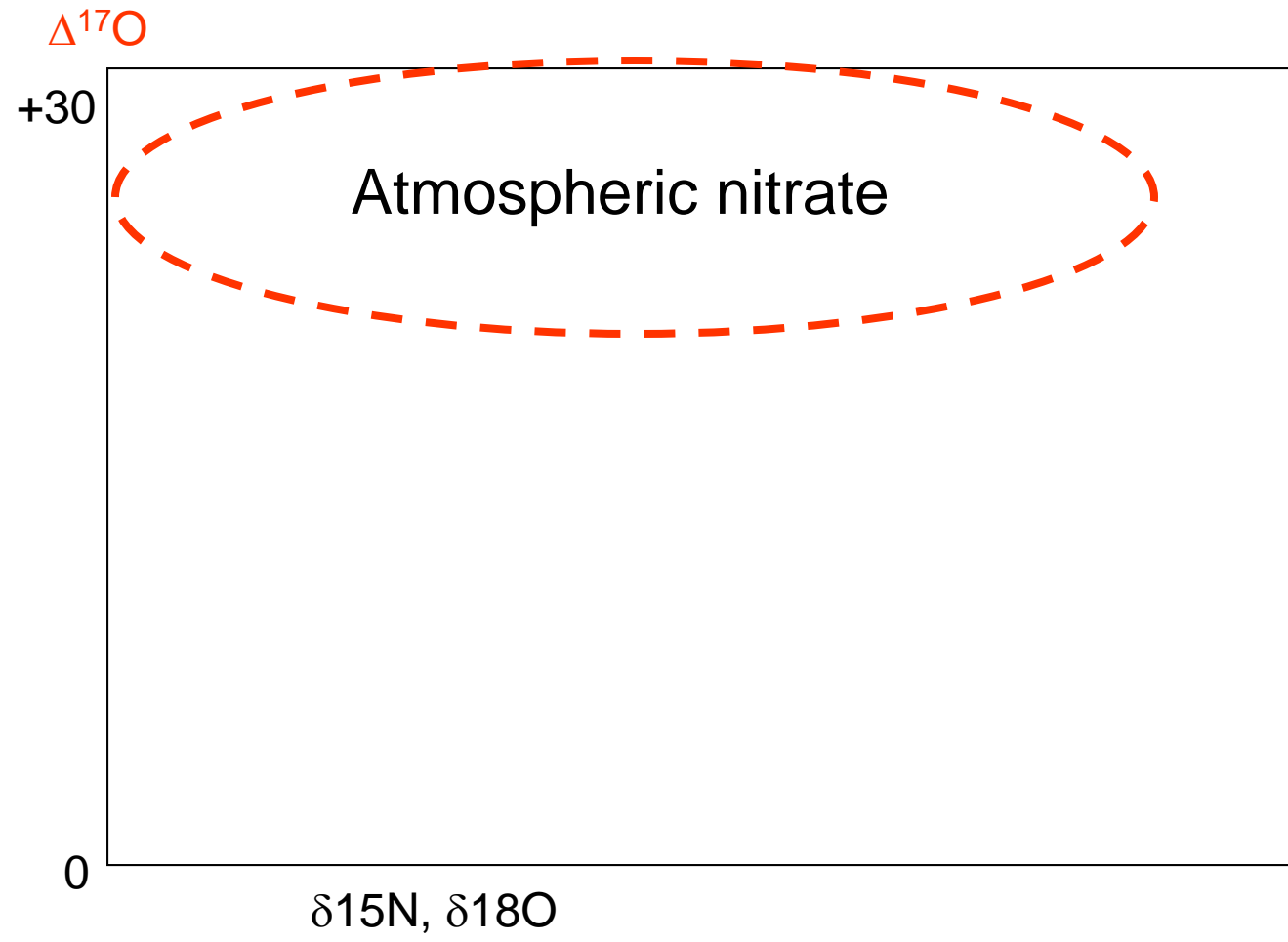-10 -5   0   5   10   15   20   25   30   35   40
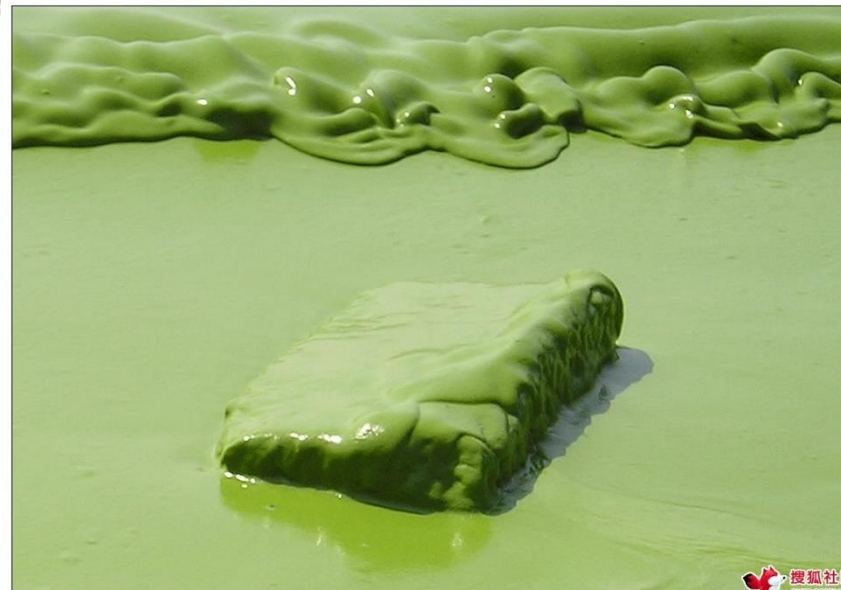
δ^{15}N (‰)

NO$_3^-$ in two dimension: δ^{15}N + δ^{18}O

We need an extra dimension!

NO$_3^-$ in two dimension: δ^{15}N + δ^{18}O + Δ^{17}O

A 3rd example: the perchlorate issue

Natural Perchlorate Has a Unique Oxygen Isotope Signature

HUIMING BAO*

Department of Geology & Geophysics, E235 Howe-Russell
Geoscience Complex, Louisiana State University,
Baton Rouge, Louisiana 70803

BAOHUA GU

Environmental Sciences Division, Oak Ridge National
Laboratory, 1 Bethel Valley Road, Oak Ridge, Tennessee 37381

Perchlorate is known to be a minor component of the
hyperarid Atacama Desert salts, and its origin has long

difficulties encountered in extracting an
quantities of perchlorate from soil deposits
quantities of nitrate and other salt impur
    The presence of natural or atmospher
the environment obviously has far-reach
ranging from public health issues to huge lia
be imposed by agricultural and environmen
Controversy exists with respect to perchlora
in those cases in which the sources of per
nation are not readily identifiable. For ex
were raised about traces of perchlorate
some commercial fertilizers, although suc
was later found to be associated with
imported from Chile (9−11). Recent studie
some potash minerals obtained from th
States, Canada, and Bolivia contain perchlo
additional studies and confirmation of t
necessary.

