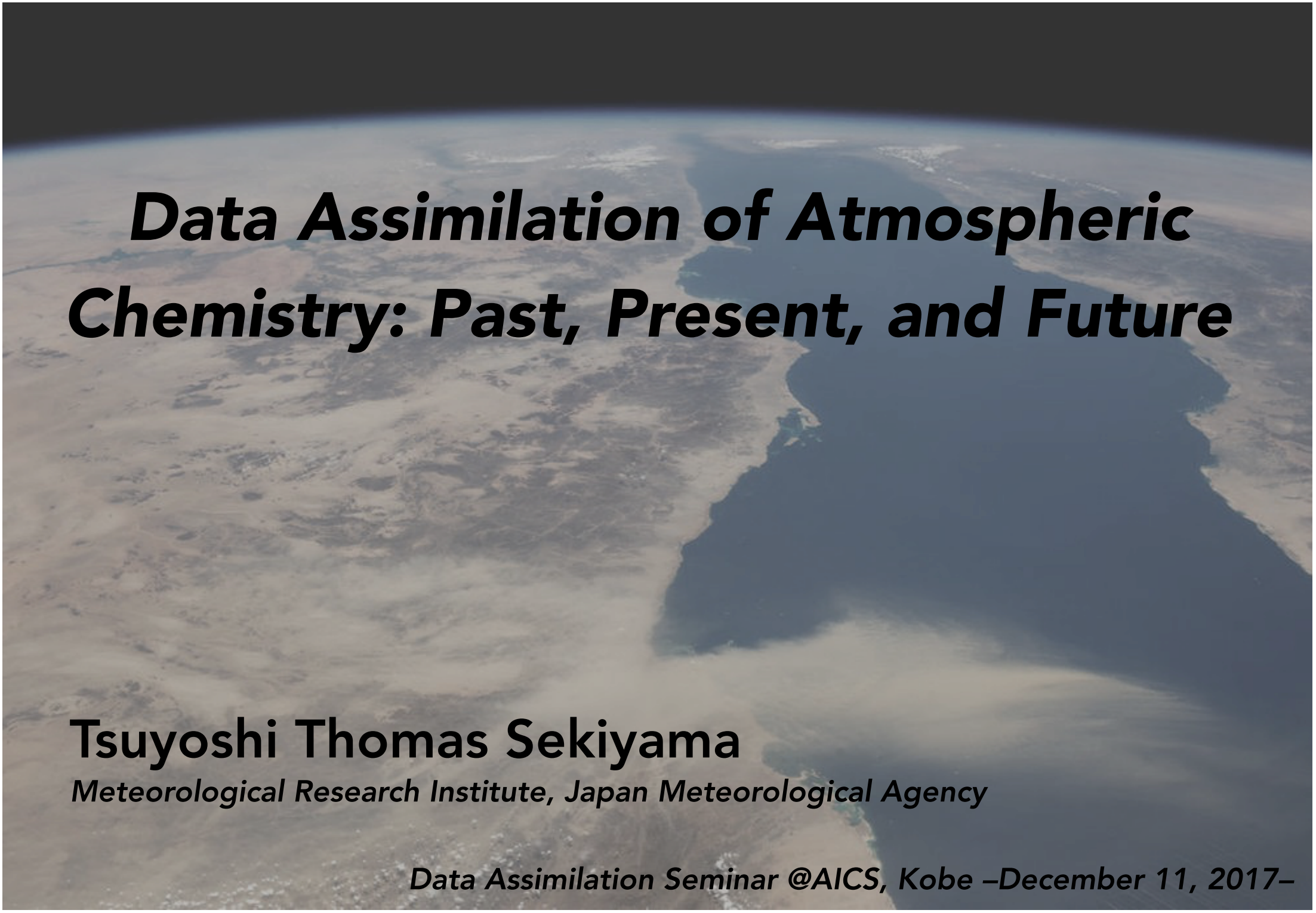

Data Assimilation of Atmospheric Chemistry: Past, Present, and Future

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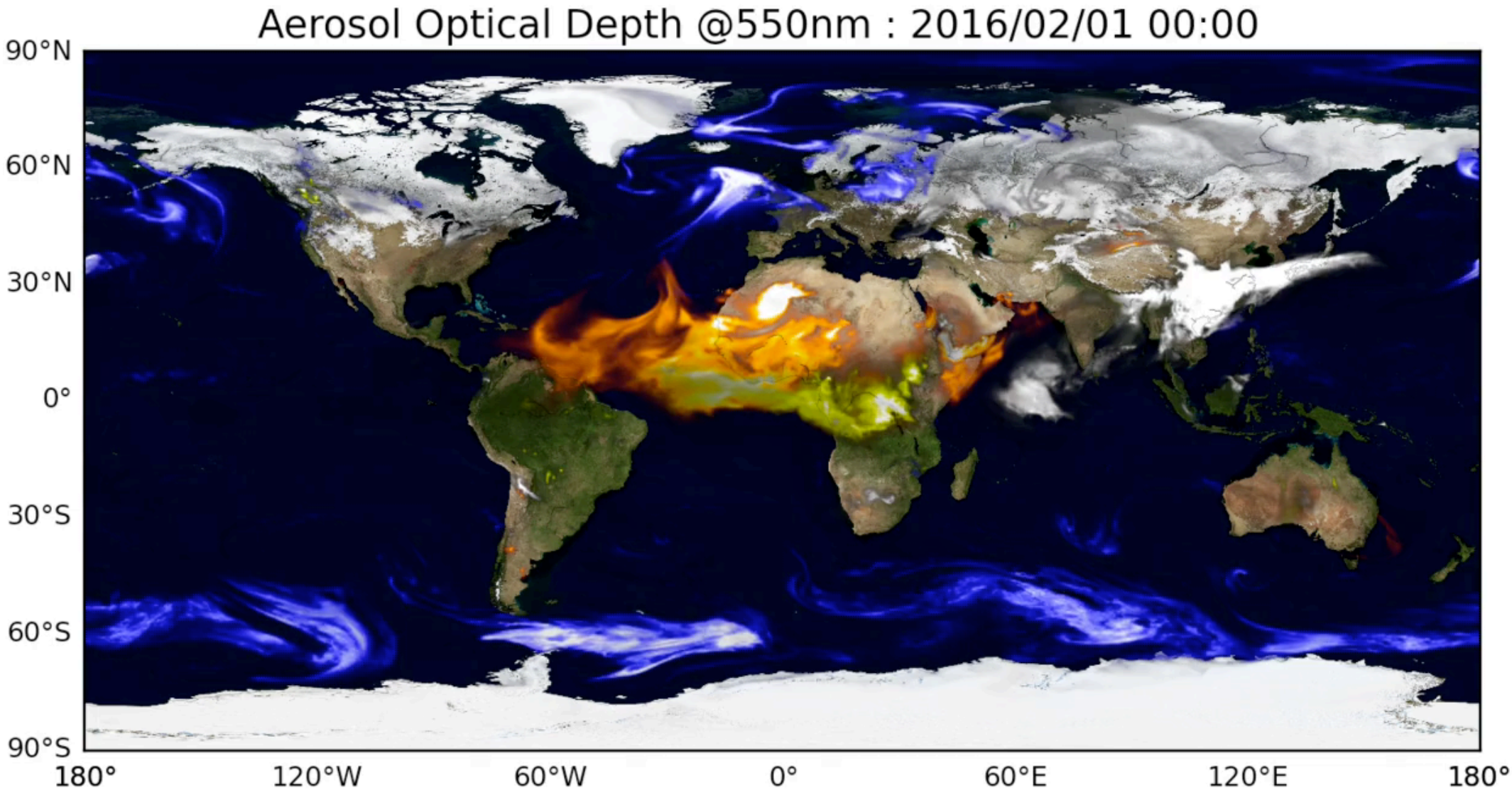
Data Assimilation Seminar @AICS, Kobe –December 11, 2017–

Data Assimilation of Atmospheric Chemistry: Past, Present, and Future

Contents

- What's atmospheric chemistry (AC) ?
  - ➜ difference between NWP and AC modeling
- Dawn of AC data assimilation
  - ➜ from the 1990s to the 2000s
- Status quo of AC data assimilation
  - ➜ contribution to environment and health issues
- Future of AC data assimilation
  - ➜ integration with NWP

What's atmospheric chemistry?



MRI/JMA aerosol model (MASINGAR mk2)

What's atmospheric chemistry?

mineral dust (Kosa)

black/organic carbons (biomass)

sulfate (≈PM2.5)

sea-salt

What's atmospheric chemistry?

