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WACCM development at Leeds University

Wuhu Feng[1,2,3]

(w.feng@leeds.ac.uk)

Acknowledgments:

John Plane[1], Martyn Chipperfield[2], Daniel Marsh[3],Chuck Bardeen[3], Doug Kinnison[3], Roland Garcia[3], Anne Smith[3], Michael Mills[3], Francis Vitt[3], Diego Janches[4], Erin Dawkins[4], David Nesvorny[5], Pekka Verronen[6], Chet Gardner[7], Josef Hoffner[8], Timo Viehl[8], David Newman[9] , Tamas Kovacs[1], James Brooke[1], Sandip Dhomse[2], Steven Pickering[2], Ryan Neely[2], Anja Schmidt[2] **….**

School of Chemistry
FACULTY OF MATHEMATICS and PHYSICAL SCIENCES
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National Centre for Atmospheric Science
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CESM Activities at Leeds

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CESM development at different HPCx:

1) UK world-class national supercomputer www.archer.ac.uk

2) UK eight Universities (Northern region) HPC: n8hpc.org.uk

3) Leeds University Advanced Research Computing; arc1, arc2, (arc3 in 2016)

Main research activities:

Two Schools (Chemistry, Earth and Environment), NCAS:

1)Metals, MSP, interactions and deposition: *Plane, Chipperfield, Feng (2010-*

2)Ozone and vegetation interaction: *Arnold and Pickering (2012?-*

3)Ice sheet during last deglaciation: Gregoria (2013?-

4)Volcanic eruption: *Schmidt and Neely* (2015-

Model strategy: WACCM is one key tool

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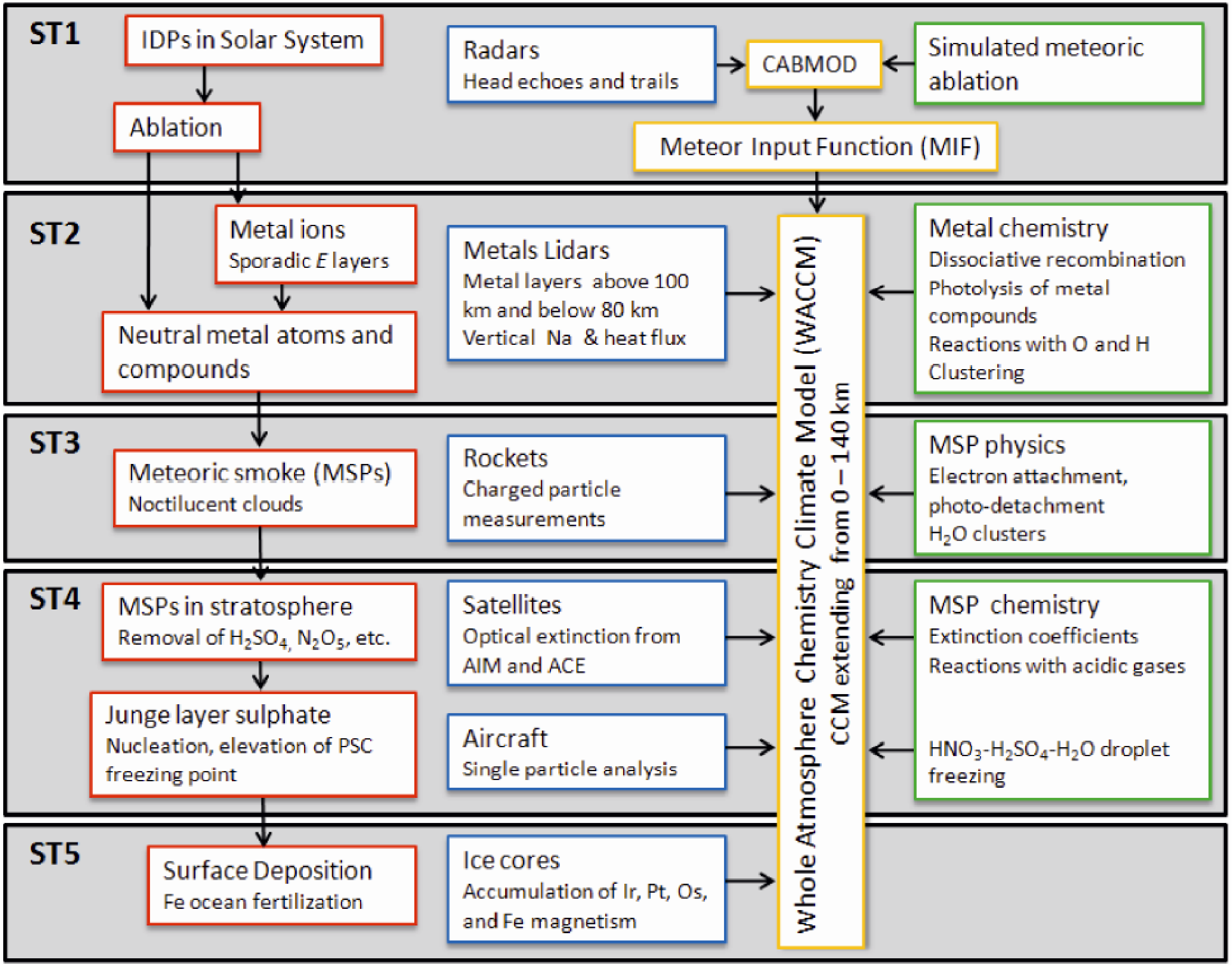

VolcanEESM & Improving the Representation of Stratospheric Aerosol in CESM

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Collaboration between WACCM group, Leeds School of Earth Environment, MIT & PNNL

- Background: Recent efforts have led to interactive representation of stratospheric aerosol in WACCM5 by extending the Model Aerosol Model into the stratosphere. (Mills et al. 2016)

- The new model capability necessitates **a new 4D SO2 forcing** file **to represent** the emissions of **volcanic eruptions from 1850 to present**.

Schmidt and Neely led development of the new VolcanEESM database (Volcanic *ic* ***E****missions of* SO_2 *for* ***E****arth* ***S****ystem* ***M****odels****)***

Hosted at the UK's Centre for Environmental Data Analysis

For more information and to download the new database please see: http://doi.org/10/f3kxt5 or contact Neely & Schmidt

Our research studies using WACCM

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1) Multi-scale Modelling of Mesospheric Metals (4M): (2010-2013)
John Plane, Martyn Chipperfield, Wuhu Feng, Erin Dawkins
Have added 6 metal chemistry (extra ~200 reactions) into WACCM

2) Cosmic Dust in the Terrestrial Atmosphere (CODITA): (2012-2017)
John Plane, Martyn Chipperfield, Wuhu Feng, James Brooks
Self-consistent 3D global model of MSP from metal chemistry

3) Atmospheric impact of close cometary encounter: (2015-2018)
John Plane, Wuhu Feng, Martyn Chipperfield, Piers Forster, Natasha Aylett
Effects of a Halley comet (siding spring):radiative balance+chemistry

4) Middle Atmosphere Processes&Lifetime Evaluations (MAPLE): (2012-2014)
Martyn Chipperfield, John Plane, Tamas Kovacs, Wuhu Feng, Sandip Dhomse
New estimation of lifetime of long-lived species (SF6, CFC115, NF3)

5) NOx/HOx production & impacts on stratospheric O_3 (NOHO): (2013-2016)
John Plane, Wuhu Feng, Tamas Kovacs, Martyn Chipperfield
Incorporated FMI D-region chemistry and Mechanism reduction

6) Modelling Studies of metal layer in the thermosphere: (2016?--)
John Plane, Wuhu Feng, 1 PhD student
Adding metal chemistry into WACCM-X

