Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Modelling nitric acid uptake by mineral dust using parameterizations of different complexity

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EGU General Assembly 2022
11622

May 24th 2022

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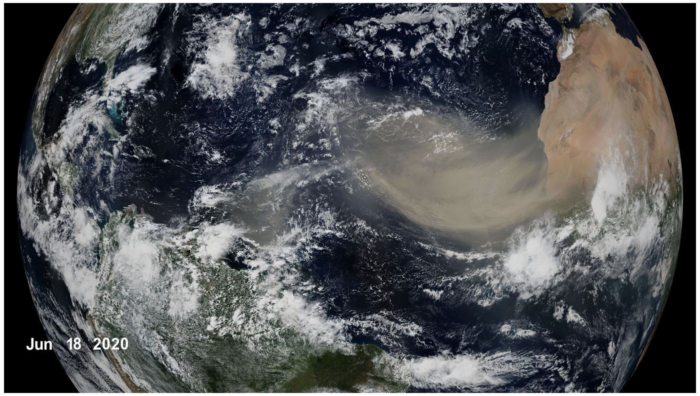


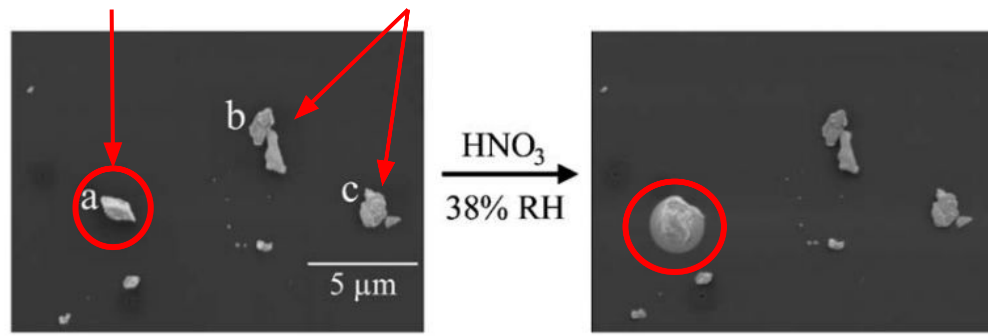
Source: NASA's Goddard Space Flight Center (December 2021)

Source: oizom.com (May 2022)