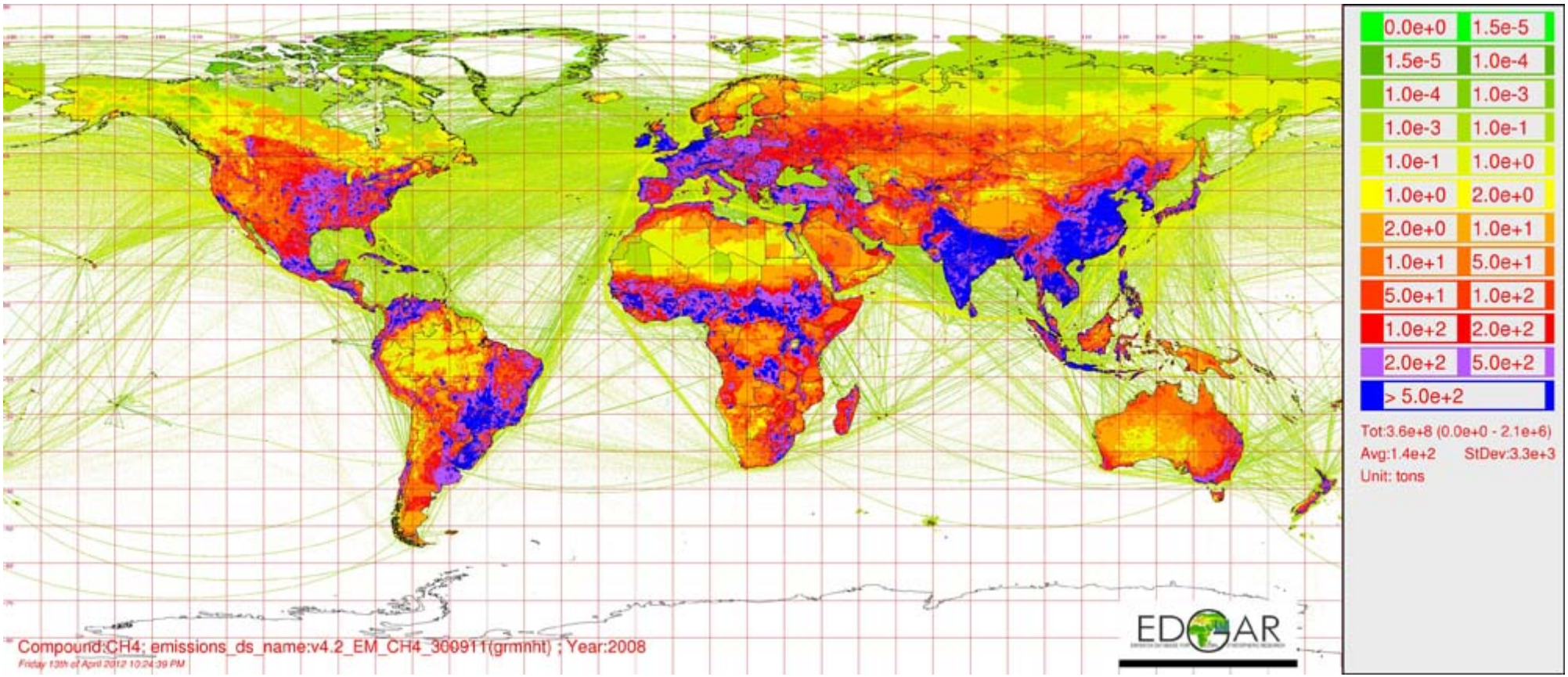
- Not classical chemistry.
- Rather, geophysics or meteorology.
- Investigates the production, reaction, loss, advection, diffusion, emission, and deposition of atmospheric constituents.
- Targets all the gas molecules and aerosol particles in the troposphere, stratosphere, and mesosphere.
  ➜ for example: ozone, greenhouse gases, black carbon, mineral dust, volcanic ash, sulfate particles (≈PM2.5), etc.

What’s different from weather research?

What's atmospheric chemistry?

Difference #1 between NWP and AC modeling

- Complicated Emissions

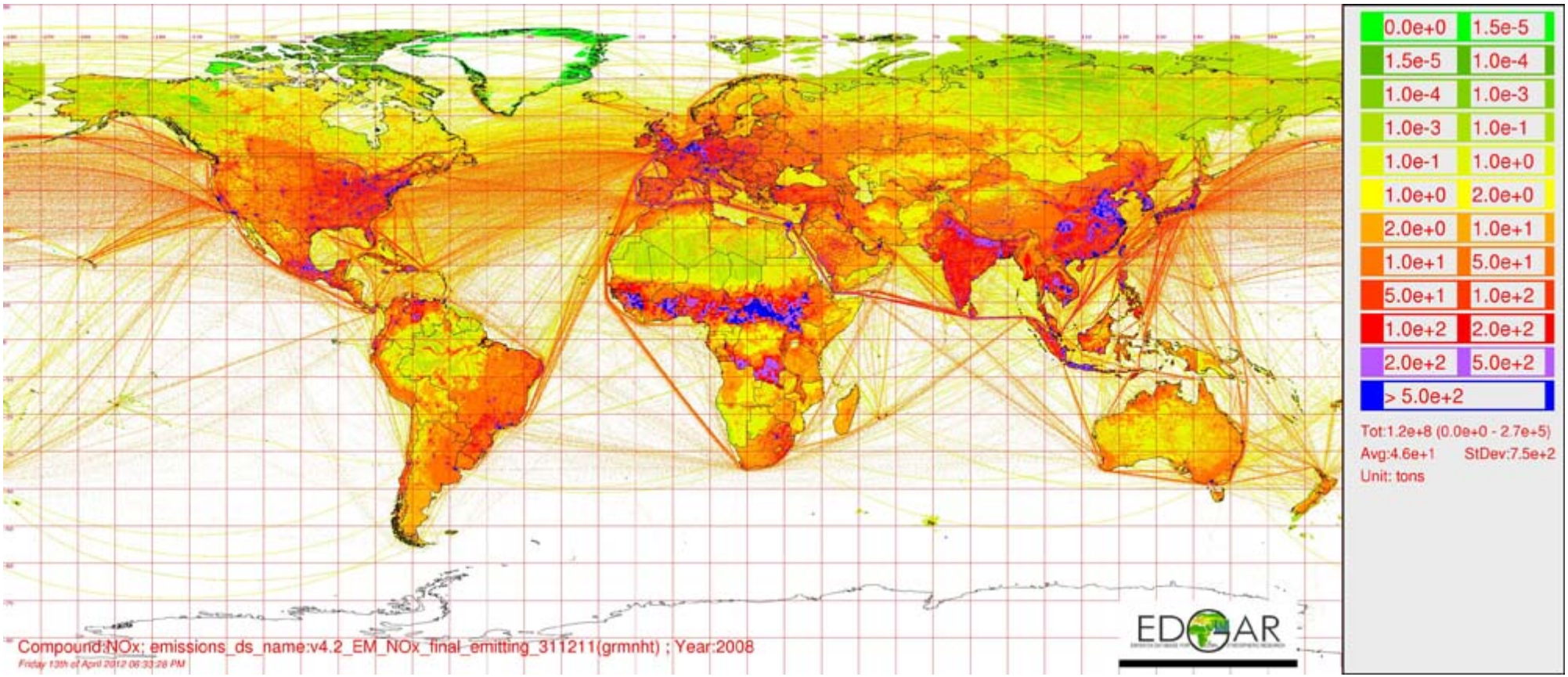


Methane (CH_4) emission

What's atmospheric chemistry?

Difference #1 between NWP and AC modeling

- Complicated Emissions

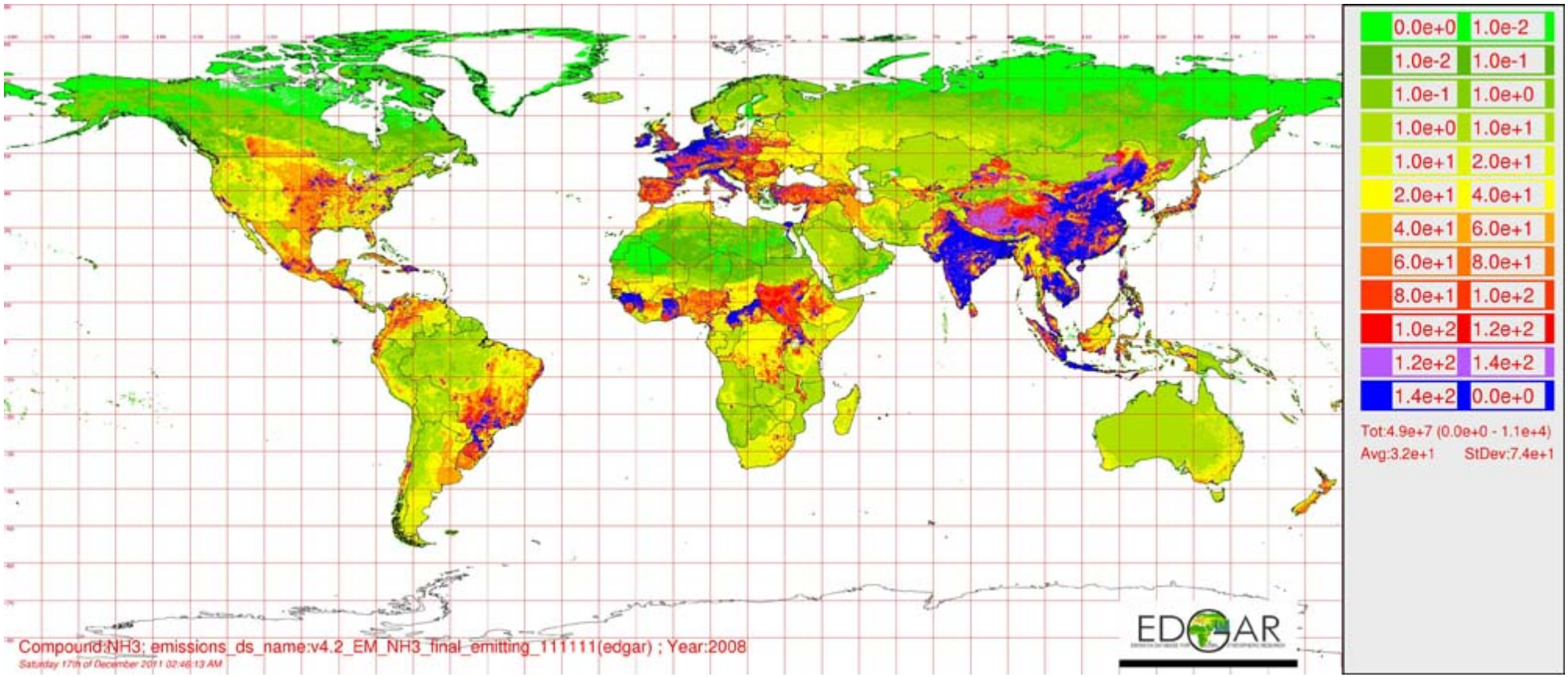


Nitrogen oxides (NO_X) emission

What's atmospheric chemistry?