Selected WACCM publications: www.env.leeds.ac.uk/~earfw

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1. Marsh et al., *JGR*, 2013: First WACCM-Na model
2. Feng et al., *JGR*, 2013: WACCM-Fe(differential ablation, Sensitivity MIF, PMC, gravity waves..)
3. Plane et al. *GRL*, 2014: WACCM-K(50 years puzzle on different behaviours for Na and K).
4. Dawkins et al., *GRL*, 2014. WACCM-K (first satellite retrieval of K) .
5. Gardner et al., *JGR*, 2014: WACCM-Na (inferring cosmic dust influx into atmosphere)
6. Totterdill et al. *JPC*, 2014: WACCM-Na and WACCM-K (metals with NF3)
7. Chu et al., *JGR*, 2014: WACCM-Fe (wind shear theory examination)
8. Langowski et al., *ACP*, 2015: WACCM-Mg (SCIMACHY Mg and Mg+ with model results)
9. Huang et al., *GRL*, 2015: WACCM-Na and WACCM-Fe (Vertical fluxes of Fe and Na)
10. Dunker et al., JASTP, 2015: WACCM-Na (Lidar, Model using GEOS5 and MERRA)
11. Frankland et al., *JASTP*, 2015: WACCM/CARMA (Uptake of HNO3 with MSP)
12. Plane et al., *Chem. Rev.*, 2015: WACCM-Na, WACCM-Fe, WACCM-Mg, WACCM-K (Overview)
13. Totterdill et al. *JPC*, 2015: WACCM-Na and WACCM-K (Metals with CFC115 and SF6)
14. Feng et al., *GRL*, 2015: WACCM-K (Diurnal variations)
15. Dawkins et al., *JGR*, 2015: WACCM-K, WACCM-Na (Global data from obs and model)
16. Bones et al., *JPC*, 2015: WACCM-Fe (Dissociative recombination of FeO+ +e)
17. Carrillo-Sanchez et al., *GRL*, 2015: WACCM-metals (MIF required for model to match Obs)
18. Viehl et al., *GRL*, 2016: WACCM-Fe (bottom layer: obs, theory calculation, updated model)

WACCM/CARMA

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0-140 km (detailed chemistry/dynamics)

- GEOS5, MERRA, ECMWF

Community Aerosol and Radiation Model for Atmosphere

- Detailed microphysics, 28 bins (0.2-102 nm)

Metal chemistry for neutral and ions

Marsh et al., *JGR* (2013): WACCM-Na

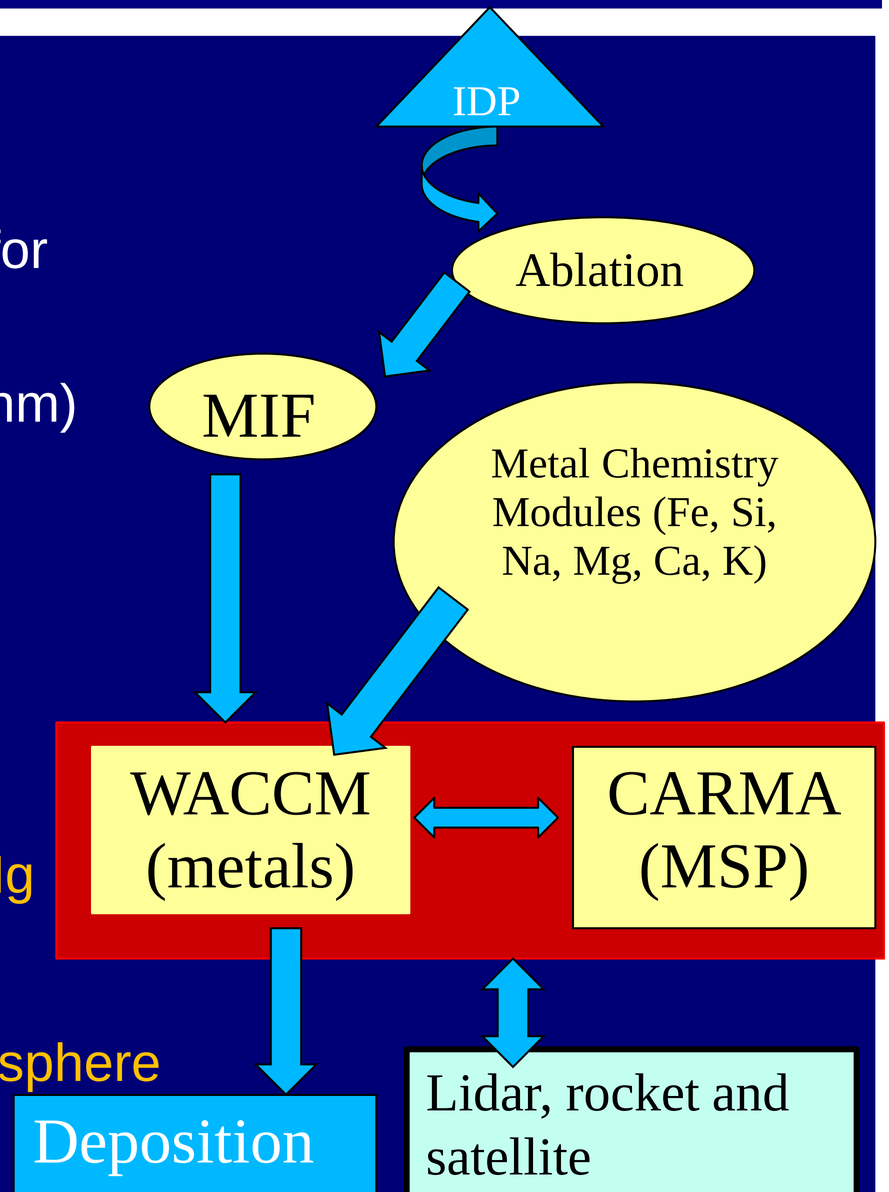
Feng et al. , *JGR* (2013): WACCM-Fe

Plane et al. , *GRL* (2014): WACCM-K

Langowski et al. , *ACP* (2015): WACCM-Mg

Plane et al. (*Submitted*): WACCM-Si

Plane et al., *Chem. Rev.*(2015): The Mesosphere and Metals: Chemistry and Changes



Interplanetary Dust Particle distributions

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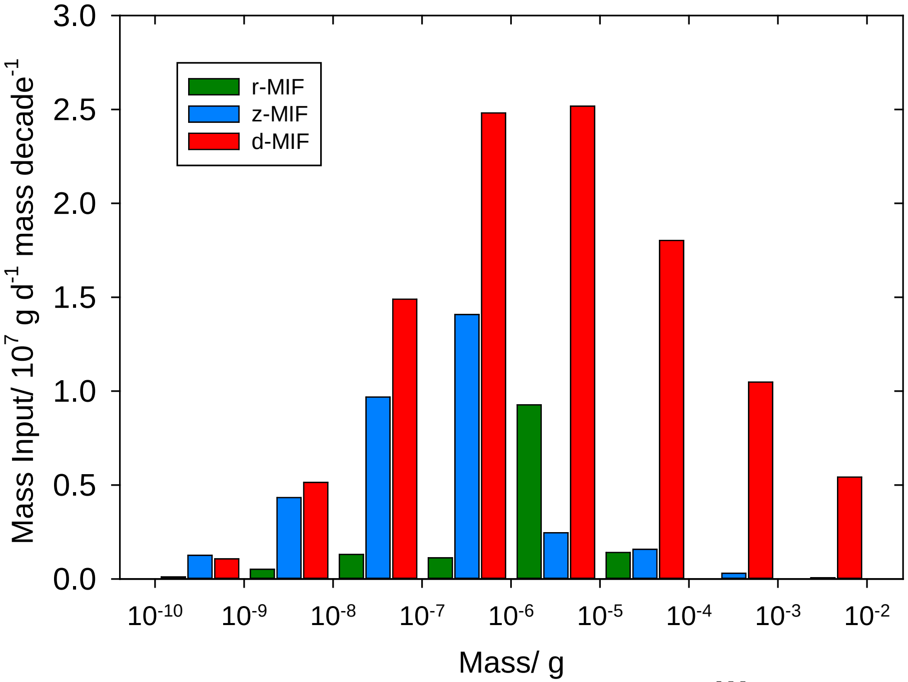
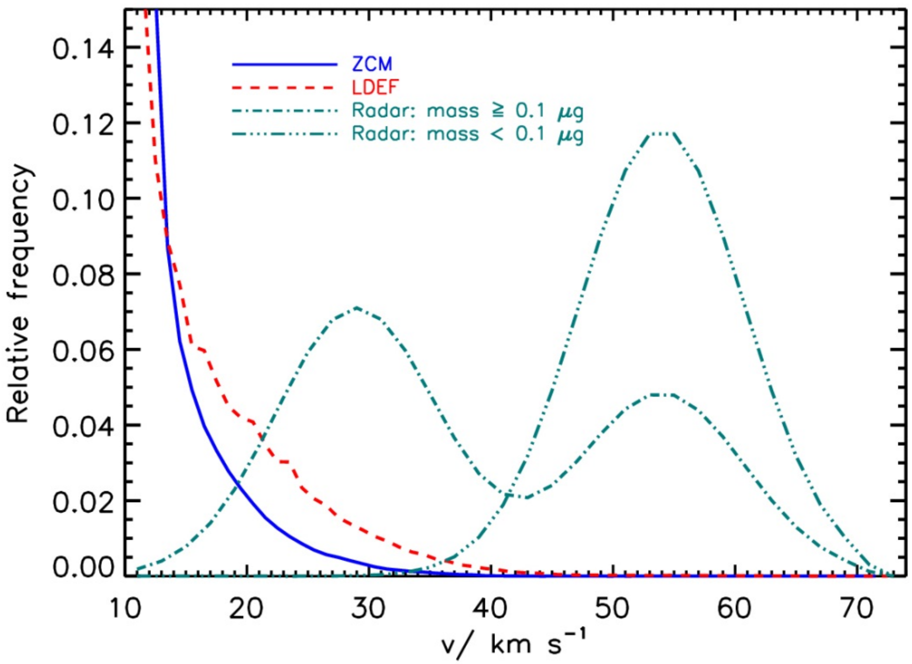