Perchlorate ion: ClO_4^-
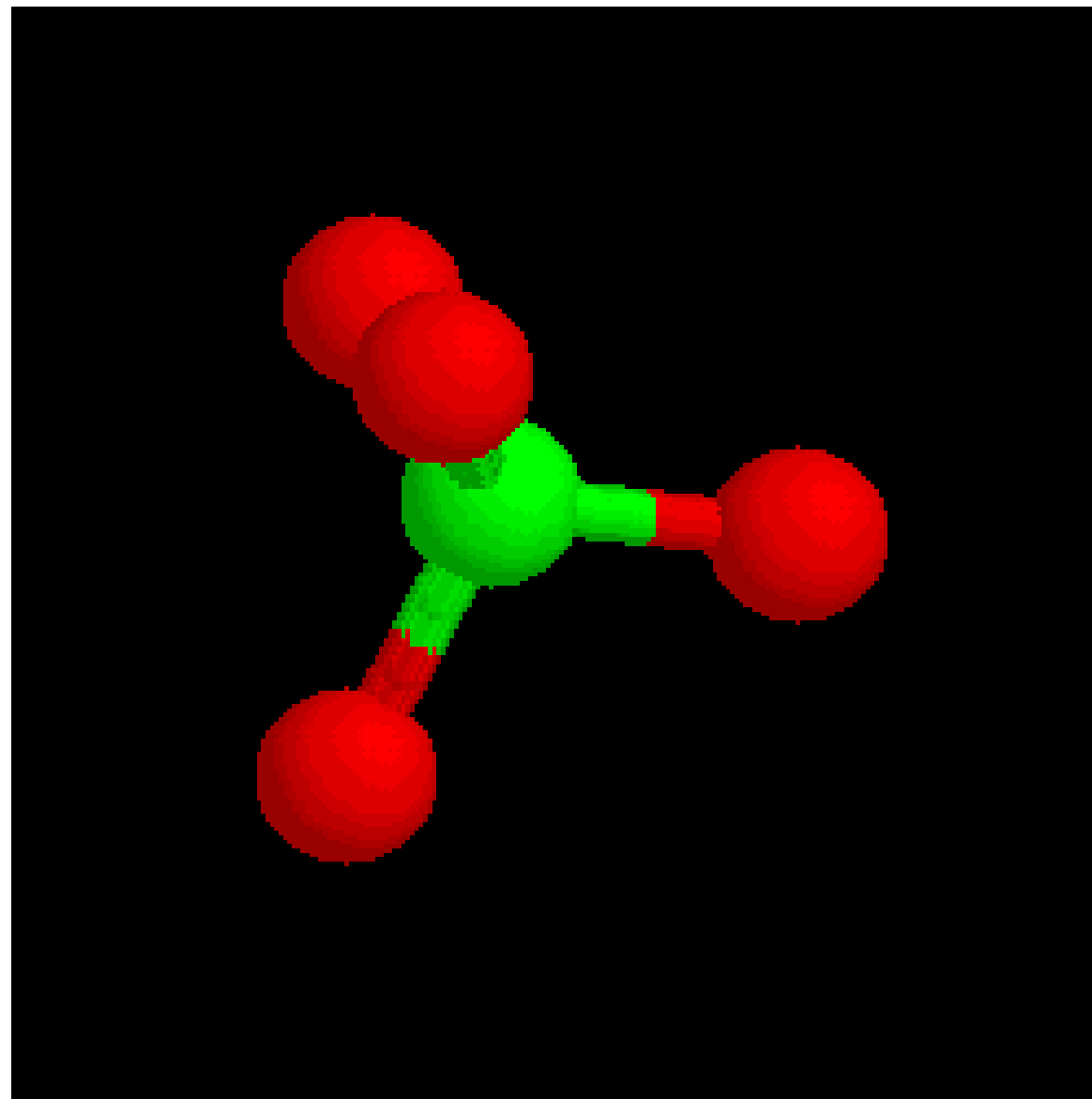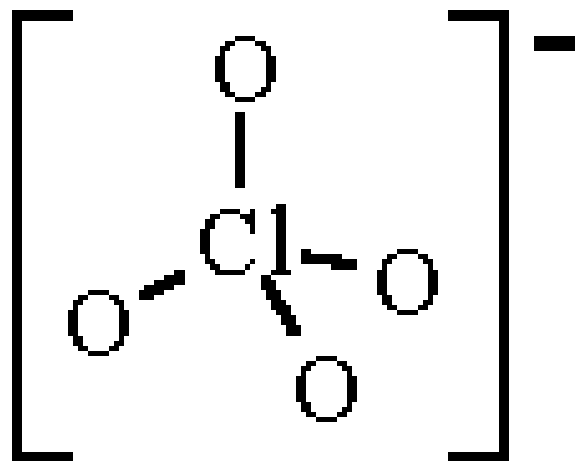
Primary oxidizer in the solid propellant for rockets and missiles
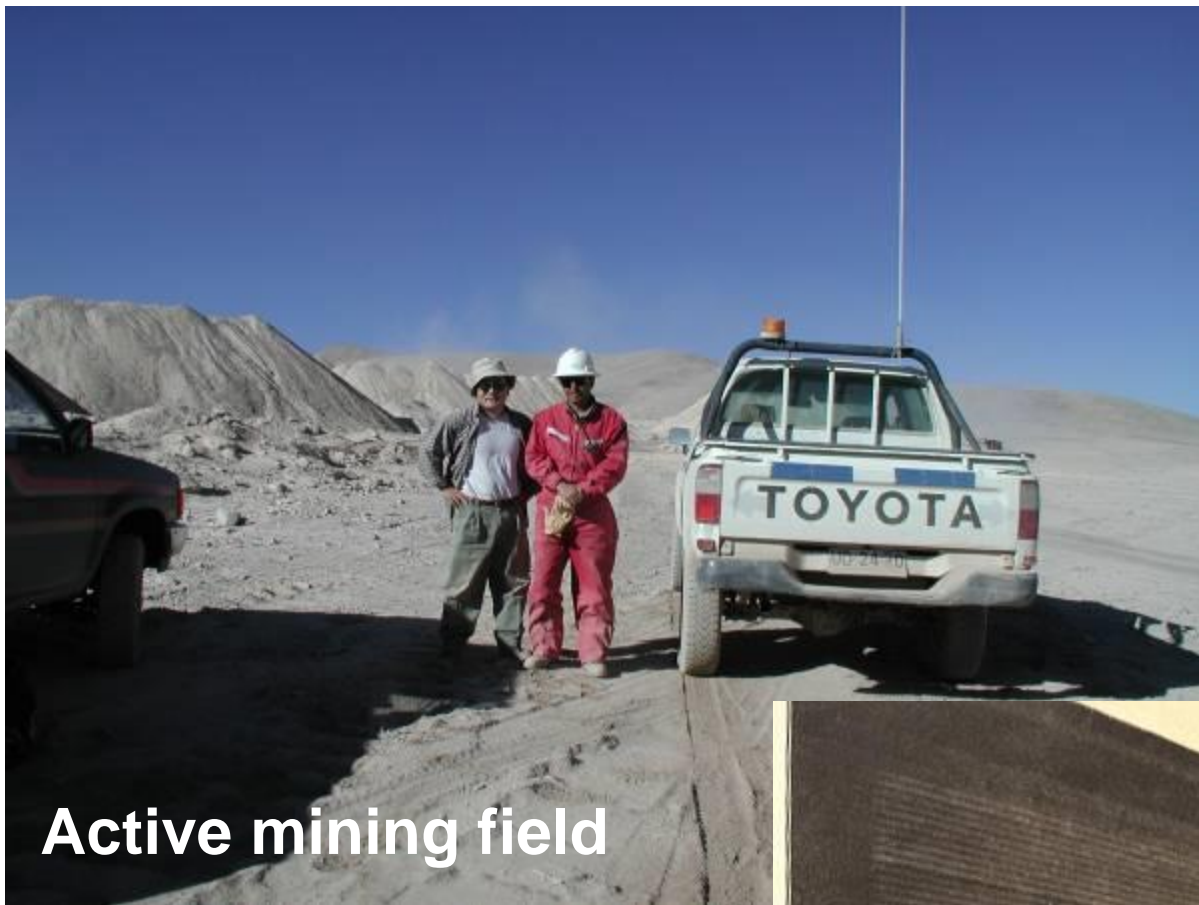
Active mining field