Difference #1 between NWP and AC modeling

- Complicated Emissions

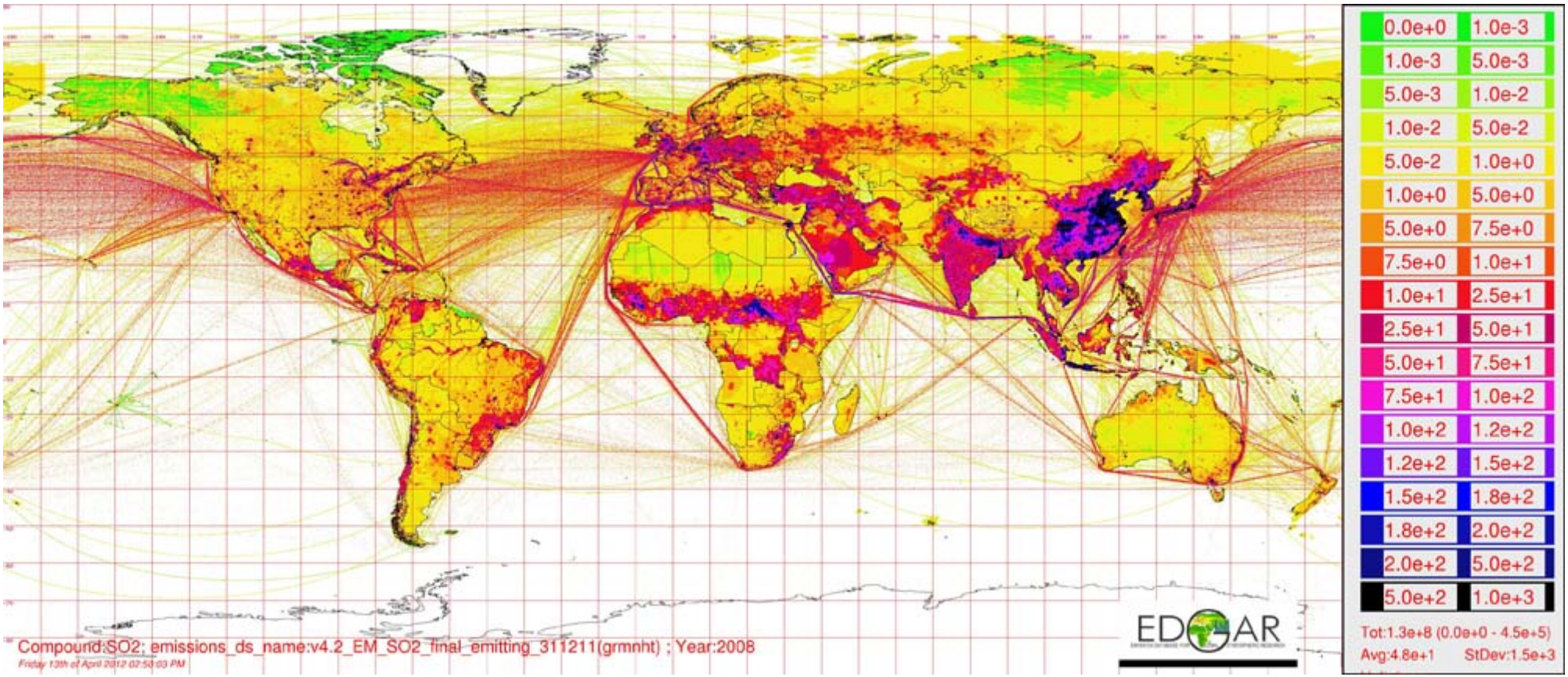


Ammonia (NH_3) emission

What's atmospheric chemistry?

Difference #1 between NWP and AC modeling

- Complicated Emissions

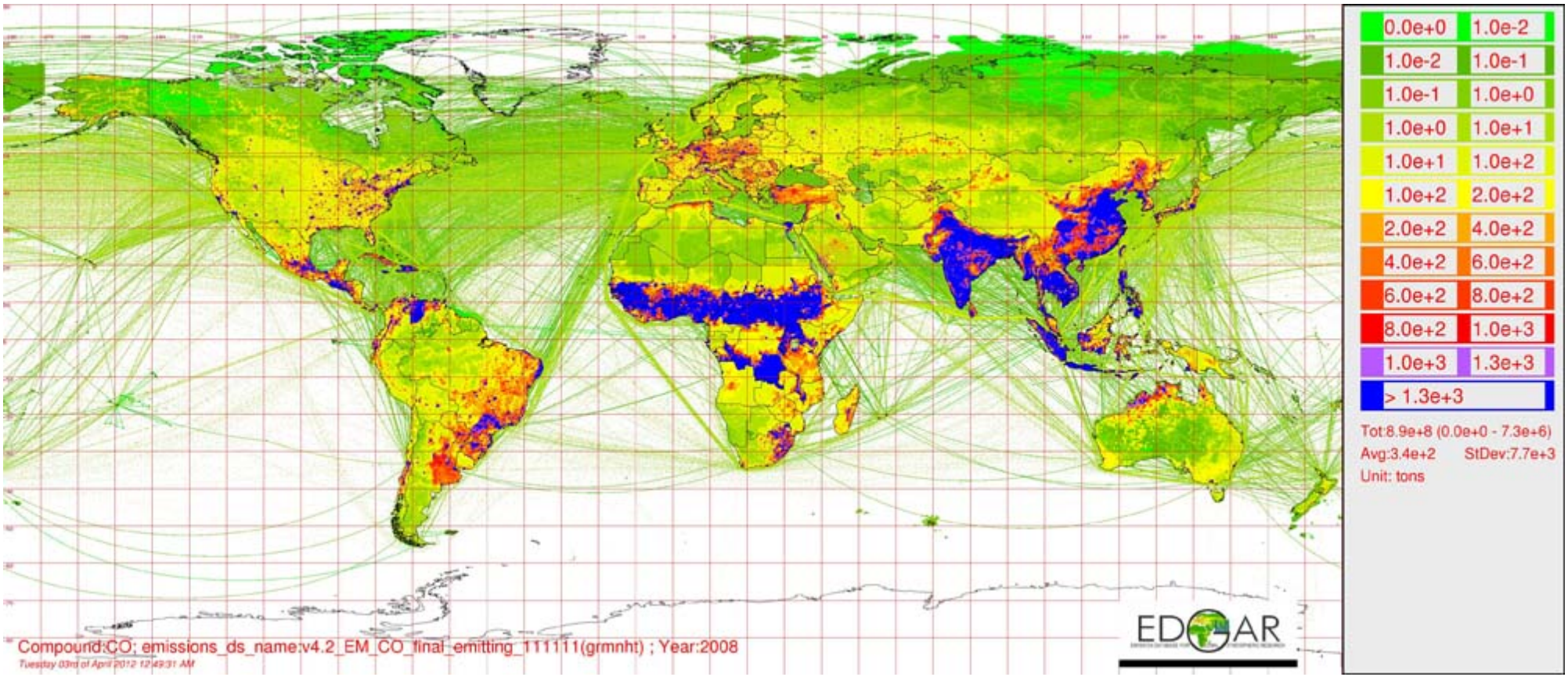


Sulfur dioxide (SO_2) emission

What's atmospheric chemistry?