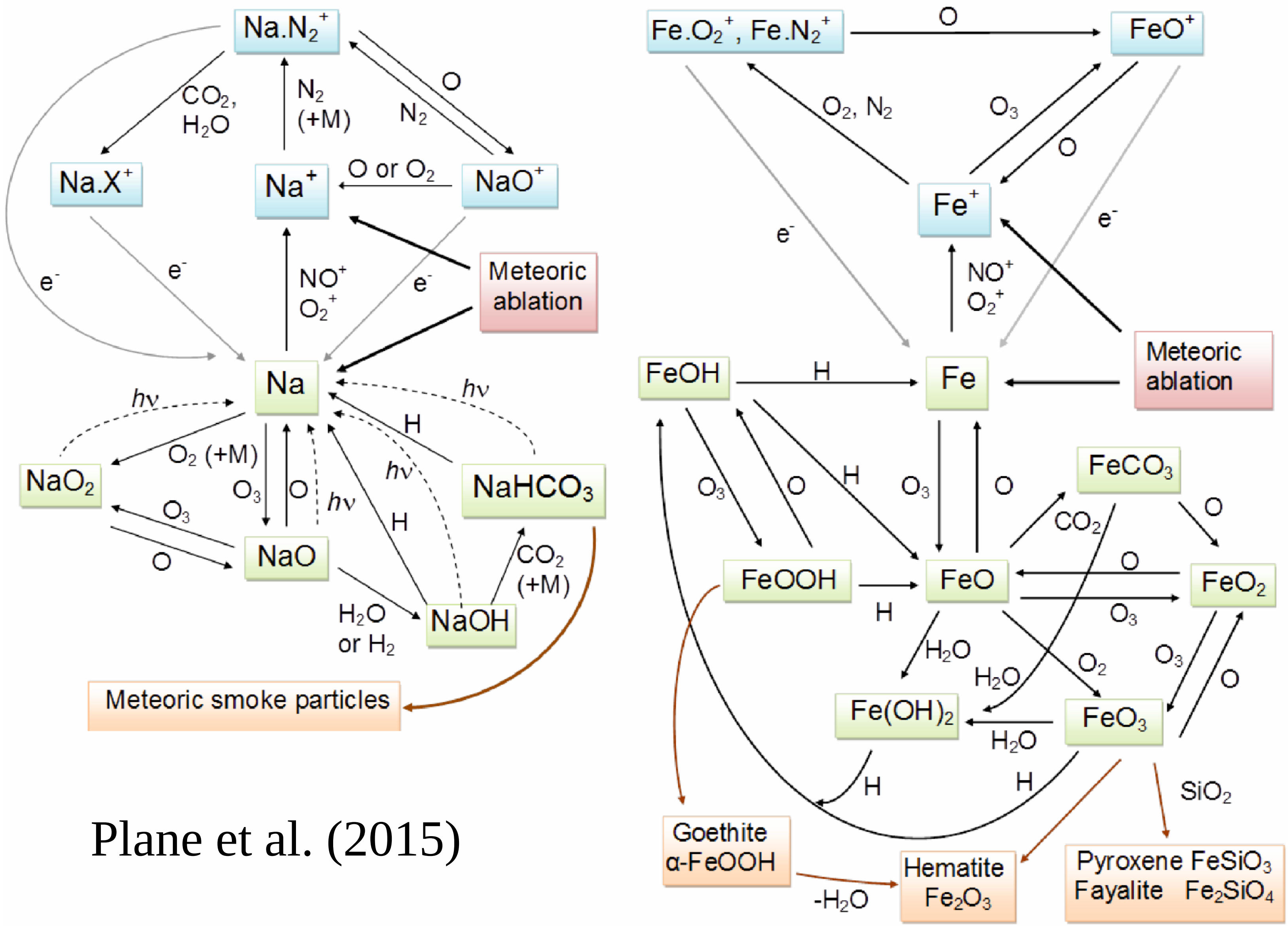


Carrillo-Sanchez et al., *GRL,* (2015)

z-MIF (Nesovrny et al., 2011): infra-red observations of the Zodiacal Dust Cloud
r-MIF (Janches et al., 2014): meteor observations made with high performance/large aperture radars
d-MIF (Love and Brownlee, 1993): Long Duration Exposure Facility (spaceborne dust detector)

- The size and velocity of cosmic dust particles entering the Earth's atmosphere is uncertain
- r-MIF: 14±3 t/day, z-MIF: 34±17 t/day, d-MIF: 110±55 t/day

Example: 2 Most Observed Metal Chemistry



Plane et al. (2015)

Global picture (Na, K, Mg, Mg^+)

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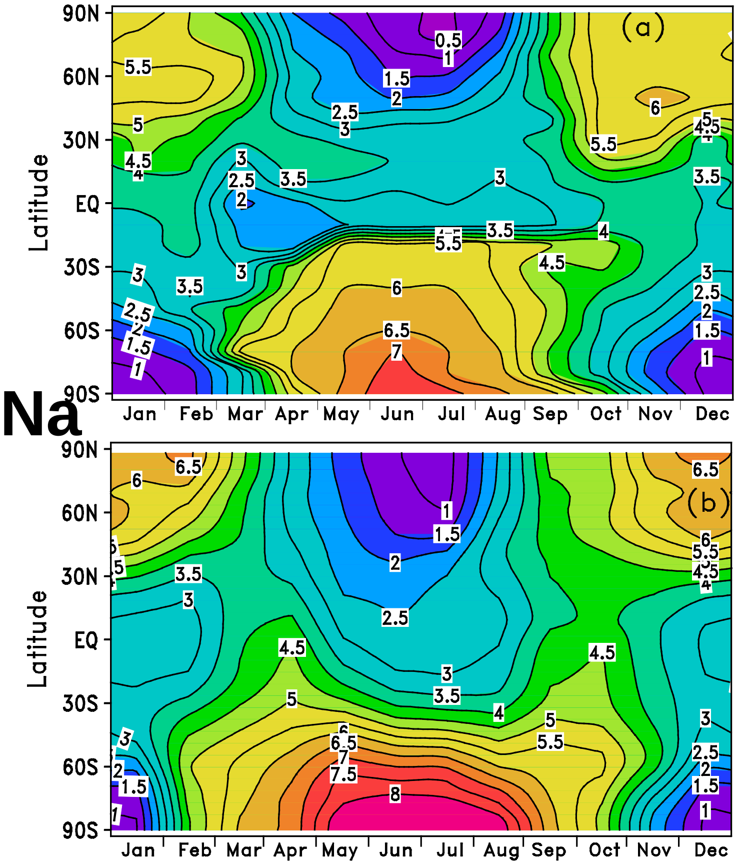
Marsh et al., *JGR*(2013)