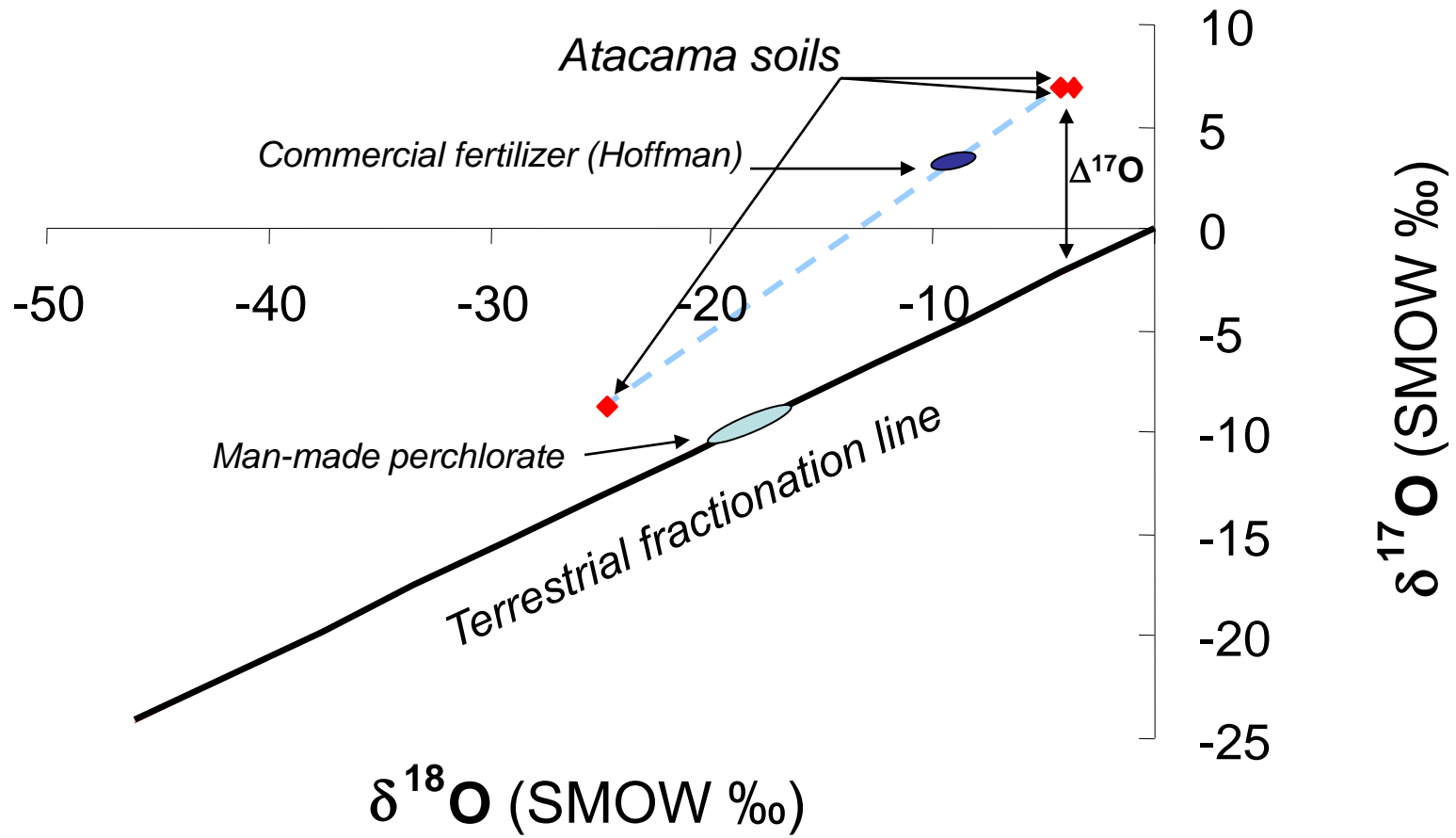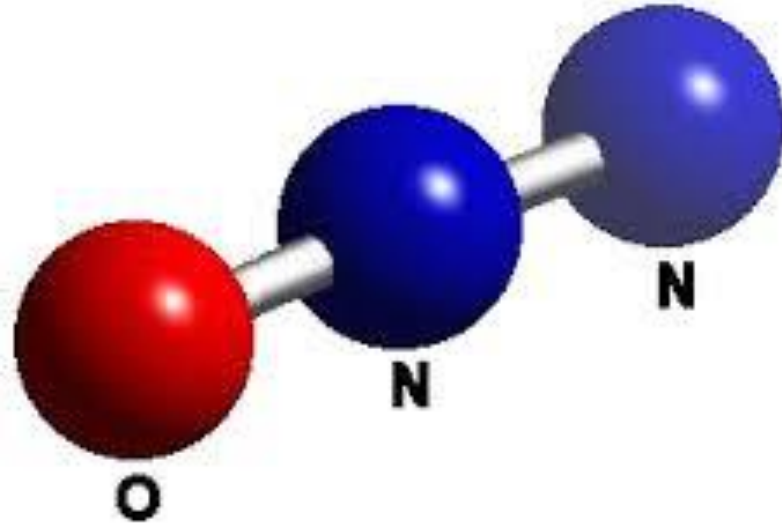
Chile was a major nitrate exporter