Difference #1 between NWP and AC modeling

- Complicated Emissions



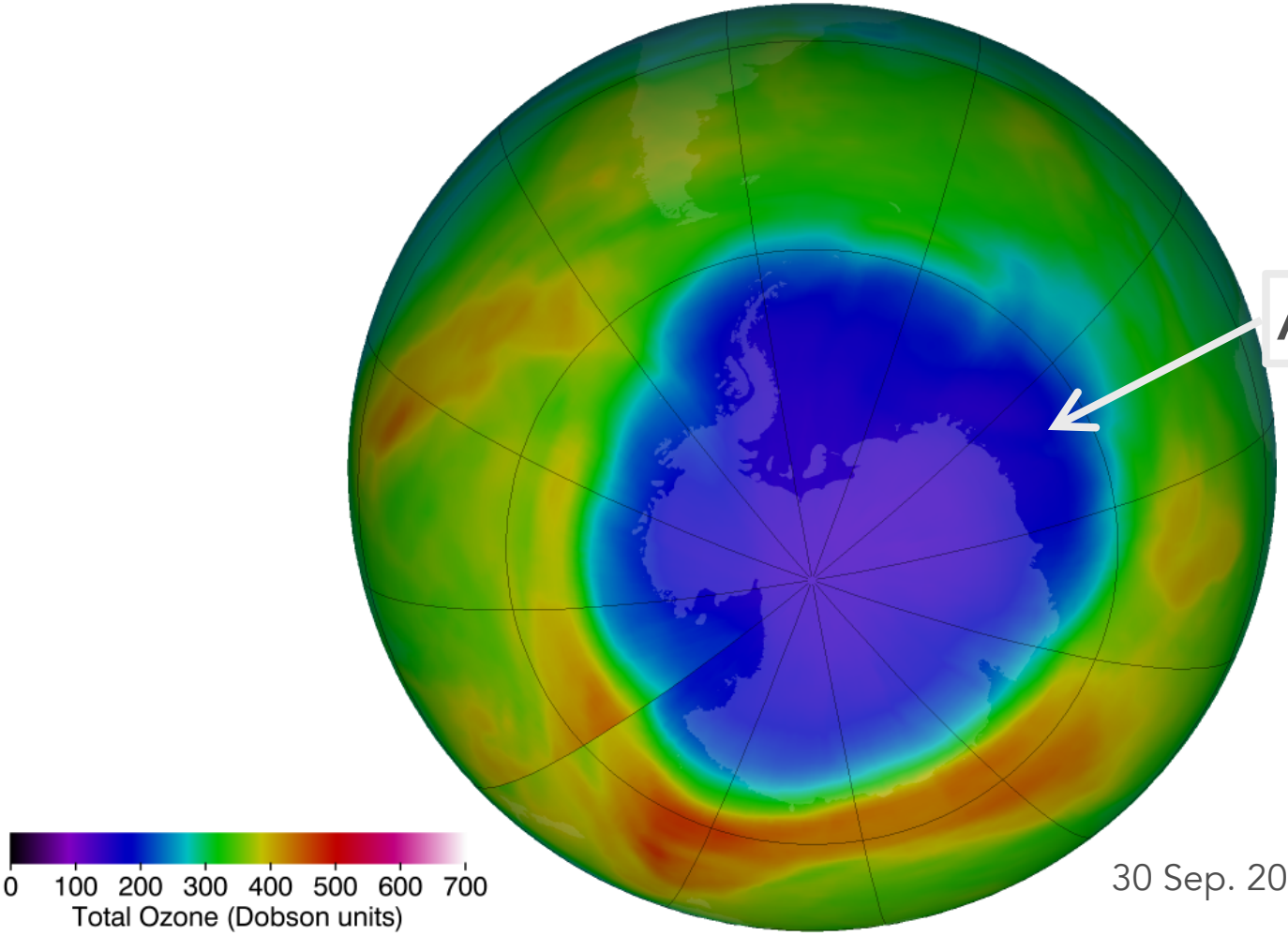
Carbon monoxide (CO) emission

We want to know the true emissions.

What's atmospheric chemistry?

Difference #2 between NWP and AC modeling

- many variables, many reactions



30 Sep. 2017 ©NASA

Polar Stratospheric Cloud (PSC)

Chemical species included in the JMA/MRI ozone chemistry model

Table 1. Names of chemical species

Long-lived species		
01…N_2O	02…CH_4	03…H_2O
04…NO_y	05…HNO_3	06…N_2O_5
07…Cl_y	08…O_x	09…CO
10…OClO	11…CO_2	12…Passive tracer
13…HCl	14…$ClONO_2$	15…HOCl
16…Cl_2	17…H_2O_2	18…$ClNO_2$
19…HBr	20…$BrONO_2$	21…NO_x
22…HO_2NO_2	23…ClO_x	24…BrO_x
25…Cl_2O_2	26…HOBr	27…CCl_4 (CFC−10)
28…$CFCl_3$ (CFC−11)	29…CF_2Cl_2 (CFC−12)	30…Br_y
31…CH_3Cl	32…CH_3Br	33…CF_2ClBr (Halon−1211)
34…CF_3Br (Halon−1301)	35…COF_2	36…HF
37…CH_2O	38…CH_3OOH	39…C_2H_6
40…CH_3CHO	41…C_2H_5OOH	42…PAN ($CH_3C(O)OONO_2$)
43…$CH_3C(O)OOH$	44…C_3H_8	45…ACET ($CH_3C(O)CH_3$)
46…C_3H_7OOH	47…HACET ($CH_3C(O)CH_2OH$)	48…MGLY ($CH_3C(O)CHO$)
49…C_2H_4	50…GLY ALD ($HOCH_2CHO$)	51…GPAN ($HOCH_2C(O)OONO_2$)
52…GC(O)OOH ($HOCH_2C(O)OOH$)	53…C_3H_6	54…ONIT ($CH_3C(O)CH_2ONO_2$)
55…POOH (HOC_3H_6OOH)	56…C_4H_{10}[a]	57…C_5H_8 (isoprene)
58…MACR[b]	59…ISON[c]	60…ISOPOOH[d]
61…NALD[e]	62…MACROOH[f]	63…MPAN[g]
64…$C_{10}H_{16}$ (terpenes)		

Short-lived species			
01…$O(^1D)$	02…OH	03…Cl	04…$O(^3P)$
05…O_3	06…HO_2	07…NO_2	08…NO
09…Br	10…N	11…ClO	12…BrO
13…NO_3	14…BrCl	15…H	16…CH_3O_2
17…$C_2H_5O_2$	18…$CH_3C(O)O_2$	19…$C_3H_7O_2$	20…$ACETO_2$ ($CH_3C(O)CH_2O_2$)
21…EO_2 ($HOC_2H_4O_2$)	22…EO (HOC_2H_4O)	23…$GC(O)O_2$ ($HOCH_2C(O)O_2$)	24… PO_2 ($HOC_3H_6O_2$)
25…$ISOPO_2$[a]	26…$MACRO_2$[b]		

Deushi and Shibata (2011)

Chemical reactions calculated in the JMA/MRI ozone chemistry model

Table 2. Gas Phase Reactions

No.	Reactions
Oxygen reactions	
hk_1	$O + O + M \rightarrow O_2 + M$
hk_2	$O + O_2 + M \rightarrow O_3 + M$
hk_3	$O + O_3 \rightarrow 2O_2$
hk_4	$O^{1D} + N_2 \rightarrow O + N_2$
hk_5	$O^{1D} + O_2 \rightarrow O + O_2$
Odd hydrogen reactions	
a_1	$H + O_2 + M \rightarrow HO_2 + M$
a_{1at}	$O^{1D} + H_2O \rightarrow 2OH$
a_2	$H + O_3 \rightarrow OH + O_2$
a_{2at}	$O^{1D} + CH_4 \rightarrow 0.75CH_3O_2 + 0.25CH_2O + 0.75OH + 0.4HO_2 + 0.05H_2$
a_{3at}	$O^{1D} + H_2 \rightarrow OH + H$
a_5	$OH + O \rightarrow H + O_2$
a_6	$OH + O_3 \rightarrow HO_2 + O_2$
a_{6b}	$HO_2 + O_3 \rightarrow OH + 2O_2$
a_7	$HO_2 + O \rightarrow OH + O_2$
a_8	$OH + OH \rightarrow H_2O + O$
a_9	$OH + OH + M \rightarrow H_2O_2 + M$
a_{10}	$H_2O_2 + O \rightarrow OH + HO_2$
a_{17}	$OH + HO_2 \rightarrow H_2O + O_2$
a_{19}	$OH + H_2 \rightarrow H_2O + H$
a_{23a}	$H + HO_2 \rightarrow 2OH$
a_{23b}	$H + HO_2 \rightarrow H_2 + O_2$
a_{23c}	$H + HO_2 \rightarrow H_2O + O$
a_{24}	$H_2 + O \rightarrow OH + H$
a_{26}	$HO_2 + NO \rightarrow NO_2 + OH$
a_{27}	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$
a_{30}	$OH + H_2O_2 \rightarrow H_2O + HO_2$
a_{36}	$OH + CO \rightarrow CO_2 + HO_2$
Odd nitrogen reactions	
b_3	$NO_2 + O \rightarrow NO + O_2$
b_4	$NO + O_3 \rightarrow NO_2 + O_2$
b_6	$N + NO \rightarrow N_2 + O$
b_7	$N + O_2 \rightarrow NO + O$
b_9	$NO_2 + O_3 \rightarrow NO_3 + O_2$
b_{12}	$NO_2 + NO_3 + M \rightarrow N_2O_5 + M$
b_{22}	$NO_2 + OH + M \rightarrow HNO_3 + M$
b_{23}	$NO_2 + HO_2 + M \rightarrow HO_2NO_2 + M$
b_{24}	$HO_2NO_2 + M \rightarrow HO_2 + NO_2 + M$
b_{27}	$HNO_3 + OH \rightarrow H_2O + NO_3$
b_{28}	$HO_2NO_2 + OH \rightarrow H_2O + NO_2 + O_2$
b_{32}	$N_2O_5 + M \rightarrow NO_2 + NO_3 + M$
b_{38}	$N_2O + O^{1D} \rightarrow N_2 + O_2$
b_{39}	$N_2O + O^{1D} \rightarrow 2NO$
b_{51}	$NO_3 + NO \rightarrow 2NO_2$
b_{52}	$NO_3 + HO_2 \rightarrow OH + NO_2 + O_2$
b_{53}	$N_2O_5 + H_2O \rightarrow 2HNO_3$

The underlined gas phase reactions are newly included into MRI-CCM2, but not treated in MRI-CCM1 (Shibata *et al.*, 2005).