Dawkins et al.,*GRL*(2014)

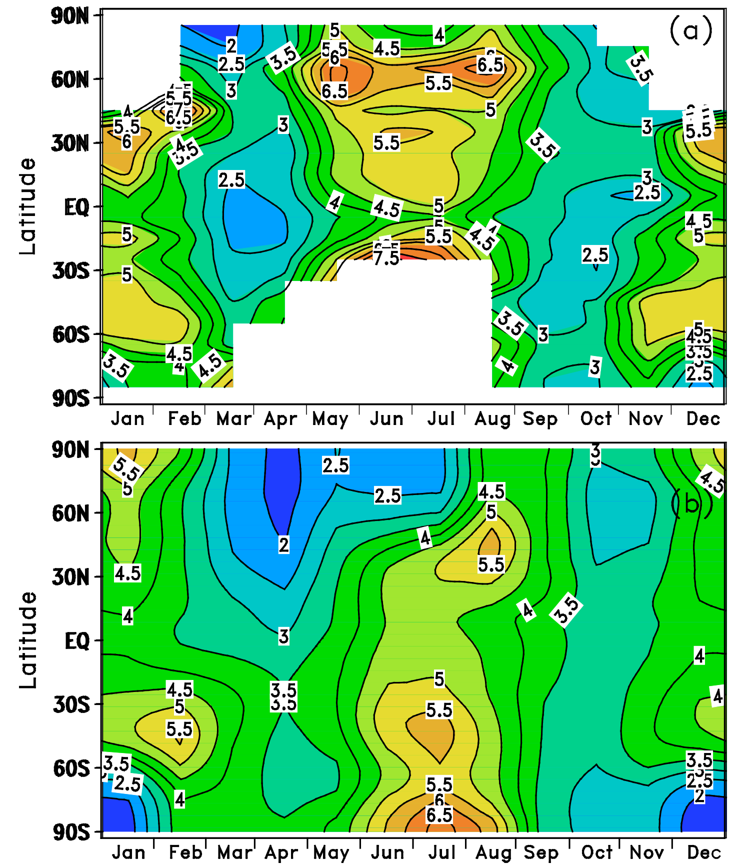
OSIRIS Satellite

Na



Model

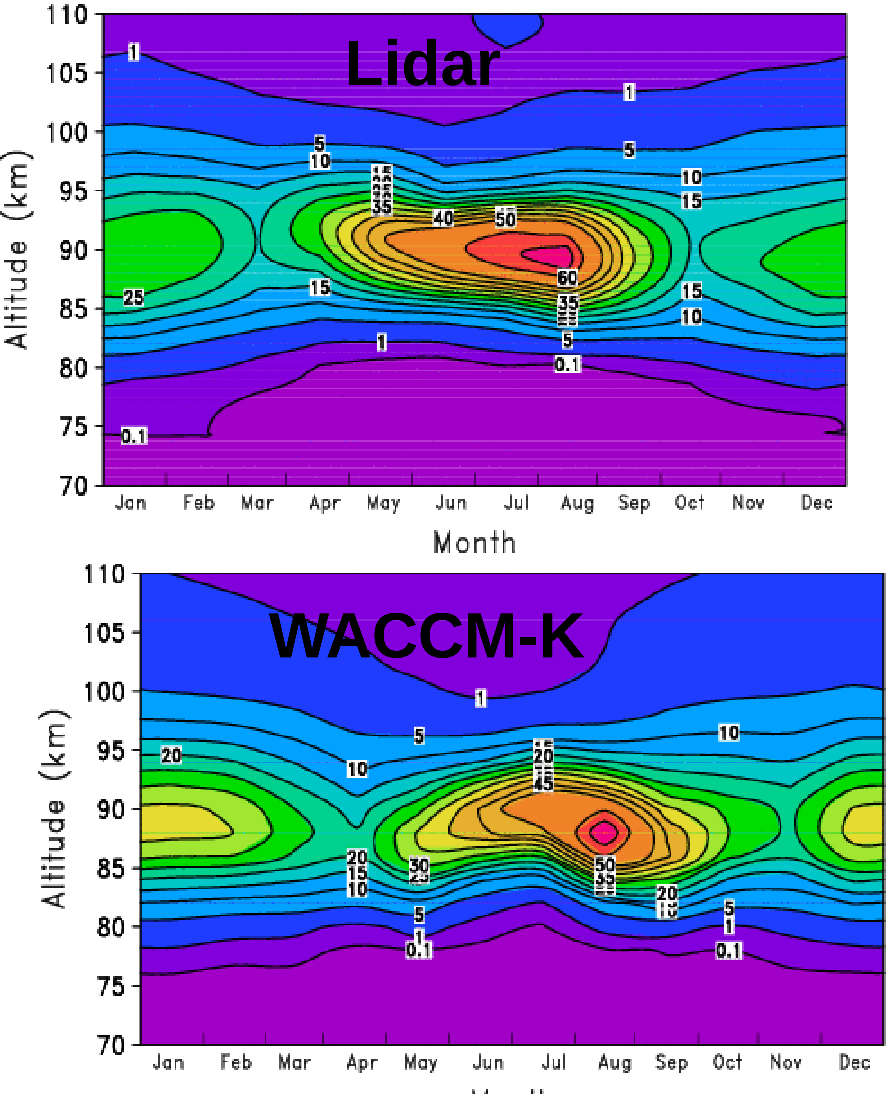
K



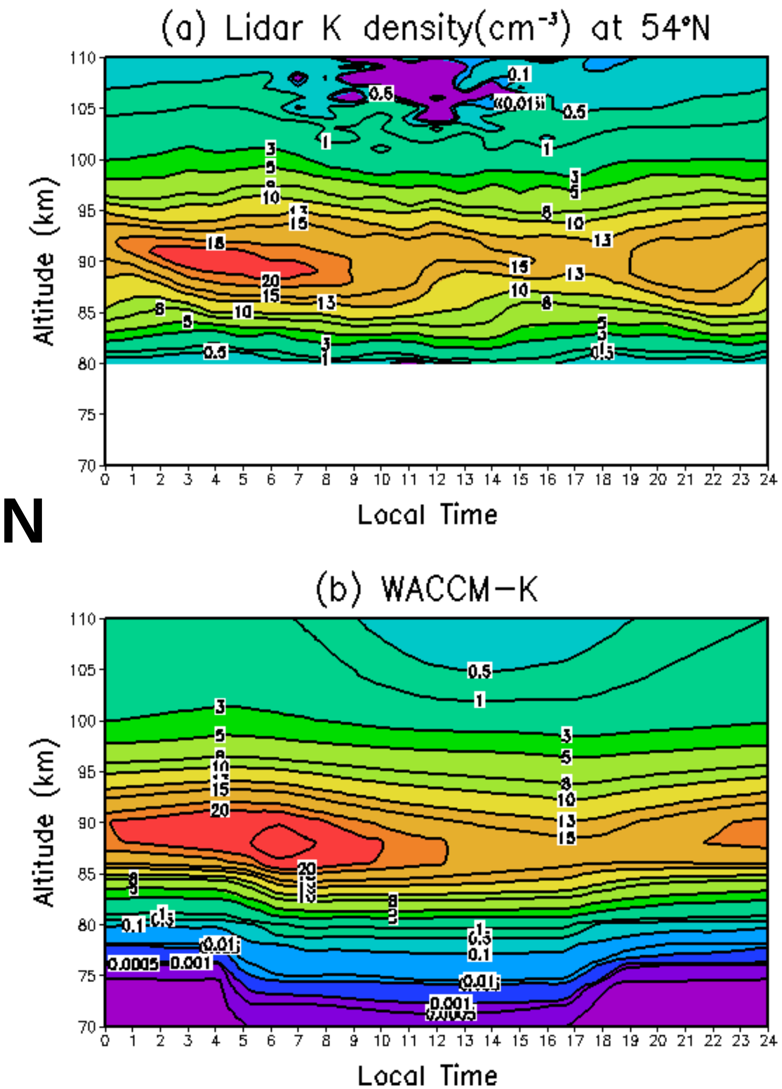
Plane et al., *GRL*(2014)