Source of perchlorate contamination:
Contaminated groundwater
or fertilizers originated from Chile?

Atacama soils

Commercial fertilizer (Hoffman)

$\Delta^{17}O$

Man-made perchlorate

Terrestrial fractionation line

$\delta^{18}O$ (SMOW ‰)

$\delta^{17}O$ (SMOW ‰)

10

5

0

-5

-10

-15

-20

-25

-50   -40   -30   -20   -10

A 4th example in soil related:

Four types of "high dimension"

H1:
Relationships among multiple stable isotope compositions of the same elements (e.g. δ¹⁸O and δ¹⁷O for O, δ³⁴S, δ³³S, and δ³⁶S for S)

$$\frac{\ln \alpha^{17}}{\ln \alpha^{18}} = \frac{(17-16)/17 \times 16}{(18-16)/18 \times 16} \times \frac{\text{force constant}}{\text{force constant *}}$$

$$\theta = 0.530$$

$$\delta^{33}S = 0.515\ \delta^{34}S$$

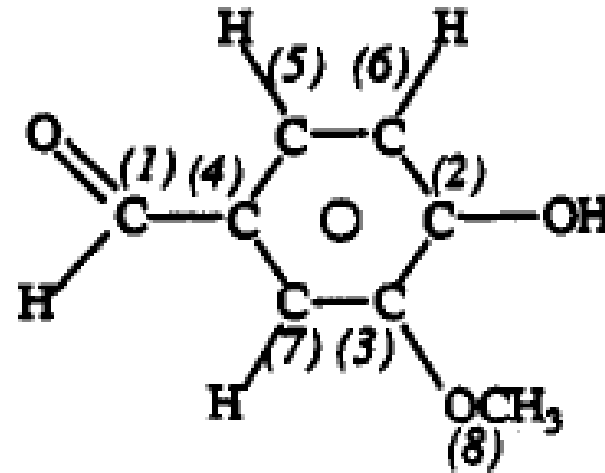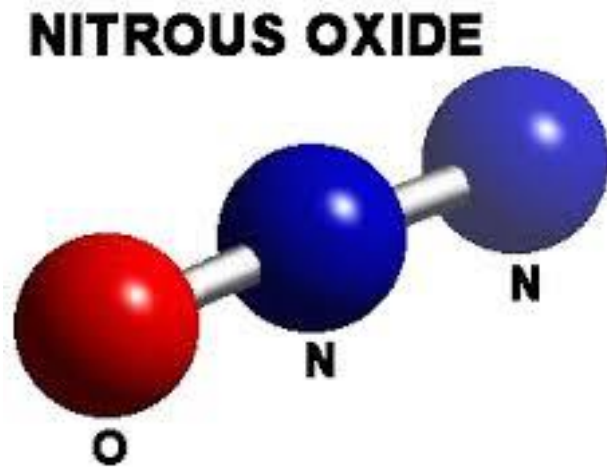$$\Delta^{33}S \equiv \delta^{33}S - 0.515\ \delta^{34}S$$

$$\delta'^{17}O = 0.5305 \times \delta'^{18}O$$

$$\Delta^{17}O \equiv \delta'^{17}O - 0.5305 \times \delta'^{18}O$$

H2:

Relationship among "site-specific" stable isotope compositions (e.g. $\delta^{15}N^\alpha$ versus $\delta^{15}N^\beta$ in $N^\alpha N^\beta O$ or N_2O in which the N^α is only boned to N^β, not to terminal O in this linear molecule)

NITROUS OXIDE

Nuclear Magnetic
Resonance Spectroscopy

H3:
Distribution among multiple isotopologues of a molecule or an ion (e.g. $^{12}C^{16}O^{16}O$, $^{12}C^{16}O^{18}O$, $^{13}C^{16}O^{18}O$ for CO_2, $^{16}O^{16}O$, $^{17}O^{16}O$, $^{18}O^{16}O$, $^{17}O^{18}O$, $^{18}O^{18}O$ for O_2)

E.g. Clumped isotope systems

The temperature-dependent mass-47 anomaly (Δ^{47}) describing the enrichment of $13C18O16O$ in $CO2$ relative to the stochastic (random) distribution is defined as follows:

$$\Delta_{47} = \left[\left(\frac{R_{47}}{R_{47^*}} - 1 \right) - \left(\frac{R_{46}}{R_{46^*}} - 1 \right) - \left(\frac{R_{45}}{R_{45^*}} - 1 \right) \right] \times 1000$$

Applications: Geothermometer; Modern atmospheric CO_2 source apportionment;
Others: 18O18O, 15N15N, 13CH3D, ...

Clumpness in non-labile molecules: O2, N2, CH4, ...