No.	Reactions
Carbon reactions	
— CH_4 oxidation —	
c_2	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$
c_3	$CH_3O_2 + NO \rightarrow CH_2O + NO_2 + HO_2$
c_4	$CH_3O_2 + CH_3O_2 \rightarrow 2CH_2O + 2HO_2 + O_2$
c_5	$CH_3O_2 + CH_3O_2 \rightarrow CH_2O + O_2 (+CH_3OH)$
c_6	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$
c_7	$CH_3OOH + OH \rightarrow 0.7CH_3O_2 + 0.3CH_2O + 0.3OH + H_2O$
c_8	$CH_2O + OH \rightarrow CO + HO_2 + H_2O$
c_9	$CH_2O + NO_3 \rightarrow CO + HO_2 + HNO_3$
— C_2H_6 oxidation and Acetaldehyde degradation—	
c_{10}	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$
c_{11}	$C_2H_5O_2 + NO \rightarrow CH_3CHO + NO_2 + HO_2$
c_{12}	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH + O_2$
c_{13}	$C_2H_5O_2 + CH_3O_2 \rightarrow 0.8CH_3CHO + 1.4CO_2 + 0.6HO_2$
c_{14}	$C_2H_5O_2 + C_2H_5O_2 \rightarrow 1.6CH_3CHO + 1.2HO_2 (+ 0.4C_2H_5OH)$
c_{15}	$C_2H_5OOH + OH \rightarrow 0.286C_2H_5O_2 + 0.714CH_3CHO + 0.714OH + H_2O$
c_{16}	$CH_3CHO + OH \rightarrow CH_3C(O)O_2 + H_2O$
c_{17}	$CH_3CHO + NO_3 \rightarrow CH_3C(O)O_2 + HNO_3$
c_{18}	$CH_3C(O)O_2 + NO \rightarrow CH_3O_2 + CO_2 + NO_2$
c_{19}	$CH_3C(O)O_2 + NO_2 + M \rightarrow PAN + M$
c_{20}	$PAN + M \rightarrow CH_3C(O)O_2 + NO_2 + M$
c_{21}	$CH_3C(O)O_2 + HO_2 \rightarrow CH_3C(O)OOH + O_2$
c_{22}	$CH_3C(O)O_2 + HO_2 \rightarrow O_3 (+CH_3COOH)$
c_{23}	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)O_2 + H_2O$
c_{24}	$CH_3C(O)O_2 + CH_3O_2 \rightarrow CH_3O_2 + CH_2O + CO_2 + HO_2 + O_2$
c_{25}	$CH_3C(O)O_2 + CH_3O_2 \rightarrow CH_2O + O_2 (+ CH_3COOH)$
c_{26}	$CH_3C(O)O_2 + CH_3C(O)O_2 \rightarrow 2CH_3O_2 + 2CO_2 + O_2$
c_{73}	$PAN + OH \rightarrow CH_2O + CO_2 + NO_3$

Table 2. (continued)

No.	Reactions
— C_3H_8 oxidation —	
c_{27}	$C_3H_8 + OH \rightarrow C_3H_7O_2 + H_2O$
c_{28}	$C_3H_7O_2 + NO \rightarrow 0.24C_2H_5O_2 + 0.09CH_3CHO + 0.18CO + 0.7ACET + 0.6CO_2 + NO_2 + HO_2$
c_{29}	$C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH + O_2$
c_{30}	$C_3H_7O_2 + CH_3O_2 \rightarrow 0.8C_2H_5O_2 + 0.3CH_3CHO + 0.2ACET + 0.6CO + 0.6CO_2 + HO_2$
c_{31}	$C_3H_7OOH + OH \rightarrow 0.667ACET + 0.157C_2H_5O_2 + 0.053CH_3CHO + 0.142C_2H_5O_2 + 0.106CO + 0.035CO_2 + 0.843OH + 0.157H_2O$
c_{32}	$ACET + OH \rightarrow ACETO_2 + H_2O$
c_{33}	$ACETO_2 + NO \rightarrow CH_3C(O)O_2 + CH_2O + NO_2$
c_{34}	$ACETO_2 + HO_2 \rightarrow HACET + O_2$
c_{35}	$ACETO_2 + CH_3O_2 \rightarrow 0.2HACET + 0.5MGLY + 0.3CH_3C(O)O_2 + 0.8CH_2O + 0.3HO_2 + O_2 (+ 0.5CH_3OH)$
c_{36}	$MGLY + OH \rightarrow CH_3C(O)O_2 + CO$
c_{37}	$MGLY + NO_3 \rightarrow CH_3C(O)O_2 + CO + HNO_3$
c_{38}	$HACET + OH \rightarrow 0.323ACETO_2 + 0.677MGLY + 0.677OH$
c_{71}	$C_3H7O_2 + C_3H7O_2 \rightarrow 2.4CH_3CHO + 1.2HO_2 + O_2 (+ 0.4C_3H_7OH)$
c_{74}	$ACETO_2 + ACETO_2 \rightarrow 0.37MGLY + 1.26CH_3C(O)O_2 + 1.26CH_2O + O_2 (+ CH_3C(O)CH_2OH)$
— C_2H_4 oxidation —	
c_{39}	$C_2H_4 + OH + M \rightarrow 0.75EO_2 + 0.5CH_2O + 0.25HO_2 + M$
c_{40}	$EO_2 + NO \rightarrow EO + NO_2$
c_{41}	$EO + O_2 \rightarrow GLY ALD + HO_2$
c_{42}	$EO \rightarrow 2CH_2O + HO_2$
c_{43}	$C_2H_4 + O_3 \rightarrow CH_2O + 0.5CO + 0.12HO_2 + 0.12OH$
c_{44}	$GLY ALD + OH \rightarrow 0.8GC(O)O_2 + 0.4CO + 0.2HO_2 + 0.2H_2$
c_{45}	$GC(O)O_2 + NO_2 + M \rightarrow GPAN + M$
c_{46}	$GPAN + M \rightarrow GC(O)O_2 + NO_2 + M$
c_{47}	$GC(O)O_2 + NO \rightarrow CH_2O + CO_2 + HO_2 + NO_2$
c_{48}	$GC(O)O_2 + HO_2 \rightarrow 0.7GC(O)O_2H + 0.3O_3 (+ 0.3CH_3COOH)$
c_{49}	$GC(O)O_2 + CH_3O_2 \rightarrow 2CH_2O + CO_2 + 2HO_2$
c_{50}	$GC(O)O_2 + CH_3O_2 \rightarrow CH_2O (+ CH_3COOH)$
c_{51}	$GC(O)O_2 + GC(O)O_2 \rightarrow 2CH_2O + 2CO_2 + 2HO_2$
c_{52}	$GC(O)O_2H + OH \rightarrow 0.5GC(O)O_2 + 0.5CH_2O + 0.5CO_2 + 0.5OH$
c_{70}	$EO_2 + EO_2 \rightarrow EO + 0.5GLY ALD + O_2 (+ 0.5HOC_2H_4OH)$
— C_3H6 oxidation —	
c_{53}	$C_3H_6 + OH + M \rightarrow PO_2 + M$
c_{54}	$C_3H_6 + O_3 \rightarrow 0.08CH_4 + 0.5CH_3CHO + 0.31CH_3O_2 + 0.54CH_2O + 0.56CO + 0.19HO_2 + 0.33OH (+ 0.25CH_3COOH)$
c_{55}	$C_3H_6 + NO_3 \rightarrow ONIT$
c_{56}	$PO_2 + NO \rightarrow CH_3CHO + CH_2O + HO_2 + NO_2$
c_{57}	$PO_2 + HO_2 \rightarrow POOH + O_2$
c_{58}	$POOH + OH \rightarrow 0.5PO_2 + 0.5HACET + 0.5OH + H_2O$
c_{60}	$ONIT + OH \rightarrow MGLY + NO_2$
c_{61}	$EO_2 + HO_2 \rightarrow 0.667POOH + O_2$
c_{72}	$PO_2 + PO_2 \rightarrow 0.75GLY ALD + CH_3CHO + CH_2O + HO_2 (+ 0.5HOC_3H_6OH)$
— C_4H10 oxidation —	
c_{62}	$C_4H_{10} + OH \rightarrow 0.468ISOPO_2 + 0.02C_3H_7O_2 + 0.3C_2H_5O_2 + CH_2O + HO_2 + H_2O$
— Isoprene oxidation —	
i_1	$C_5H_8 + O_3 \rightarrow 0.65MACR + 0.1MACRO_2 + 0.58CH_2O + 0.1CH_3C(O)O_2 + 0.08CH_3O_2 + 0.14CO + 0.09H_2O_2 + 0.25HO_2 + 0.25OH (+ 0.28HCOOH)$
i_2	$C_5H_8 + OH \rightarrow ISOPO_2$
i_3	$C_5H_8 + NO_3 \rightarrow ISON$
i_4	$ISOPO_2 + NO \rightarrow 0.044ISON + 0.956MACR + 0.956CH_2O + 0.956HO_2 + 0.956NO_2$
i_5	$ISOPO_2 + HO_2 \rightarrow ISOPOOH$
i_6	$ISOPO_2 + ISOPO_2 \rightarrow 2MACR + CH_2O + CO_2 + HO_2$
i_7	$ISOPOOH + OH \rightarrow MACR + CO_2 + OH$
i_8	$ISON + OH \rightarrow NALD + 0.2MGLY + 0.1CH_3C(O)O_2 + 0.1CH_2O + 2.1CO_2 + 0.1HO_2$
i_9	$MACR + OH \rightarrow MACRO_2$
i_{10}	$MACR + O_3 \rightarrow 0.9MGLY + 0.1CH_3C(O)O_2 + 0.22CO + 0.43CO_2 + 0.32HO_2 + 0.19OH (+ 0.45HCOOH)$