Airborne dust heterogeneous chemical reactions

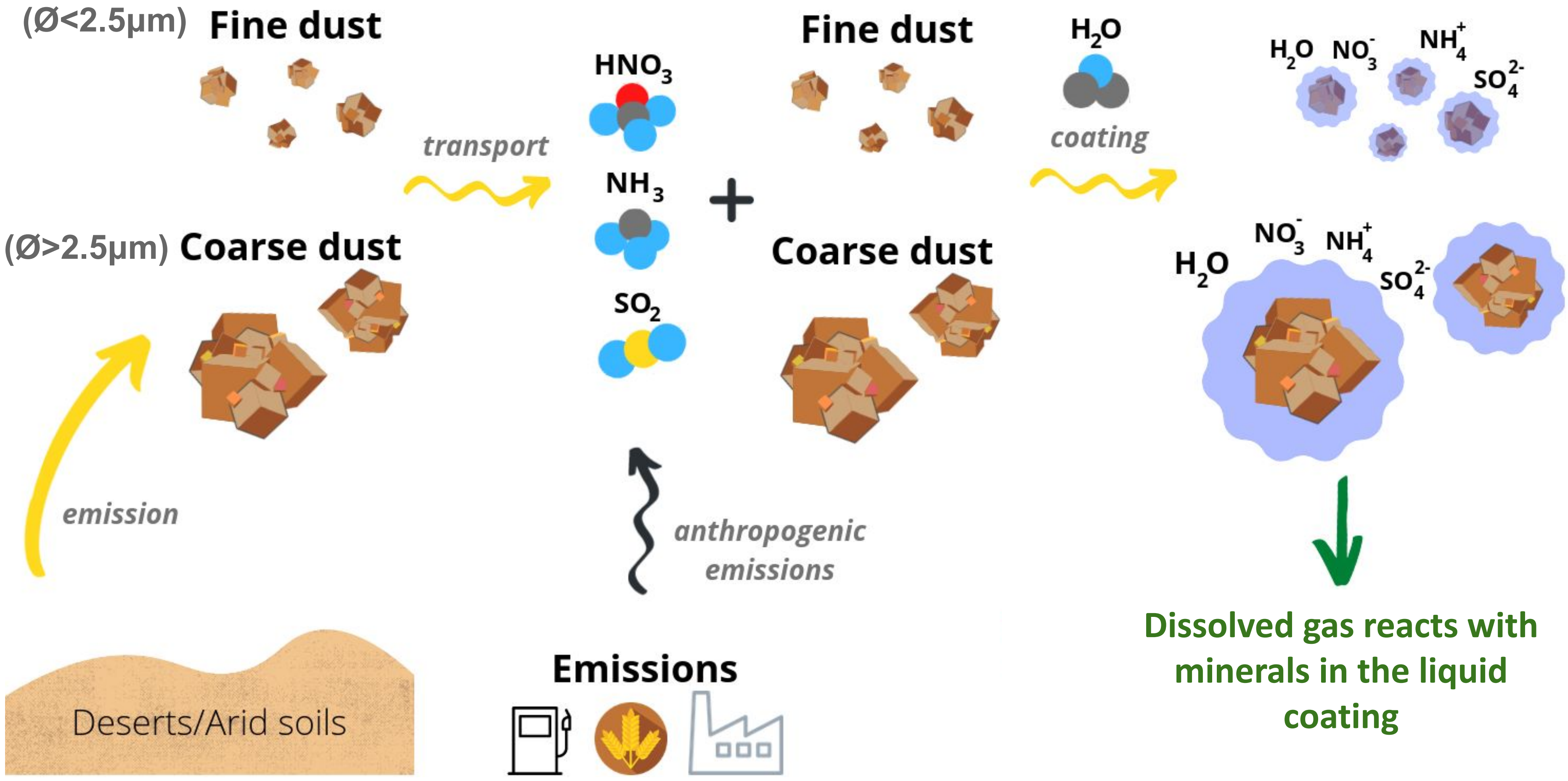
dependent on mineralogy

$CaMg(CO_3)_2$ (Dolomite) AlSi



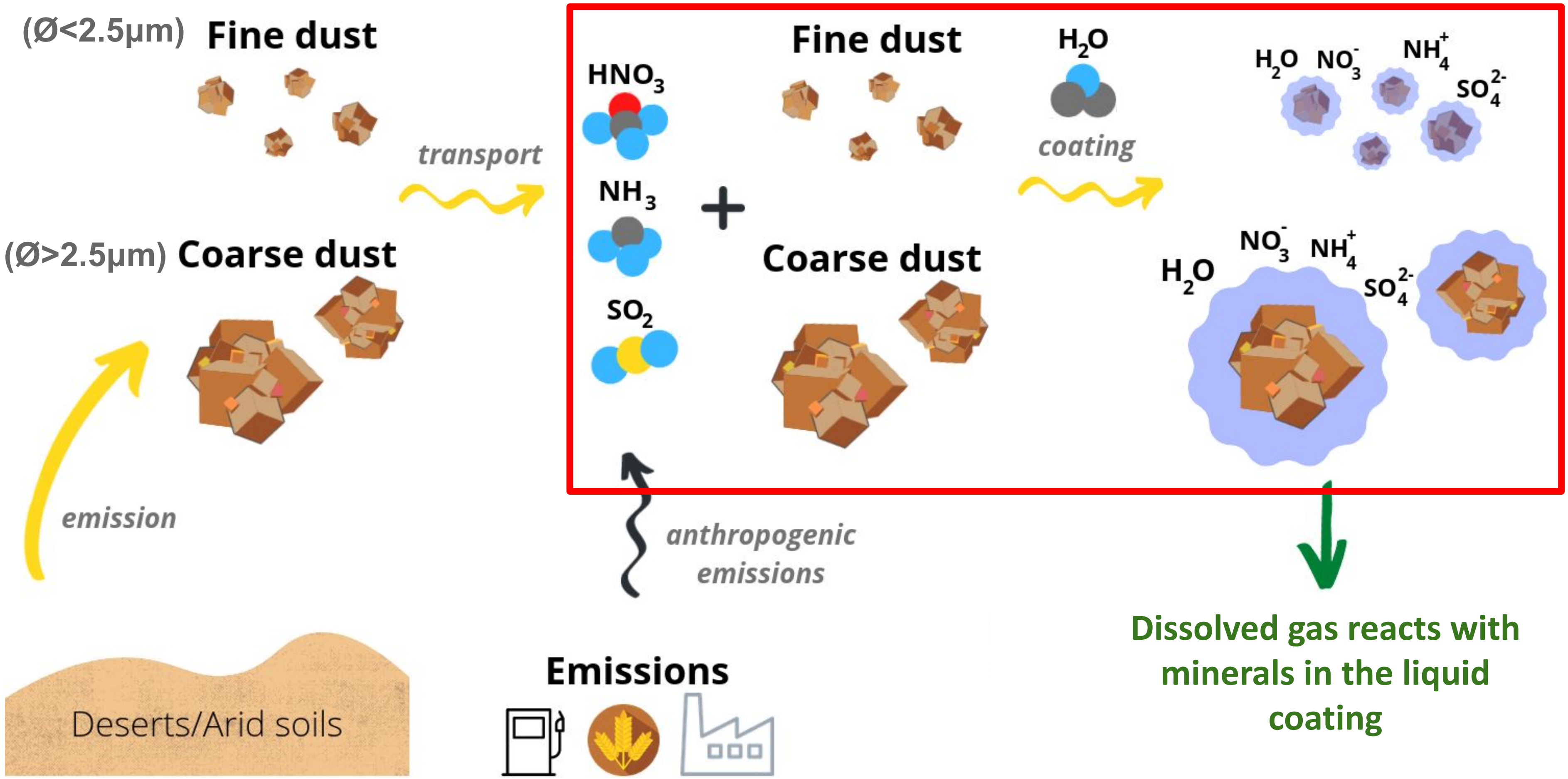
Source: Krueger et al., 2004

(1/4) Introduction: Dust heterogeneous chemistry



(1/4) Introduction: Dust heterogeneous chemistry

How to simulate this?



(2/4) Implementation in MONARCH model

MONARCH
Atmospheric chemistry model
Multiscale Online Non-hydrostatic AtmospheRe CHemistry

① FINE DUST (Ø<2.5µm)