- First time incorporates Na chemistry into WACCM
- Different seasonal behaviours seen in Na and K
- Fifty years puzzle has been explained by WACCM-K and WACCM-Na

Seasonal, Diurnal variations



54N



Plane et al. *GRL(2014)*

Feng et al. *GRL* (2015)

Sensitivity to improve the bottom layer

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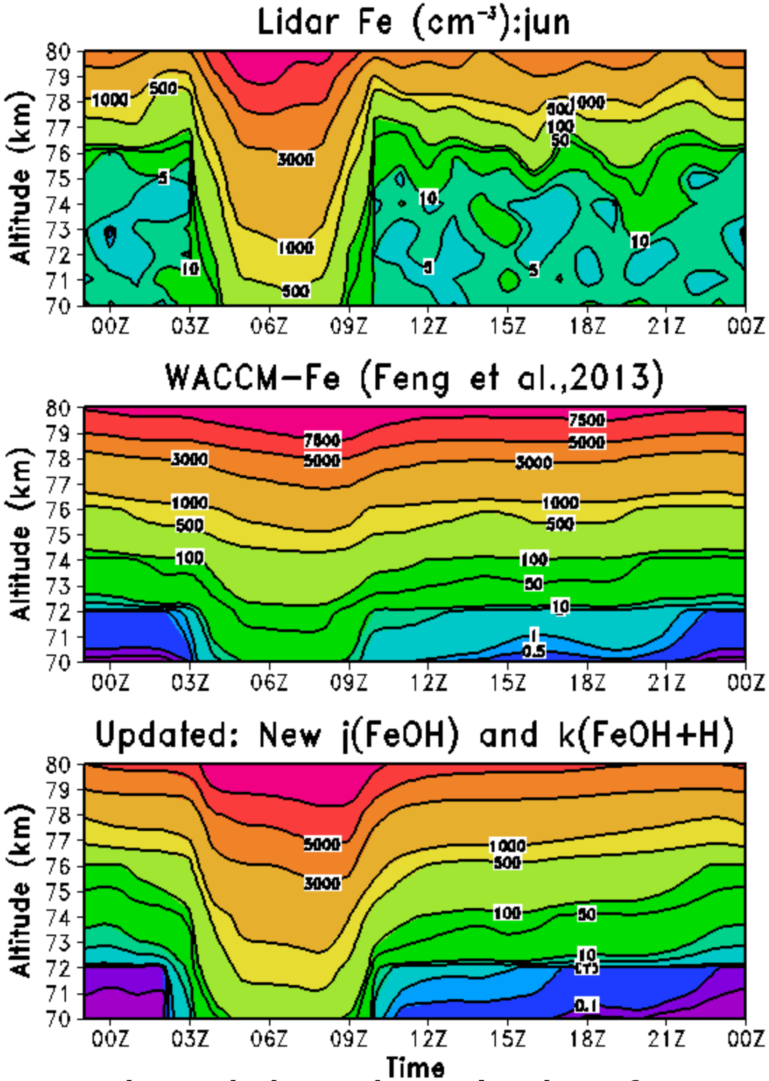

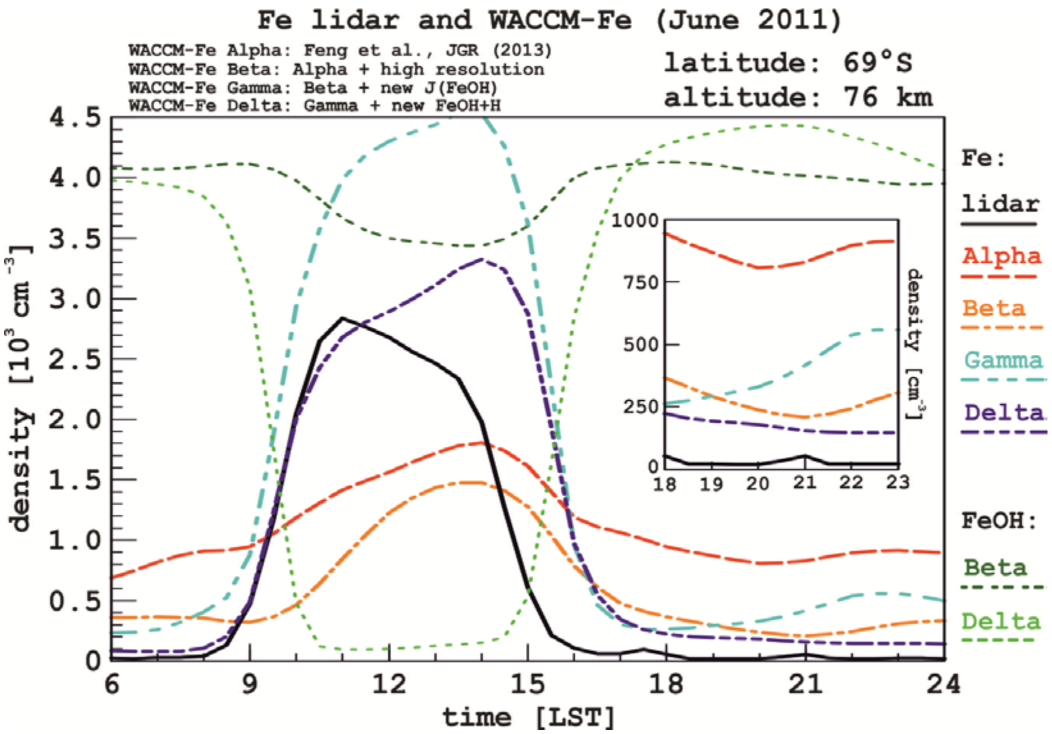

Viehl et al.,*GRL*(2016)

- Updated the photolysis of FeOH and rate coefficients of FeOH+H improves the diurnal variation of bottomside of Fe layer (69S)

SSW impacts on mesospheric metal layers

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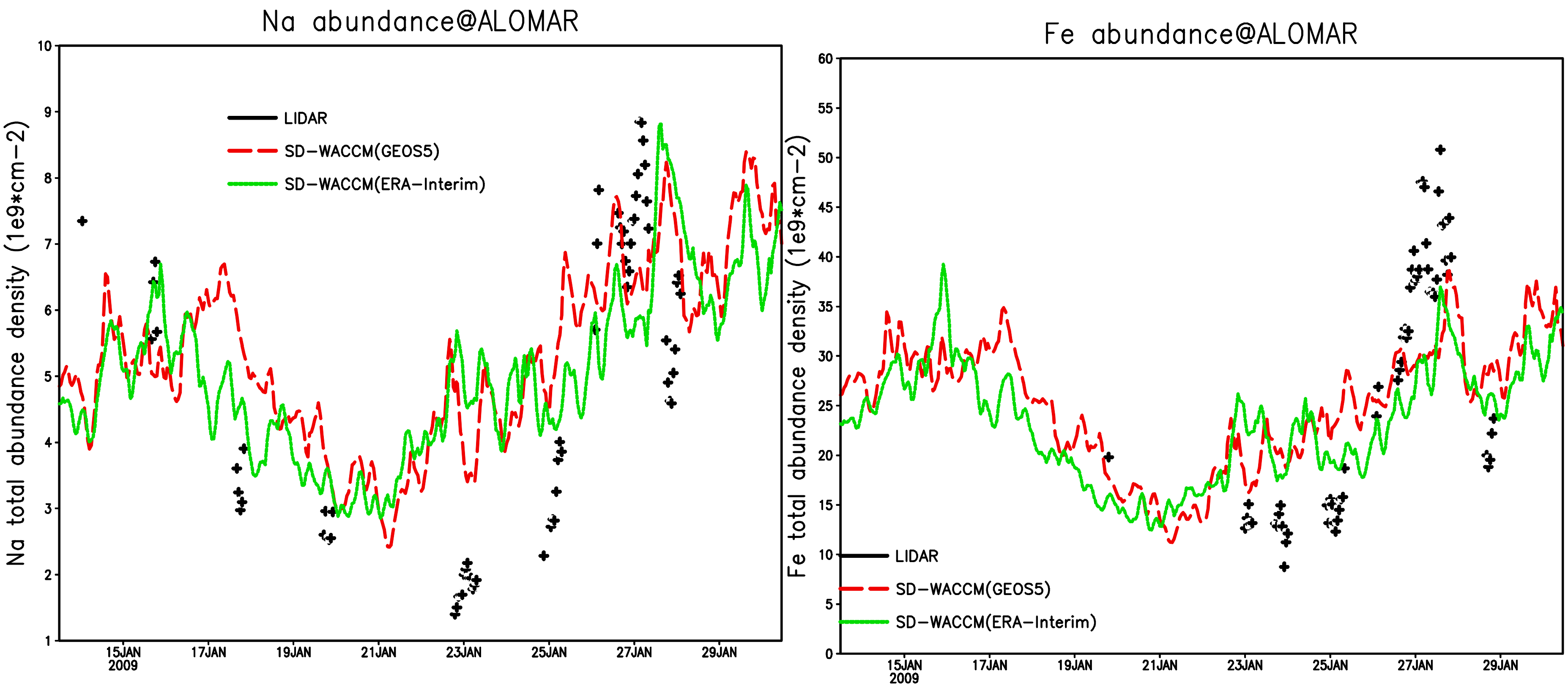