$^{16}O^{16}O$, $^{16}O^{18}O$, $^{18}O^{18}O$

$^{14}N^{14}N$, $^{15}N^{14}N$, $^{15}N^{15}N$

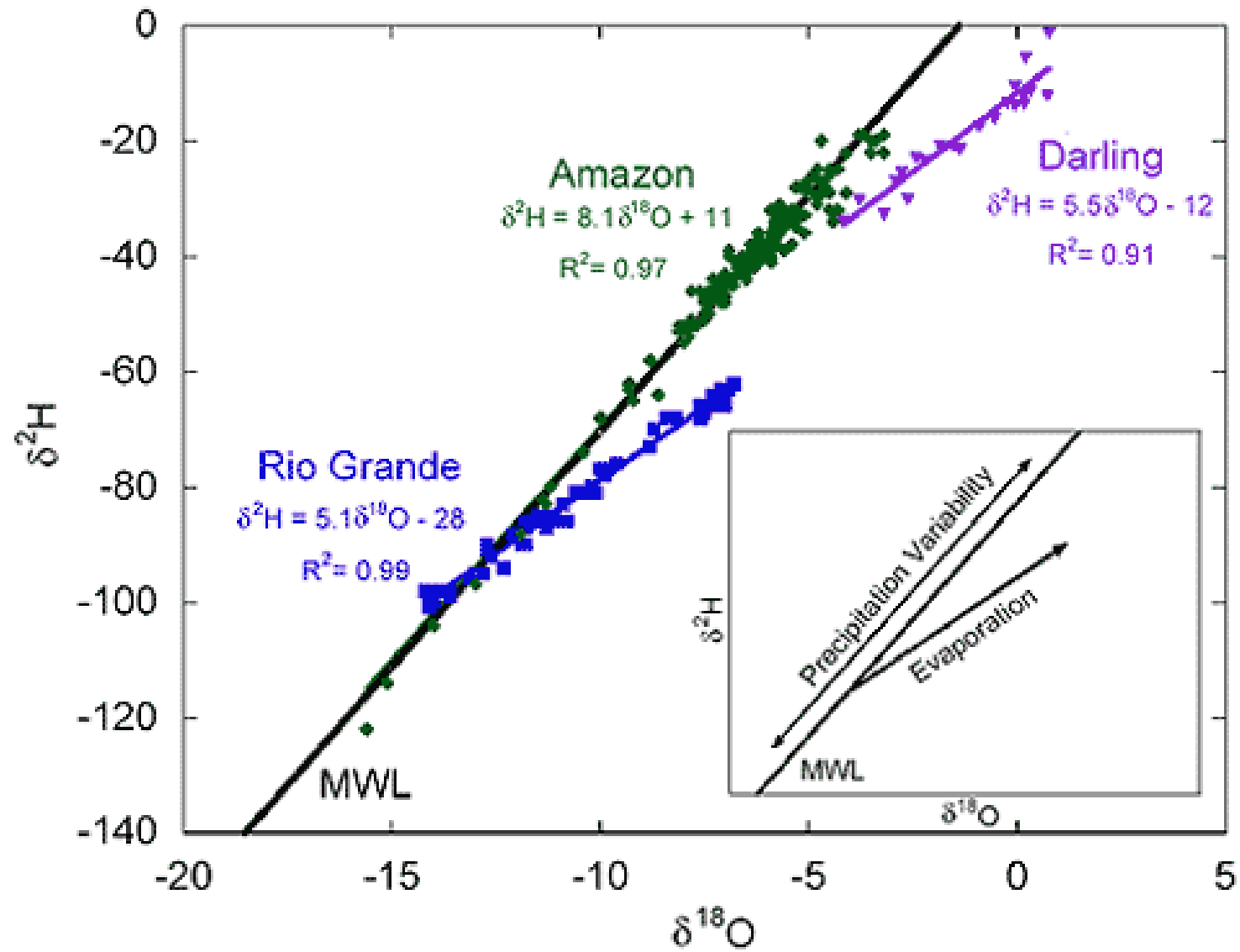$^{12}CH_4$, $^{12}CH_3D$, $^{13}CH_4$, $^{13}CH_3D$, $^{12}CH_2D_2$, $^{13}CH_2D_2$,

...