Deushi and Shibata (2011)

Chemical reactions calculated in the JMA/MRI ozone chemistry model

Table 2. (continued)

No.	Reactions
i_{11}	MACR + NO → 0.5MGLY + 0.25HACET + 0.25$CH_3C(O)O_2$ + 0.75CH_2O + 0.25CO + 0.25CO_2 + 0.75HO_2 + 0.19OH + NO_2
i_{12}	$MACRO_2$ + HO_2 → MACROOH
i_{13}	$MACRO_2$ + $MACRO_2$ → HACET + MGLY + 0.5CH_2O + 0.5CO + 0.5CO_2
i_{14}	$MACRO_2$ + NO_2 + M → MPAN + M
i_{15}	MPAN + M → $MACRO_2$ + NO_2 + M
i_{16}	MPAN + OH → 0.2MGLY + 0.1$CH_3C(O)O_2$ + 0.1CH_2O + 3.1CO_2 + 0.1HO_2 + NO_2
i_{17}	MACROOH + OH → $MACRO_2$ + H_2O
i_{18}	NALD + OH → CH_2O + CO + NO_2
— Terpenes oxidation —	
t_1	$C_{10}H_{16}$ + OH → 1.3ISOPO_2 + 0.6ACET + 1.7CO_2
t_2	$C_{10}H_{16}$ + O_3 → 1.3MACR + 0.2$MACRO_2$ + 0.2$CH_3C(O)O_2$ + 0.16CH_3O_2 + 0.18H_2O_2 + 1.16CH_2O + 0.5OH + 0.28CO + 0.5HO_2 + 1.44CO_2 (+ 0.56HCOOH)
t_3	$C_{10}H_{16}$ + NO_3 → 1.2ISOPO_2 + 4CO_2 + NO_2

No.	Reactions
Chlorine reactions	
d_0	CH_3Cl + OH → Cl + H_2O (+ products)
d_2	Cl + O_3 → ClO + O_2
d_3	ClO + O → Cl + O_2
d_4	ClO + NO → Cl + NO_2
d_5	Cl + CH_4 → HCl + CH_3O_2
d_6	Cl + H_2 → HCl + H
d_7	Cl + HO_2 → HCl + O_2
d_8	ClO + OH → Cl + HO_2
d_9	ClO + OH → HCl + O_2
d_{11}	HCl + OH → Cl + H_2O
d_{31}	ClO + NO_2 + M → $ClONO_2$ + M
d_{32}	$ClONO_2$ + O → ClO + NO_3
d_{33}	ClO + HO_2 → HOCl + O_2
d_{34}	HOCl + OH → H_2O + ClO
d_{35}	HOCl + O → OH + ClO
d_{36}	Cl + NO_2 + M → $ClNO_2$ + M
d_{37}	HOCl + Cl → OH + Cl_2
d_{60}	ClO + ClO + M → Cl_2O_2 + M
d_{61}	Cl_2O_2 +M → ClO + ClO + M
d_{62}	OClO + OH → HOCl + O_2
d_{63}	OClO + Cl → ClO + ClO
d_{64}	OClO + O → ClO + O_2
d_{64}	OClO + O → ClO + O_2
d_{65}	OClO + NO → ClO + NO_2
d_{101}	CCl_4 + O^{1D} → 4Cl (+ products)
d_{102}	$CFCl_3$ + O^{1D} → 3Cl + HF (+ products)
d_{103}	CF_2Cl_2 + O^{1D} → 2Cl + COF_2 (+ products)
d_{110}	COF_2 + O^{1D} → 2HF (+ products)
Bromine reactions	
e_2	Br + O_3 → BrO + O_2
e_3	BrO + O → Br + O_2
e_4	BrO + NO → NO_2 + Br
e_{5a}	BrO + ClO → OClO + Br
e_{5b}	BrO + ClO → Br + Cl + O_2
e_{5c}	BrO + ClO → BrCl + O_2
e_6	BrO + BrO → 2Br + O_2
e_7	Br + HO_2 → HBr + O_2
e_8	Br + OClO → BrO + ClO
e_{11}	HBr + OH → H_2O + Br
e_{13}	BrO + NO_2 + M → $BrONO_2$ + M
e_{15}	BrO + HO_2 → HOBr + O_2
e_{91}	CF_3Br + O^{1D} → Br + COF_2 + HF (+ products)
e_{92}	CF_2ClBr + O^{1D} → Br + Cl + COF_2 (+ products)
e_{93}	CH_3Br + O^{1D} → Br (+ products)