Feng et al.,*JASTP* (to be submitted)

- **Extreme scenario is good test for the model performance**
- **Model using different meteorological analysis does a good job in simulating the SSW impact on mesospheric metal layers**

Long term trend and solar cycle response

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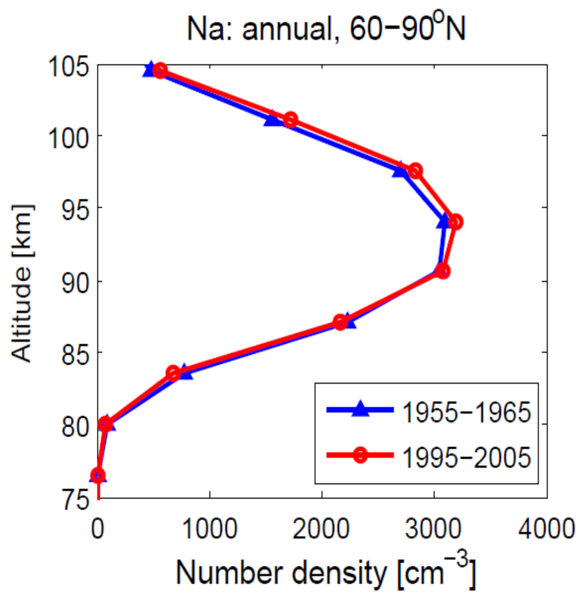

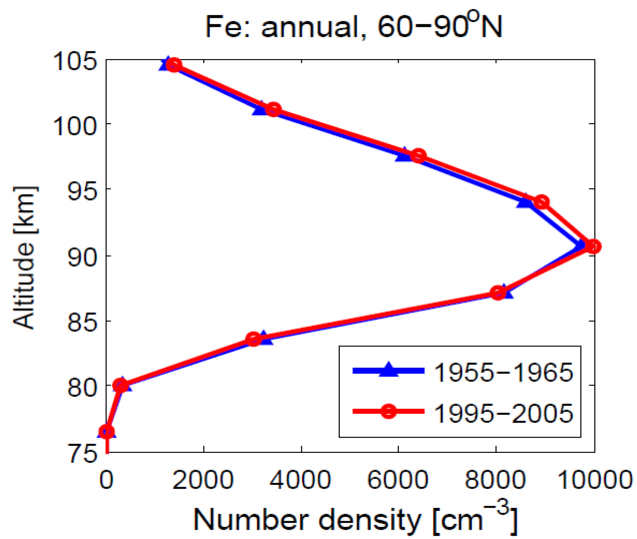

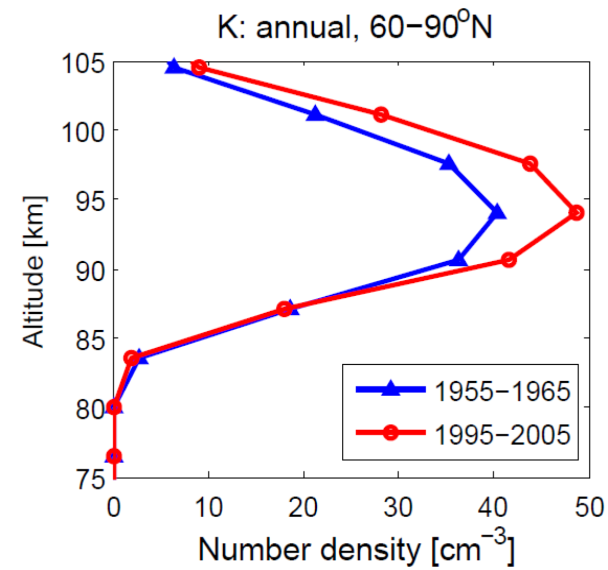

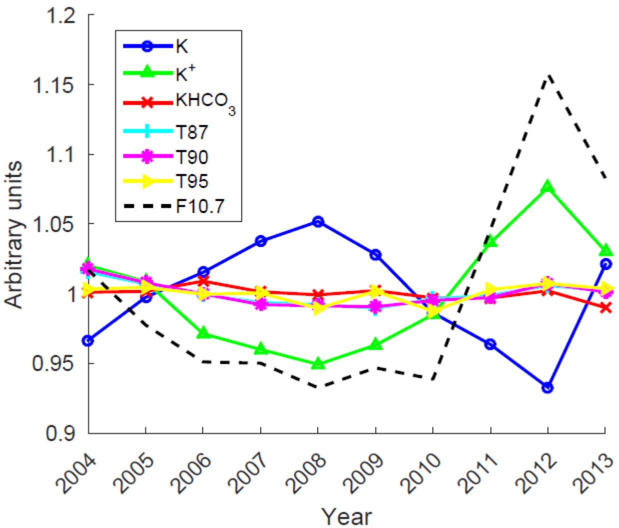

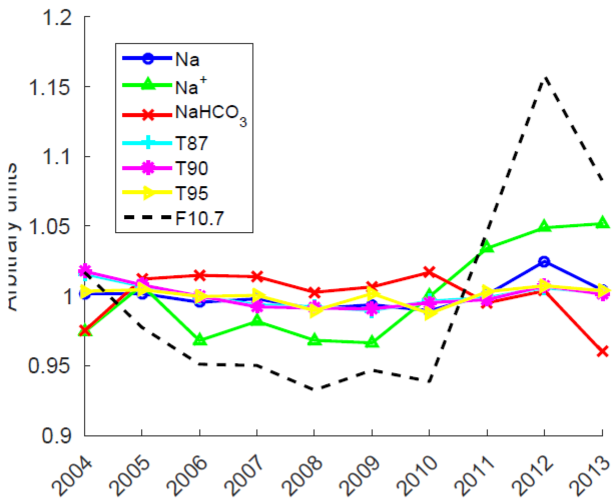

- ➢ **Significant K increases over the past 50 years while there is almost no change for Na and Fe**
- ➢ **Anti-correlation between solar flux and K but not for Na**

Dawkins et al. (to be submitted)