1. Thermodynamic equilibrium with:

1.1. **EQSAM v.03d** *(Metzger et al., 2002)*

2.1. **ISORROPIA II** *(Funtoukis and Nenes, 2007)*

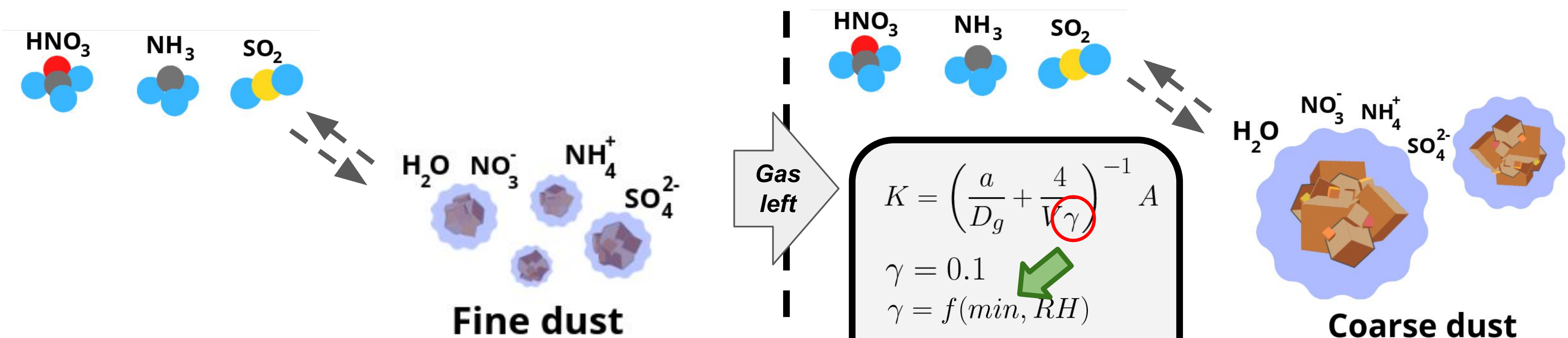
② COARSE DUST (Ø>2.5µm)

2.1. Irreversible uptake reaction with uptake coefficients = **0.1** or **f(min,RH)**

(Hauglustaine et al., 2014)

2.2. Thermodynamic equilibrium (kinetically limited) with ISORROPIA II

(Pringle et al., 2010)



$$K = \left(\frac{a}{D_g} + \frac{4}{V\gamma}\right)^{-1} A$$

$$\gamma = 0.1$$

$$\gamma = f(min, RH)$$