H4:
Relationships among isotope compositions of two or more elements in a compound (e.g. $\delta^{34}S$ and $\delta^{18}O$ in SO_4^{2-}, $\delta^{15}N$ and $\delta^{18}O$ in NO_3^-, $\delta^{56}Fe$ and $\delta^{34}S$ in FeS_2, $\delta^{30}Si$ and $\delta^{18}O$ in SiO_2, or $\delta^{44}Ca$, $\delta^{13}C$, and $\delta^{18}O$ in $CaCO_3$).
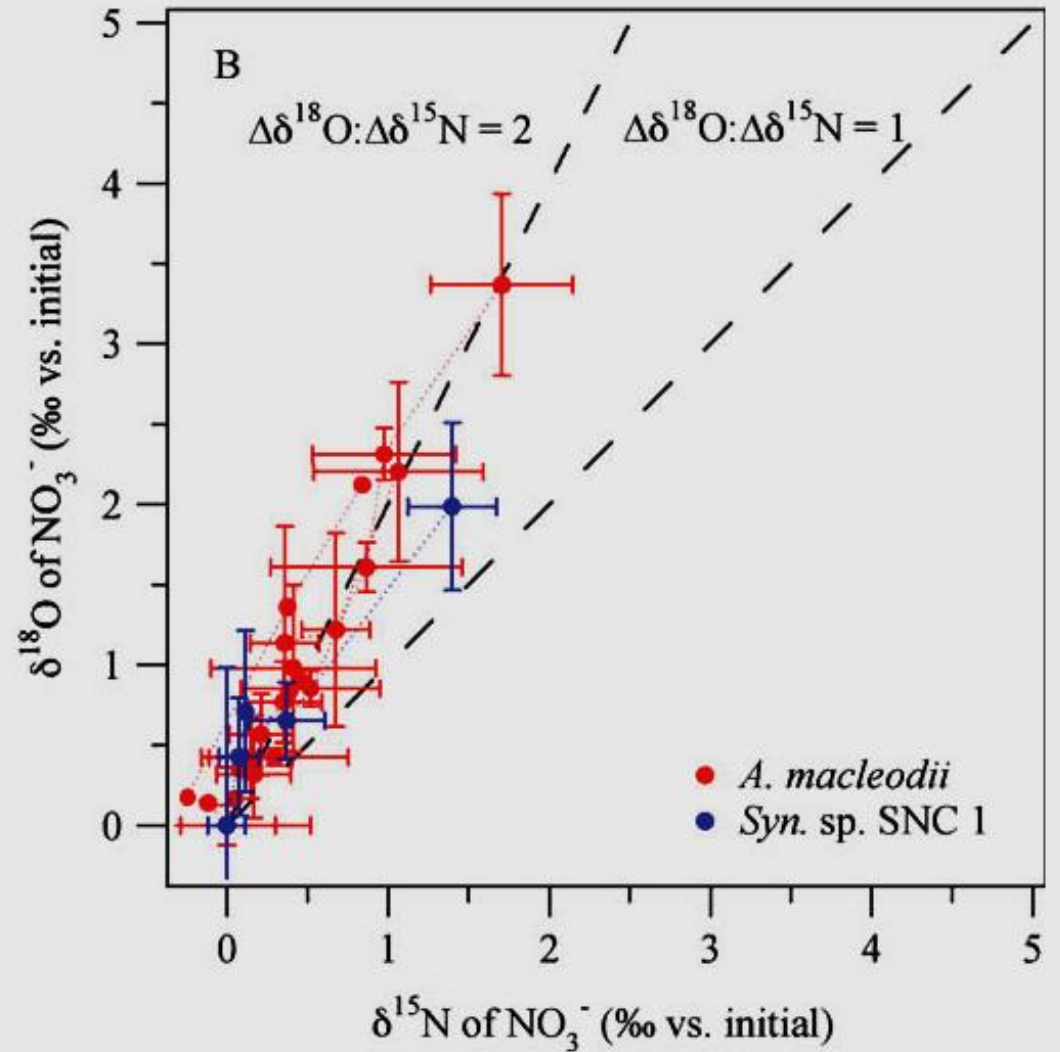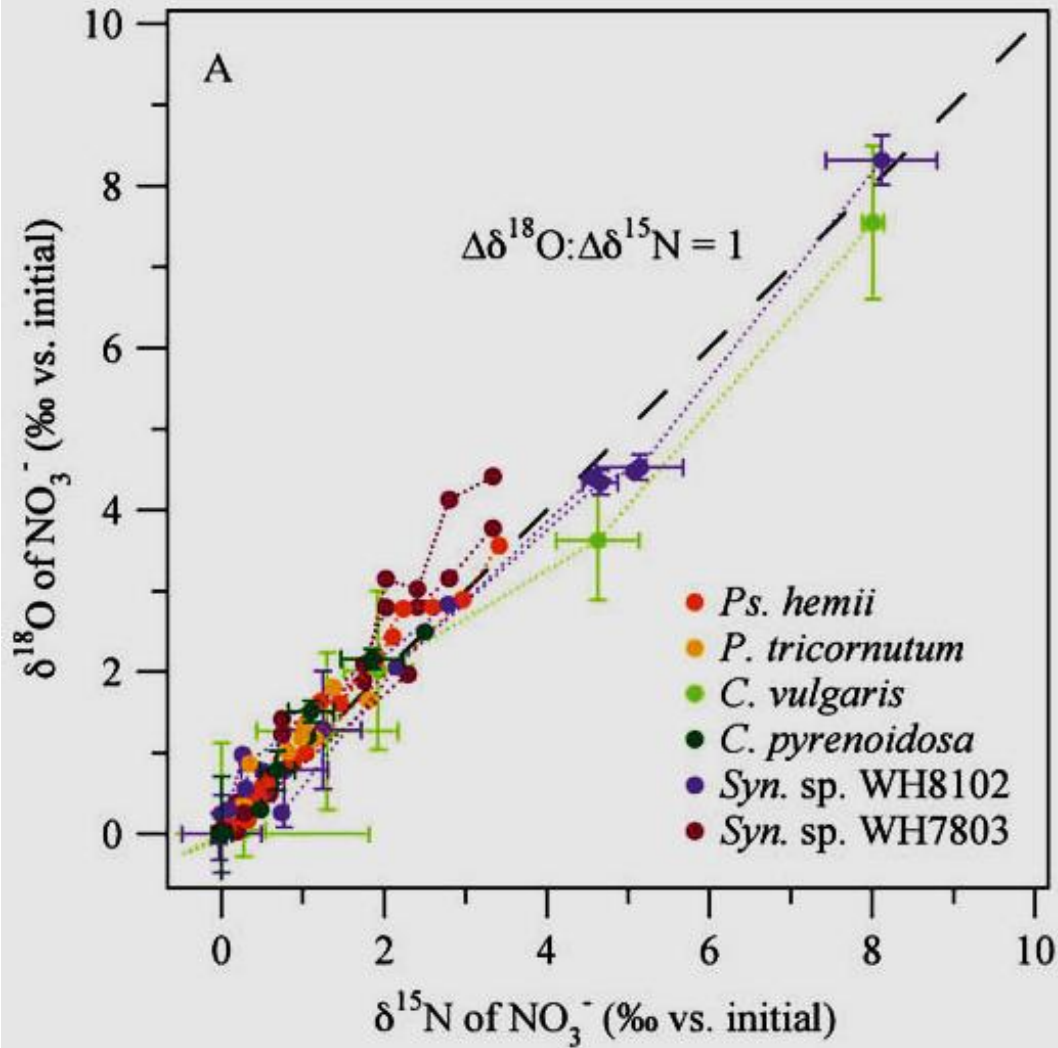
Examples of polyatomic molecules or ions: H_2O, CO_2, SO_2, CH_4, N_2O, SiO_2, CO_3^{2-}, SO_4^{2-}, NO_3^-, ClO_4^-, PO_4^{3-}, ...

A classical example: Meteoric Water Line (MWL)
Observation: $\delta D \approx 8\delta^{18}O + 10$