Metal-containing species Profiles

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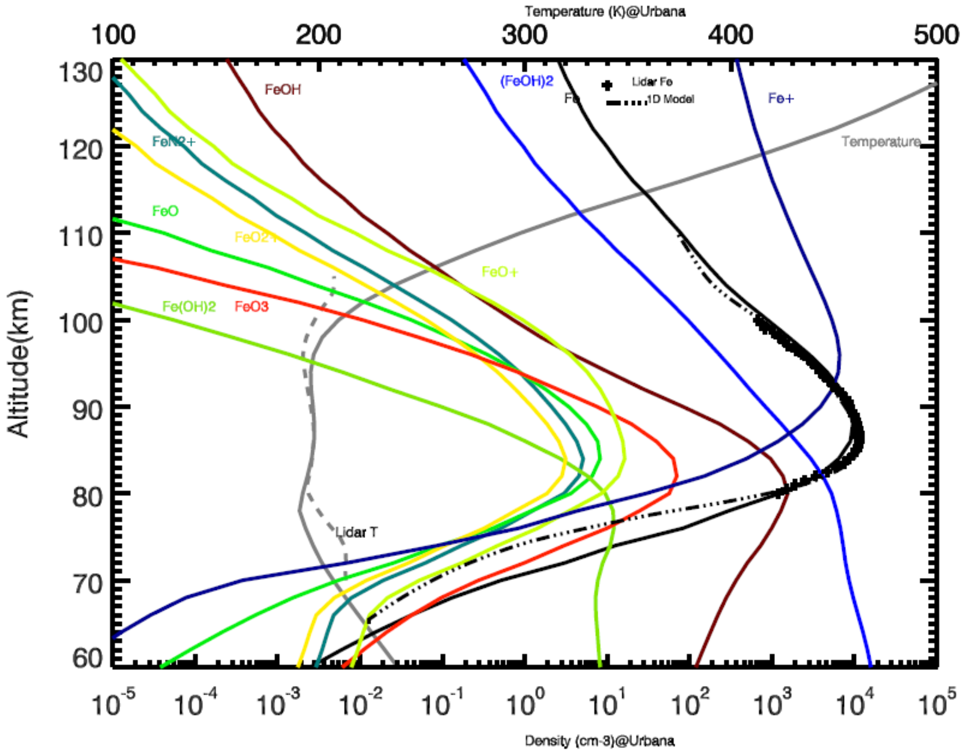
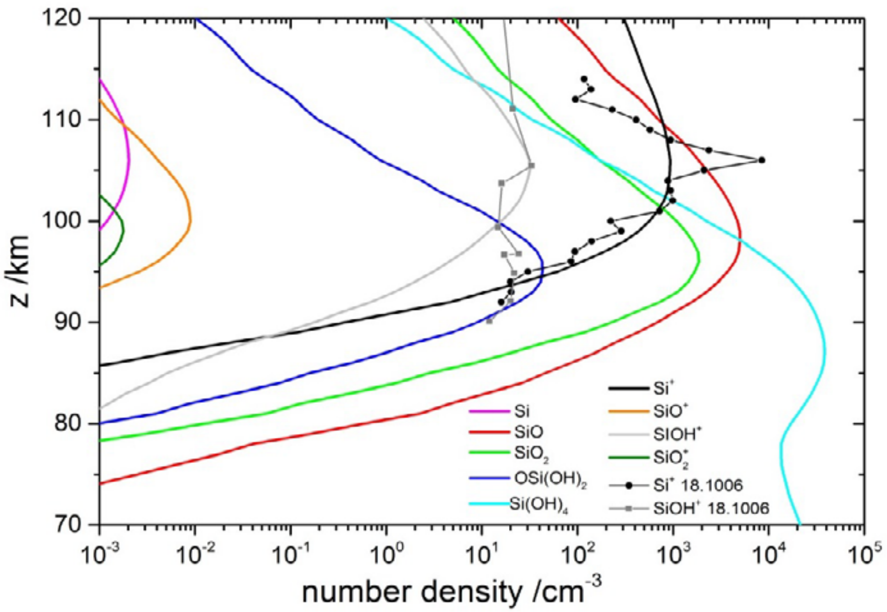


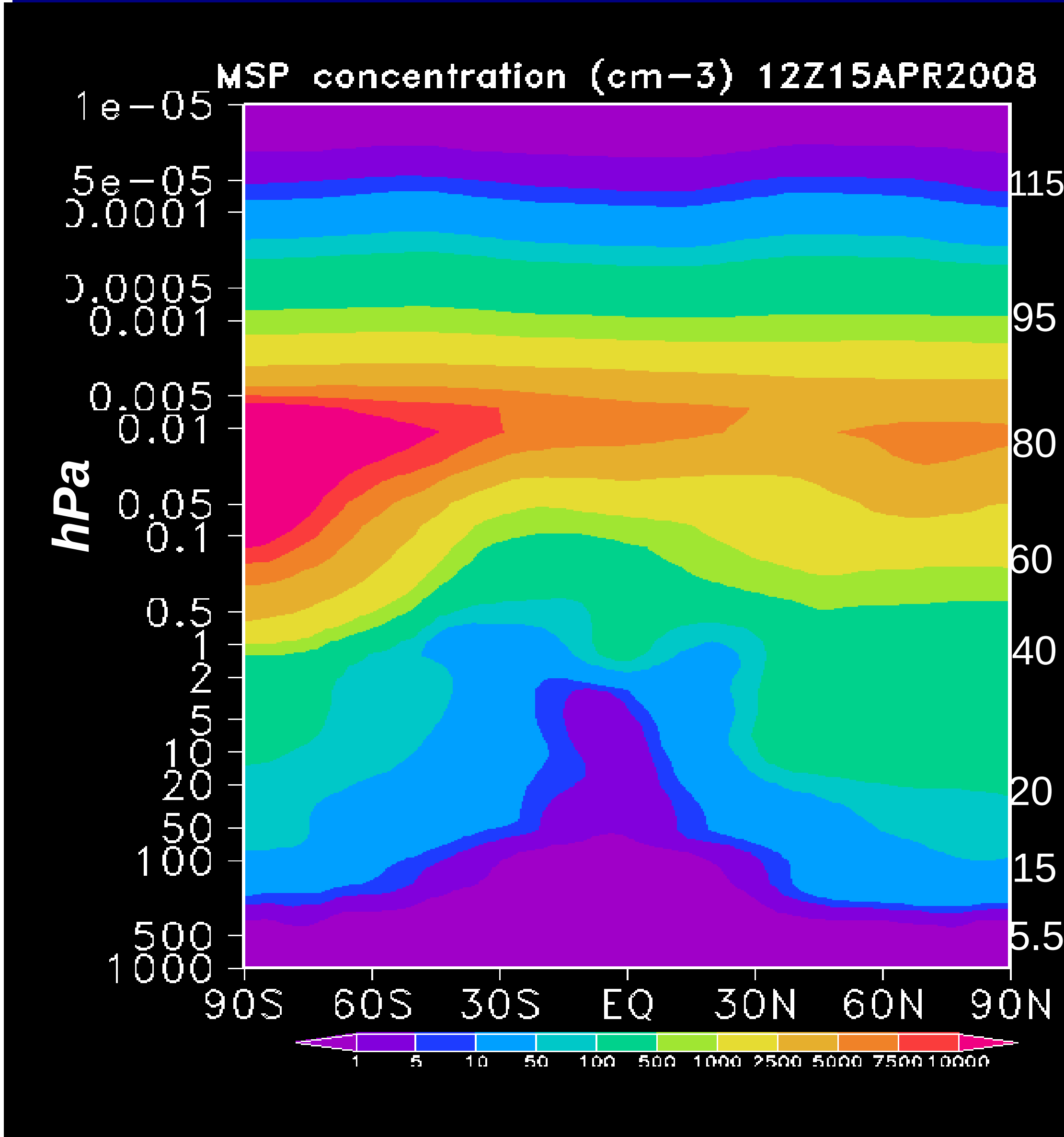
Feng et al. *JGR* (2013)



Plane et al. *JGR*(submitted)

- Quite different metal-containing species profiles
- Si^+ dominates above 110 km which is different with other metal ions
- Modelled bottom layer reservoirs species can be identified to be used for MSP explicitly.

Meteoric smoke particle concentration



- ➢The smoke material **explicitly** formed by metal chemistry enters the model in the smallest size bin (0.2 nm)
- ➢Seasonal variation in MSP concentration.
- ➢Largest MSP concentration (10,000 cm^{-3}) matches rocket data.

Summary and Conclusions

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- Meteoric metals are very useful tracers to test the atmospheric models in the upper atmosphere. Investigating different MLT metal layers within the same model will thus allow us to better understand the astronomy, chemistry and transport processes that control the different metal layers in the MLT.

- Successful adding Mesospheric metal Chemistry into a 3D NCAR CESM (WACCM4) model ----The first global model of meteoric metals. 6 metals (Na, Fe, K, Ca, Mg, Si) have been included into the model. Good simulation compared with available measurements, depending on MIF, chemistry and other processes considered.

- The first self-consistent global model of MSP from metal chemistry is still under validation. D region chemistry and MSP interaction with stratospheric aerosols are still developing.

ions transport problem?