Vlasenko et al. (2006)

(3/4) Evaluation: Dust event - Wang et al. (2017)

Significant impacts of heterogeneous reactions on the chemical composition and mixing state of dust particles: A case study during dust events over northern China

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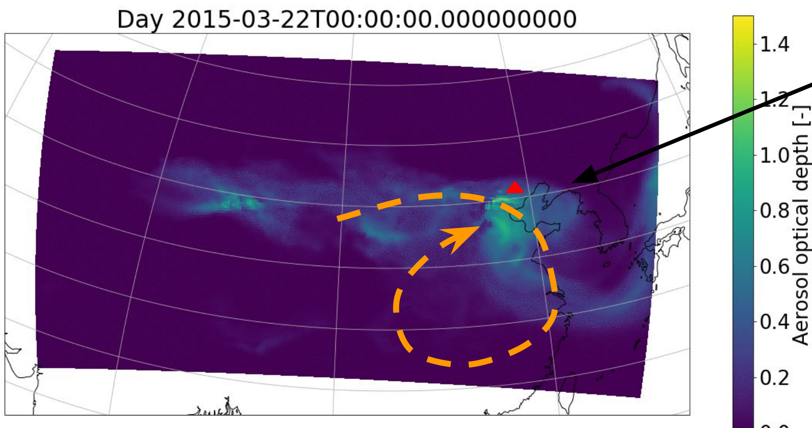
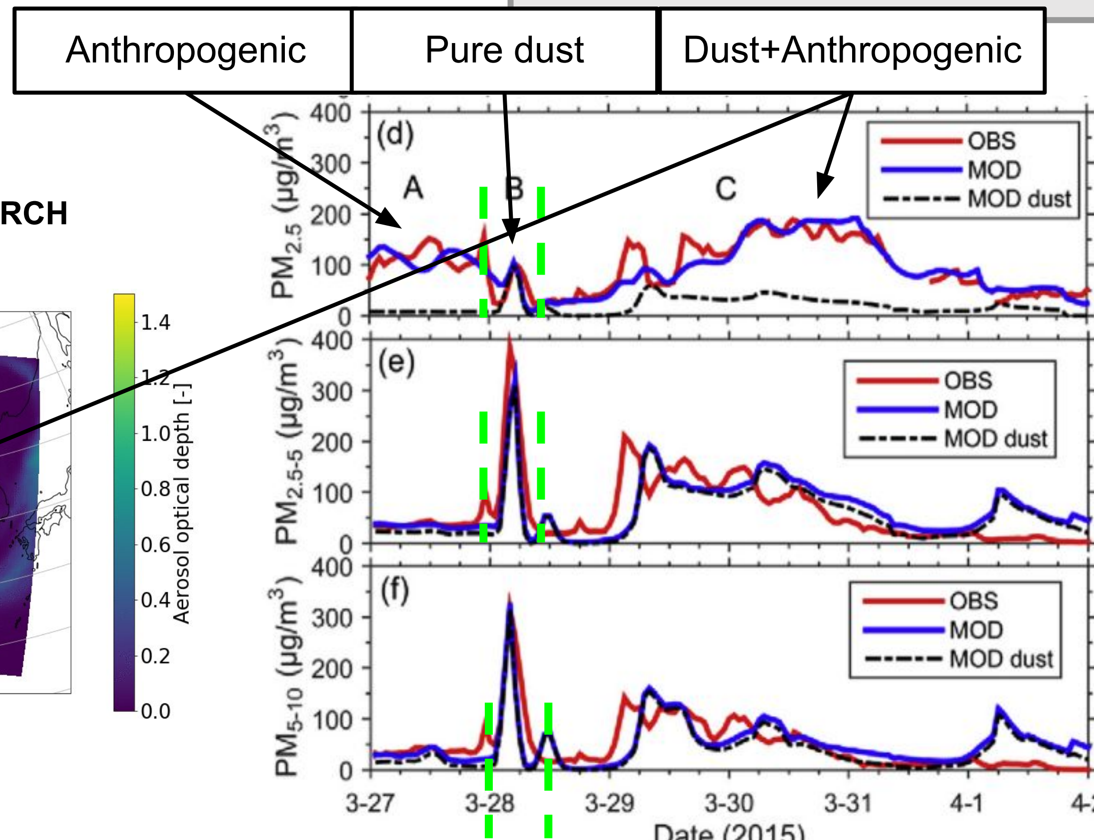
- Period: **March-April 2015**
- Obs.: **Beijing Institute of Atmospheric Physics**
- Model: **NAQPMS**
- Emissions: **MIX inventory**