Amazon
$\delta^2H = 8.1\delta^{18}O + 11$
$R^2 = 0.97$

Darling
$\delta^2H = 5.5\delta^{18}O - 12$
$R^2 = 0.91$

Rio Grande
$\delta^2H = 5.1\delta^{18}O - 28$
$R^2 = 0.99$

MWL

Precipitation Variability

Evaporation

MWL

δ^2H

$\delta^{18}O$

http://web.sahra.arizona.edu/programs/isotopes/oxygen.html

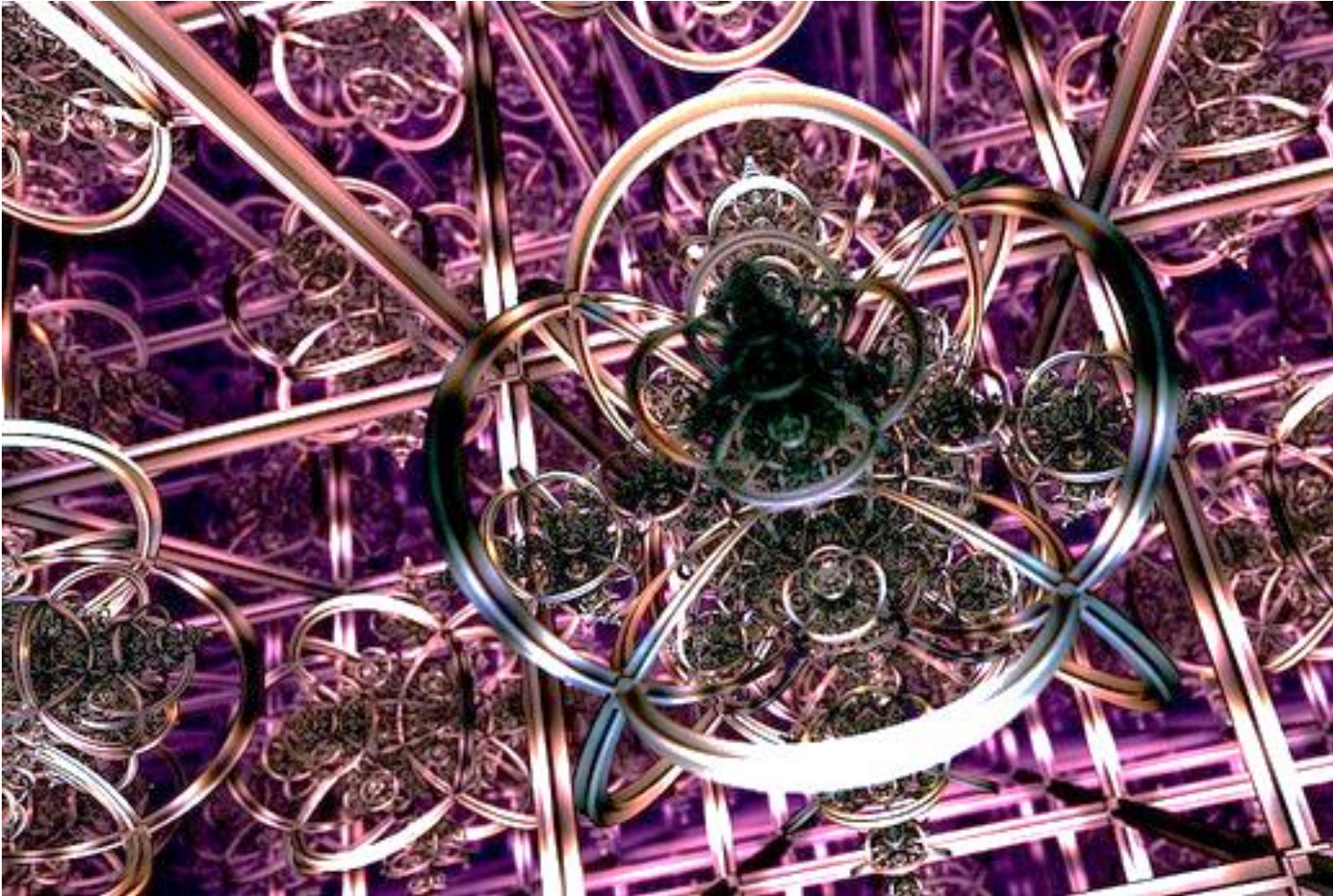# Nitrate isotope fractionation by prokaryotic plankton

Granger et al., 2010
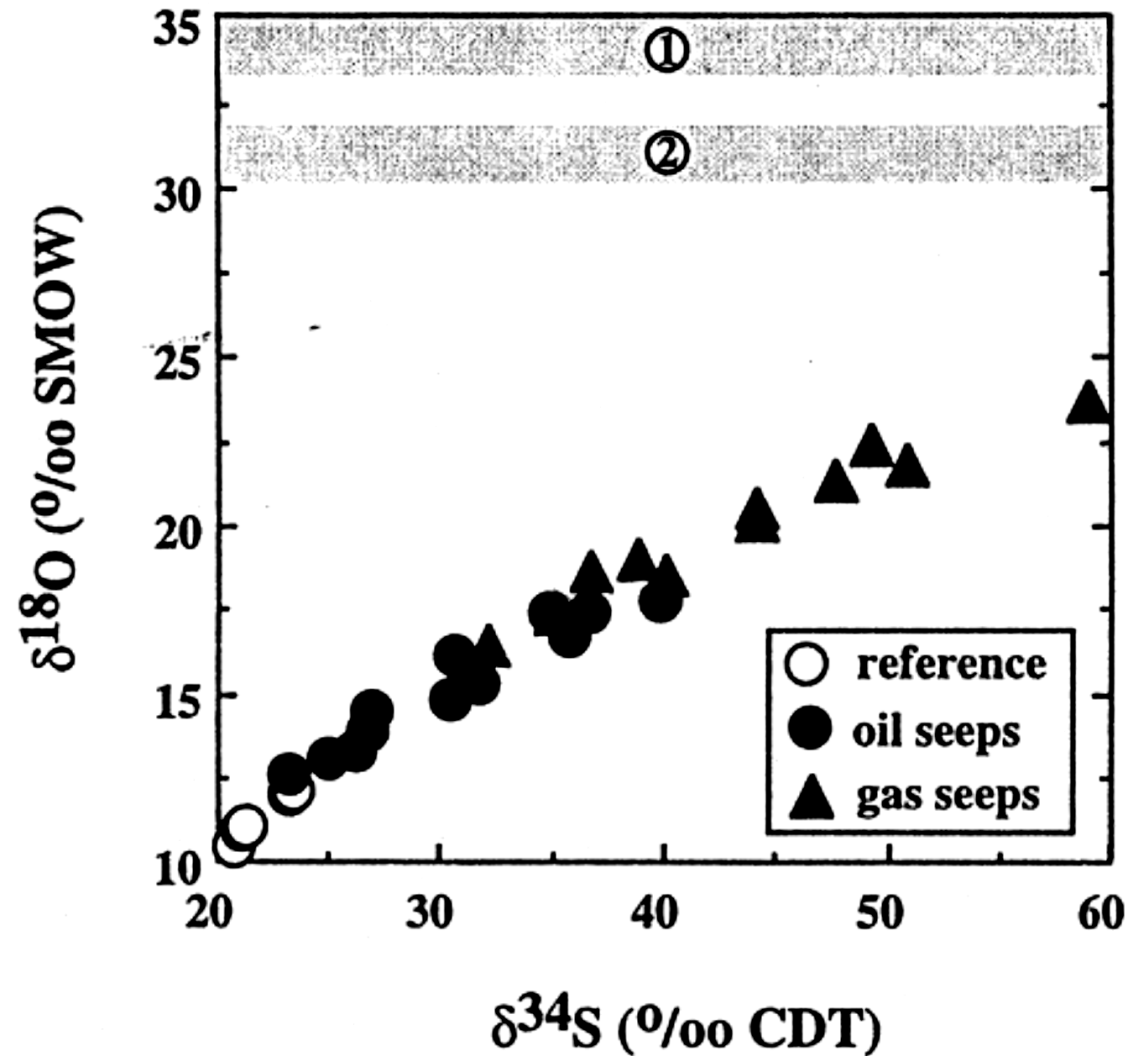
Aharon and Fu, 2003