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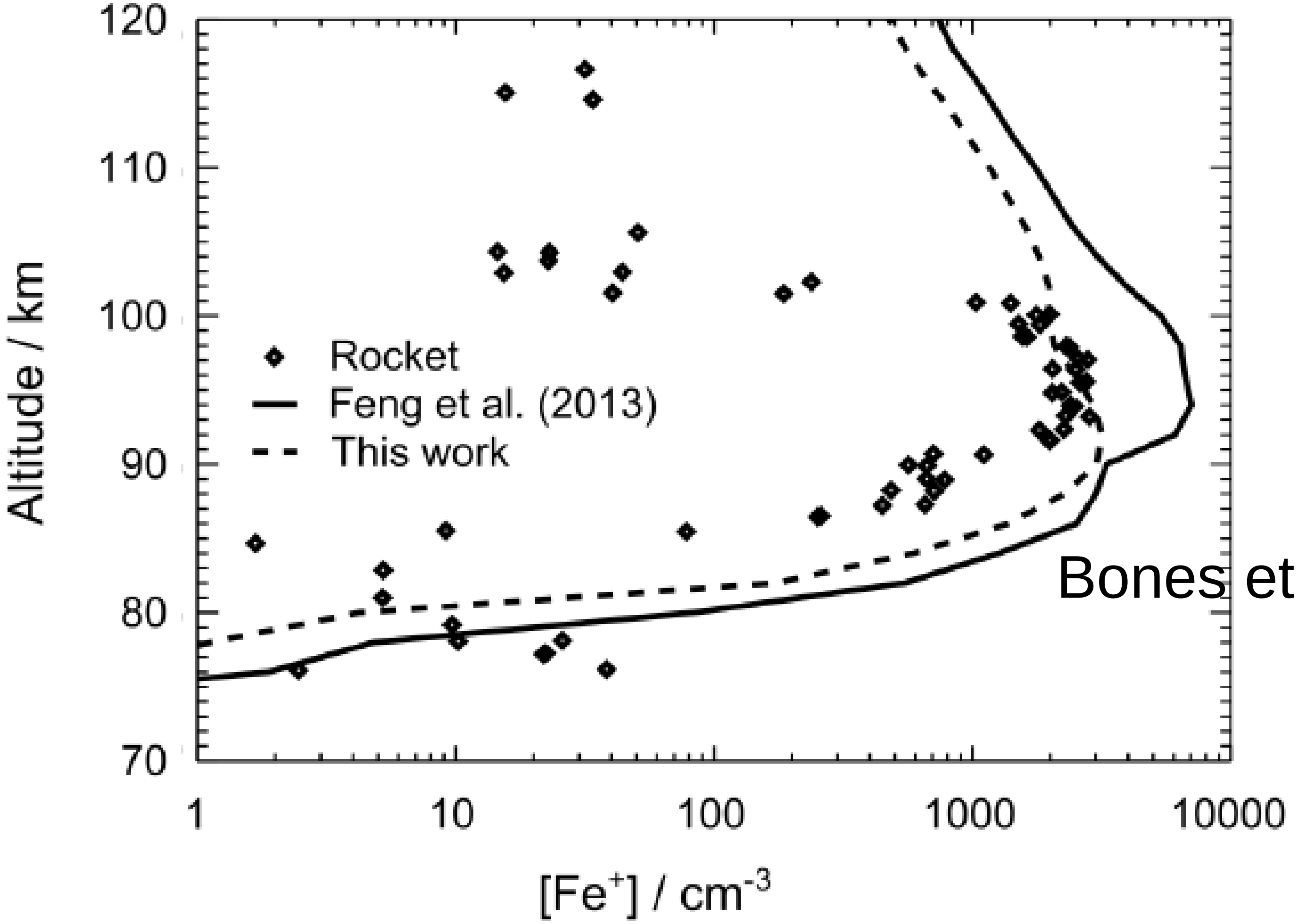

Bones et al., *JPC* (2015)

- Overestimates Fe^+ profile above 100 km, though the updated DR of FeO^+ +e improves the peak Fe^+

Deposition

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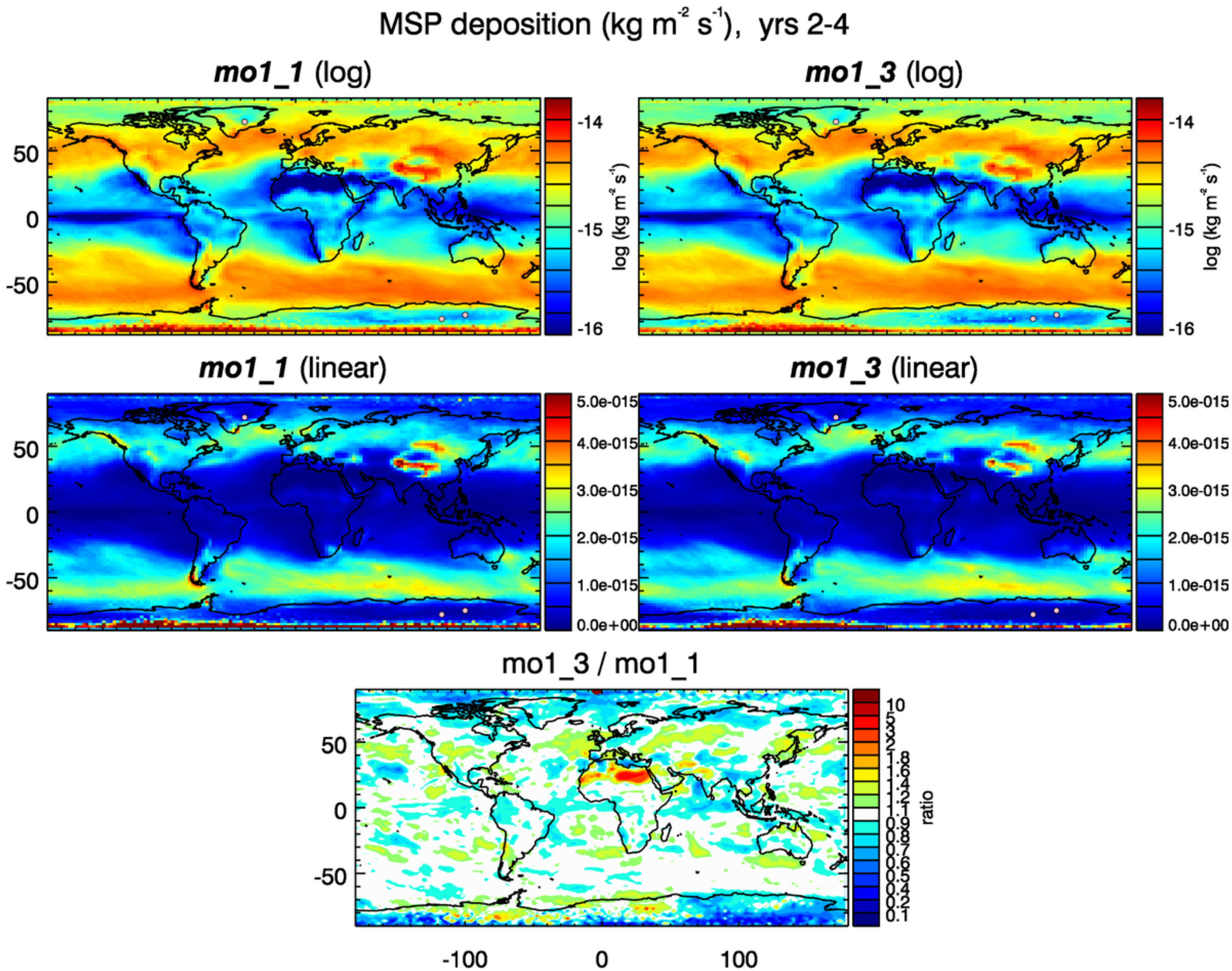

Aerosol snow scavenging coefficients (SSC) are extremely uncertain (several orders of magnitude). Changed SSC from 0.1 to a parametrisation taking radius into account (from Wang et al., Geosci. Model Dev., 7, 799 (2014)). Didn't make much difference.

mo1_3: With parametrisation.

mo1_1: SSC = 0.1

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