Dust AOD (550nm) from MONARCH

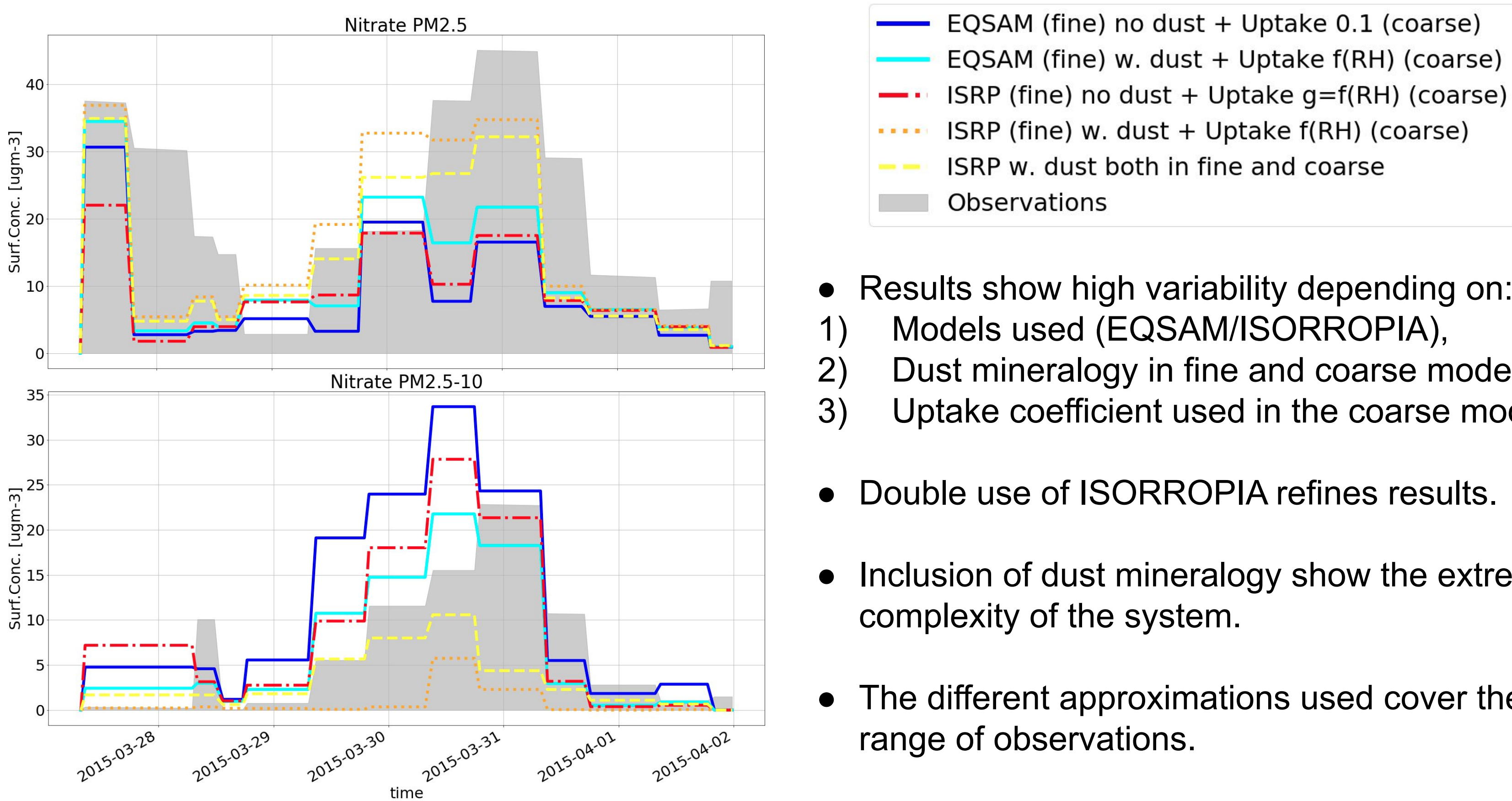




(4/4) Results and conclusions

Evaluation with **Wang et al. (2017):**

- **Dust + anthropogenic** species event over Beijing in March-April 2015.
- Average dust mineralogy: **7.7% Ca^{2+}**, **2.1% K^{+}** and **1.7% Mg^{2+}**



- Results show high variability depending on:
1) Models used (EQSAM/ISORROPIA),
2) Dust mineralogy in fine and coarse modes,
3) Uptake coefficient used in the coarse mode.

- Double use of ISORROPIA refines results.

- Inclusion of dust mineralogy show the extreme complexity of the system.

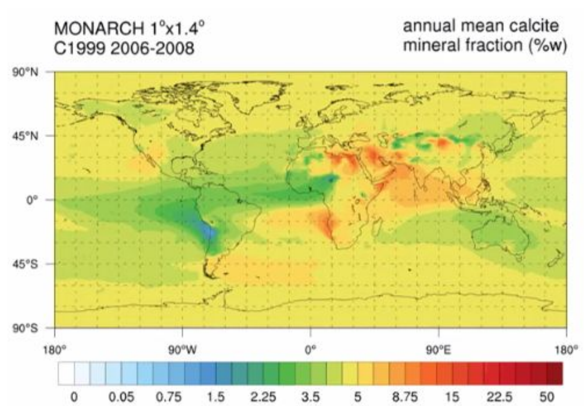
- The different approximations used cover the range of observations.

Next steps

Perform **global-scale simulations**…

Configurations and **parameterizations**

Calcite surface concentration (%)



Dust mineralogical inventories

… to understand better
✅ **the effect of dust mineralogy on dust heterogeneous chemistry**

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Thank you for your attention

This project is part of the ERC Grant:

FRAGMENT

FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe (Working package 3)

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