Table 3. Photochemical Reactions

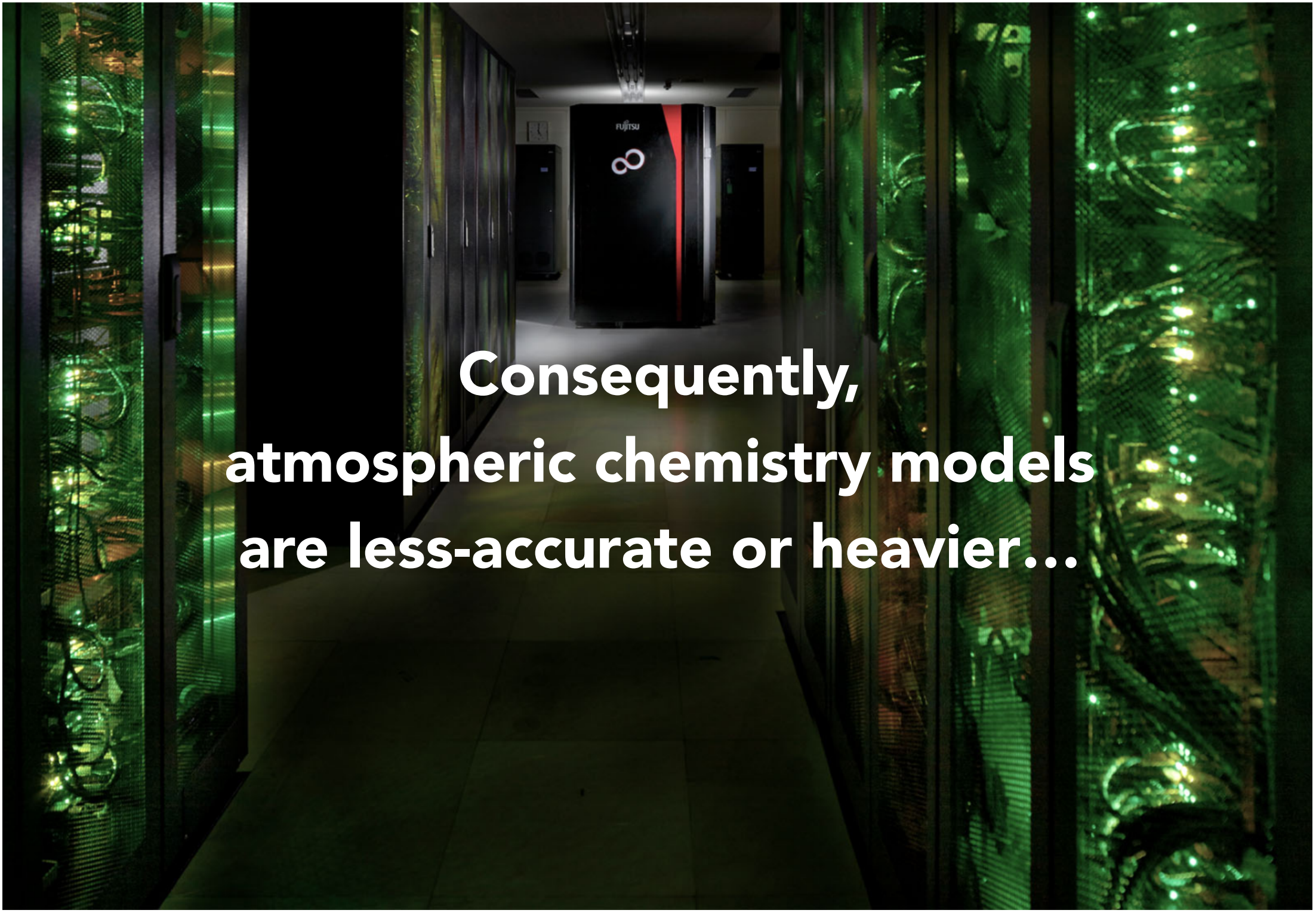
No.	Reactions	No.	Reactions
01	O_2 + hν → 2O	31*	CF_2ClBr + hν → Br + Cl + COF_2 (+ products)
02*°	O_3 + hν → O + O_2	32*	CF_3Br + hν → Br + COF_2 + HF (+ products)
03	H_2O + hν → H + OH	33*	$ClONO_2$ + hν → ClO + NO_2
04*	N_2O + hν → N_2 + O^{1D}	34	$BrONO_2$ + hν → BrO + NO_2
05	CH_4 + hν → CH_3O_2 + HO_2	35	COF_2 + hν → 2HF (+ products)
06*°	NO_2 + hν → NO + O	36	CH_3OOH + hν → CH_2O + HO_2 + OH
07*	HNO_3 + hν → NO_2 + OH	37*	CH_2O + hν → CO + 2HO_2
08	HOCl + hν → Cl + OH	38*	CH_2O + hν → CO + H_2
09	HO_2NO_2 + hν → HO_2 + NO_2	39*	PAN + hν → $CH_3C(O)O_2$ + NO_2
10*	$ClONO_2$ + hν → Cl + NO_3	40*	PAN + hν → CH_3O_2 + CO_2 + NO_3
11*	N_2O_5 + hν → NO_3 + NO_2	41	C_2H_5OOH + hν → CH_3CHO + OH + HO_2
12*	O_3 + hν → O^{1D} + O_2	42	$CH_3C(O)OOH$ + hν → CH_3O_2 + CO_2 + OH
13*	H_2O_2 + hν → 2OH	43	CH_3CHO + hν → CH_3O_2 + CO + HO_2
14	OClO + hν → O + ClO	44	CH_3CHO + hν → CH_4 + CO
15	Cl_2O_2 + hν → 2Cl + O_2	45	C_3H_7OOH + hν → 0.7ACET + 0.24$C_2H_5O_2$ + 0.09CH_3CHO + 0.18CO + OH + HO_2
16	HCl + hν → H + Cl		
17	Cl_2 + hν → 2Cl	46*	ACET + hν → $CH_3C(O)O_2$ + CH_3O_2
18	CO_2 + hν → CO + O	47*	ACET + hν → 2CH_3O_2 + CO
19	$ClNO_2$ + hν → Cl + NO_2	48	HACET + hν → $CH_3C(O)O_2$ + CH_2O + HO_2
20	$BrONO_2$ + hν → Br + NO_3	49°	MGLY + hν → $CH_3C(O)O_2$ + CO + HO_2
21	BrCl + hν → Br + Cl	50	GLY ALD + hν → CH_2O + CO + 2HO_2
22	HOBr + hν → Br + OH	51	GLY ALD + hν → CO (+CH_3OH)
23	NO + hν → N + O	52	GC(O)OOH + hν → CH_2O + CO_2 + OH + HO_2
24°	NO_3 + hν → NO_2 + O	53	POOH + hν → CH_3CHO + CH_2O + OH + HO_2
25°	NO_3 + hν → NO + O_2	54	ISOPOOH + hν → MACR + CH_2O + OH + HO_2
26*	CCl_4 + hν → 4Cl (+ products)	55*	ISON + hν → MACR + CH_2O + HO_2 + NO_2
27*	$CFCl_3$ + hν → 3Cl + HF (+ products)	56	MACR + hν → $CH_3C(O)O_2$ + CH_2O + CO + HO_2
28*	CF_2Cl_2 + hν → 2Cl + COF_2 (+ products)	57*	MPAN + hν → $MACRO_2$ + NO_2
29*	CH_3Cl + hν → Cl (+ products)	58	MACROOH + hν → 0.5HACET + 0.5MGLY + 0.5CH_2O + 0.5CO + OH + HO_2
30*	CH_3Br + hν → Br (+ products)		
		59	NALD + hν → CH_2O + CO + HO_2 + NO_2

Table 4. Heterogeneous Reactions

No.	Reactions
On sulfate, sea salt, tropospheric cloud particles	
g1	$ClONO_2$ + $(H_2O)_l$ → HOCl + HNO_3
g2	N_2O_5 + $(H_2O)_l$ → 2HNO_3
g3	$BrONO_2$ + $(H_2O)_l$ → HOBr + HNO_3
g4	HO_2 + $(H_2O)_l$ → 0.5H_2O_2 + 0.5O_2
g5	EO_2 + $(H_2O)_l$ → (2/3)POOH
g6	PO_2 + $(H_2O)_l$ → POOH
g7	$ISOPO_2$ + $(H_2O)_l$ → ISOPOOH
g8	$MACRO_2$ + $(H_2O)_l$ → MACROOH
g9	CH_3COO_2 + $(H_2O)_l$ → HO_2 (+ CH_3COOH)
g10	NO_2 + $(H_2O)_l$ → 0.5NO_2 + 0.5HNO_3
On polar stratospheric cloud particles	
het1	$ClONO_2$ + $(H_2O)_s$ → HOCl + $(HNO_3)_s$
het2	$ClONO_2$ + $(HCl)_s$ → Cl_2 + $(HNO_3)_s$
het3	N_2O_5 + $(H_2O)_s$ → $(2HNO_3)_s$
het4	N_2O_5 + $(HCl)_s$ → $ClNO_2$ + $(HNO_3)_s$
het5	HOCl + $(HCl)_s$ → Cl_2 + $(H_2O)_s$
het6	HOBr + $(HCl)_s$ → BrCl + $(H_2O)_s$

Reactions on polar stratospheric clouds (PSCs)

Deushi and Shibata (2011)

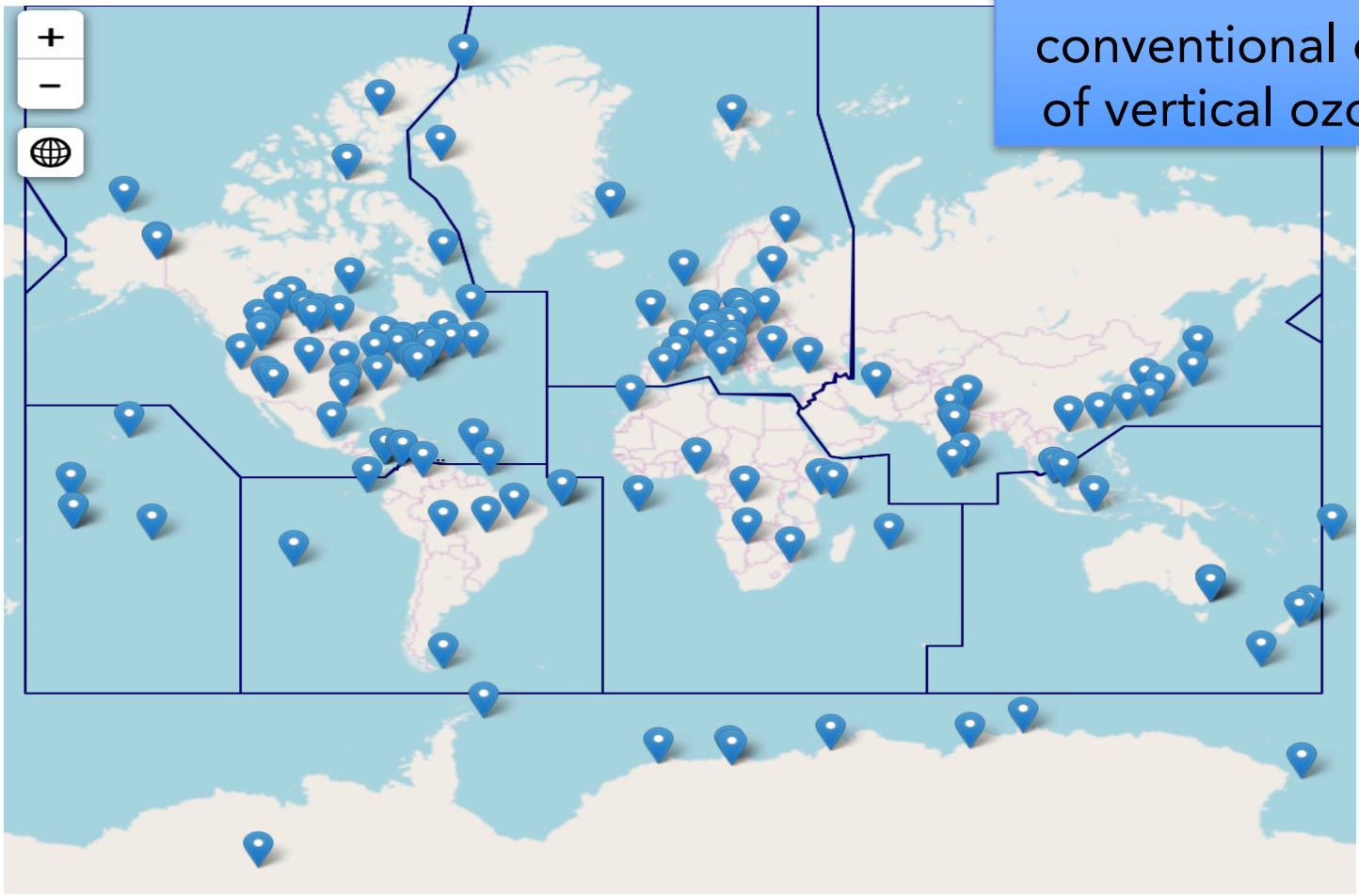

Consequently,
atmospheric chemistry models
are less-accurate or heavier…

What else?