Fig. 10. $\delta^{18}O$ vs $\delta^{34}S$ sulfate data in pore fluids from reference sediment (empty circle), oil seeps (solid circles), and gas seeps (solid triangles) display a positive relation suggesting that kinetic isotope

Looking into higher dimensions

The third eye:
Perception beyond ordinary sight

稳定同位素的δ概念

We are looking at a very small difference, i.e. a normalized ratio or a ratio of two ratios.

$$\delta = (R/R_{ref}) - 1$$

$$\delta' = \ln (R/R_{ref})$$

相对于化学反应的<u>浓度</u>等参数来说， δ已经是个高维度的概念了。

高维同位素的intrinsic关系

$\theta = \ln^{17}\alpha / \ln^{18}\alpha, \quad = \ln^{33}\alpha / \ln^{34}\alpha$

一种化合物或一个确定的过程的一个同位素系统的内在性质。

$Z = \ln^{18}\alpha / \ln^{30}\alpha, \quad = \ln^{18}\alpha / \ln^{34}\alpha$

一种化合物或一个确定的过程的两个不同同位素系统的内在性质。 $SO_4^{2-}, NO_3^{-}, SiO_2, \ldots$

The confines of triple oxygen isotope exponents in elemental and complex mass-dependent processes

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Abstract

Small differences in triple isotope relationships, or $\Delta^{17}O$ in the case of oxygen, have been increasingly used to study a range of problems including hydrological cycles, stratosphere-troposphere exchange, biogeochemical pathways and fluxes, and the Moon's origin in the geochemical and cosmochemical communities. A $\Delta^{17}O$ value depends on the triple isotope exponent θ of involved reaction steps. However, the probabilistic distribution of the intrinsic and apparent θ values has not been examined for elemental processes and for processes that are out of equilibrium or bearing reservoir-transport complexities. A lack of knowledge on the confines of θ may hamper our understanding of the subtle differences among mass-dependent processes and may result in mischaracterization of a set of mass-dependent processes as being in violation of mass-dependent rules. Here we advocate a reductionist approach and explore θ confines starting from kinetic isotope effects (*KIEs*) within the framework

Triple Oxygen Isotopes: Fundamental Relationships and Applications

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Keywords

oxygen-17, laboratory calibration, air oxygen, seawater, silicates, nonequilibrium

Abstract

The statistical mechanical basis of the triple isotope fractionation relationship

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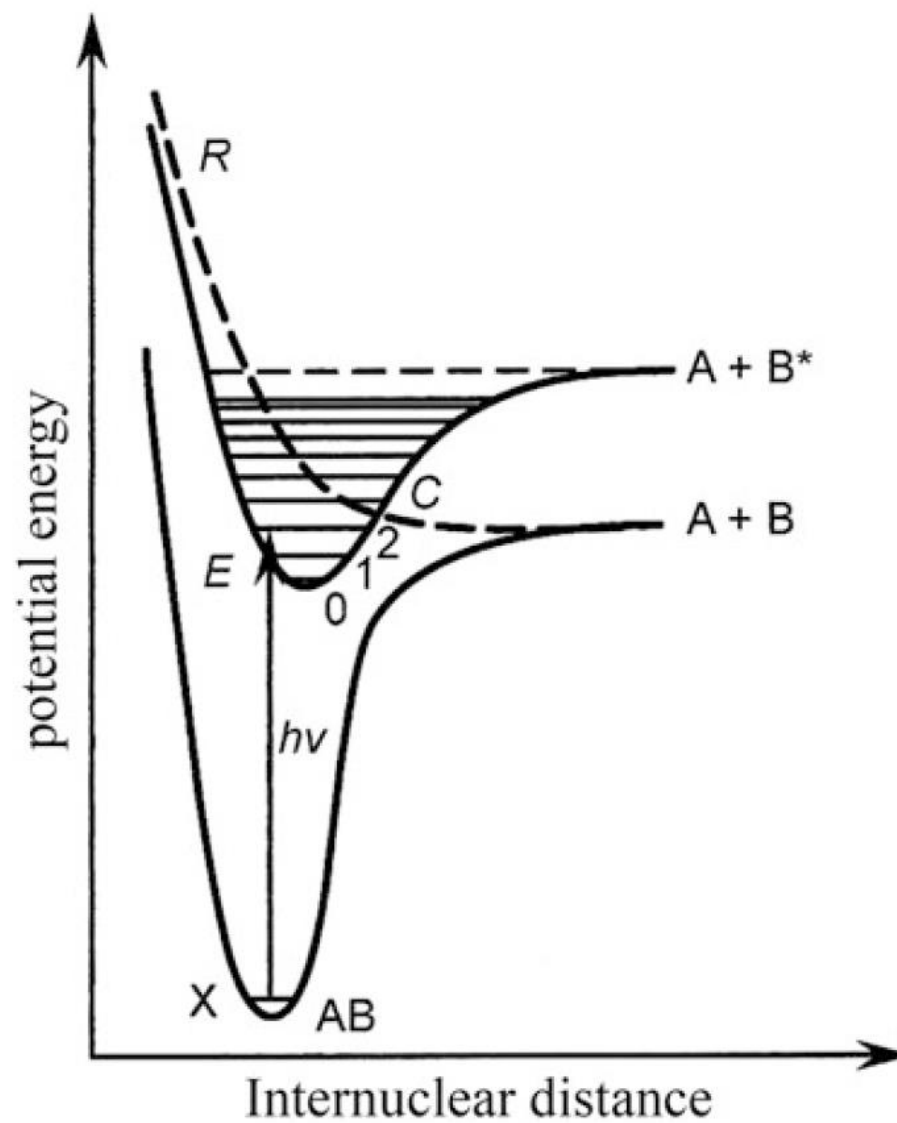## Abstract

Multiple stable isotope relationships have found a growing variety of uses in geochemistry and cosmochemistry. Approximations to the statistical-mechanical models for predicting isotope effects have led to the notion that mass fractionation laws are constrained to a "canonical" range of possible values. Despite previous work indicating that these mass frac-

Fig. 2.2 Potential energy curves for a diatomic molecule showing excitation to a bound electronic state that crosses with a repulsive state

Akimoto, 2016

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