What's atmospheric chemistry?

Difference #3 between NWP and AC modeling

- very few observations



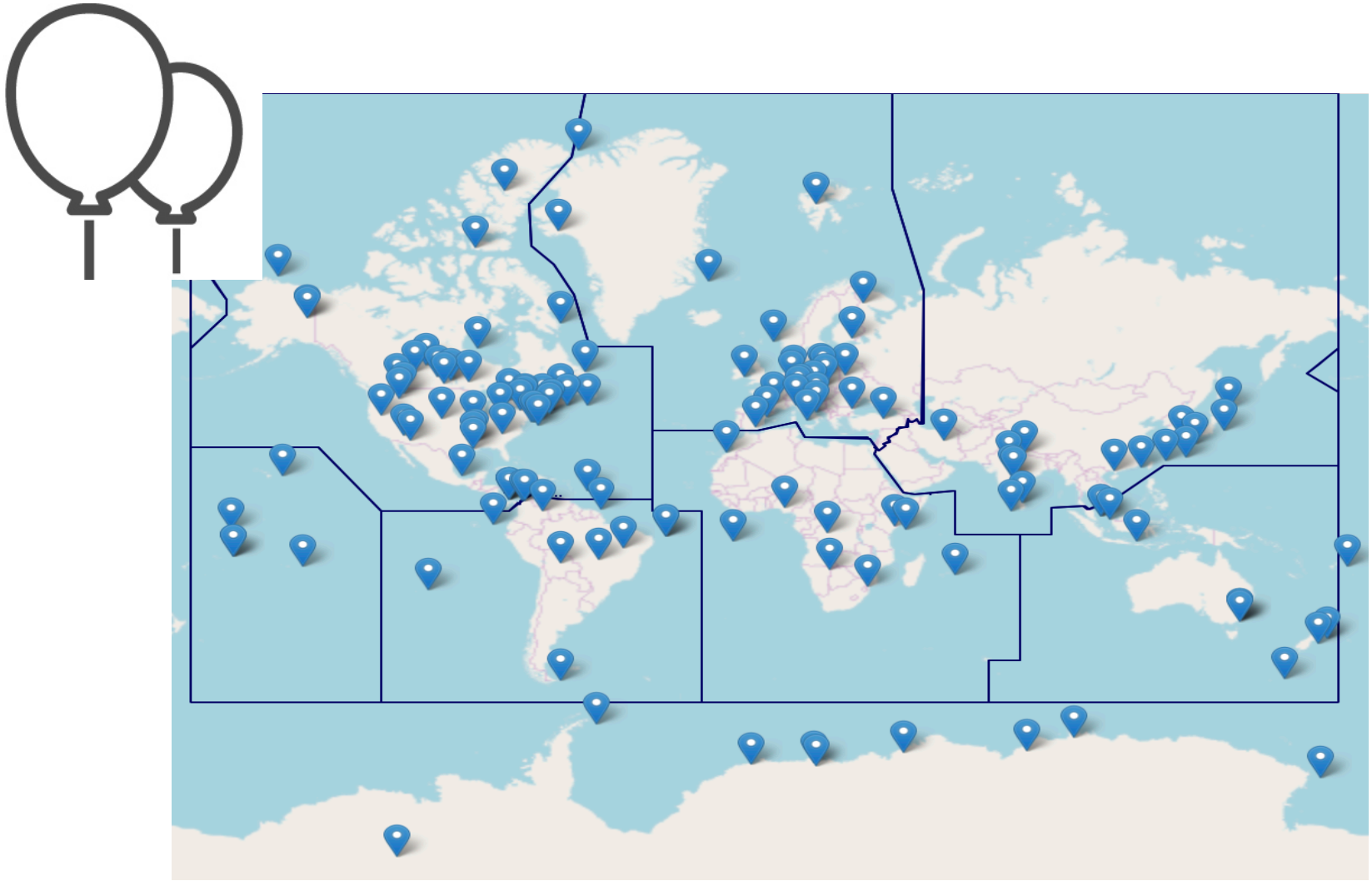
All the ozone sonde stations from 1962 to 2017 collected by WOUDC/WMO

Dawn of atmospheric chemistry data assimilation

from the 1990s to the 2000s

Expansion of observations

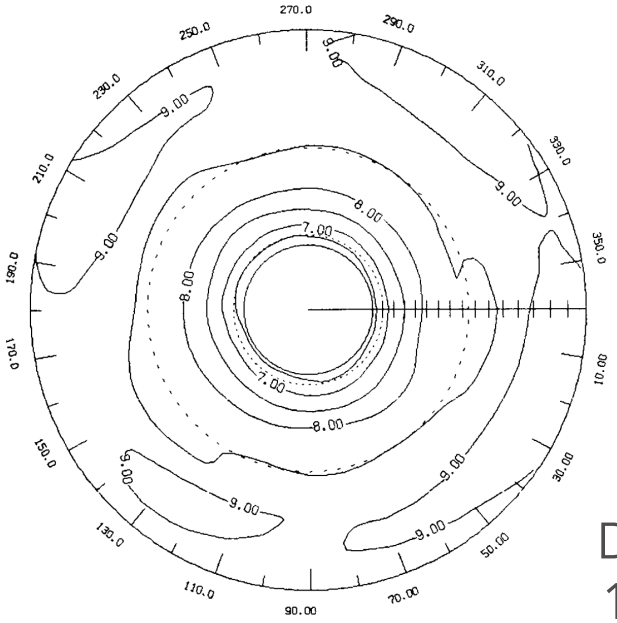
- Example: conventional ozone observations

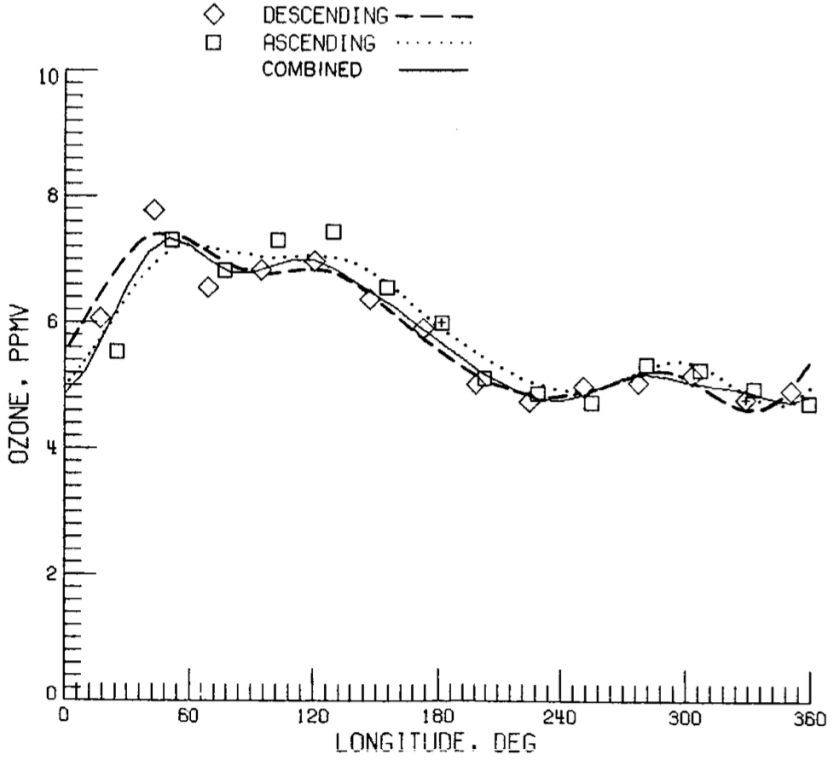


All the ozone sonde stations from 1962 to 2017 collected by WOUDC/WMO

Expansion of observations

- Example: non-conventional ozone observations





(c) At 48°N (see fig. 7 for latitude position).

Nimbus 7 LIMS ozone observations at 10 hPa on January 2, 1979 ©NASA

Data available every 4° of latitude at 100, 70, 50, 30, 16, 10, 7, 5, 3, 2, 1.5, 1, 0.7, 0.5, 0.4, 0.2, 0.1, and 0.05 hPa

Figure 6. Combined mode LAMAT ozone mixing ratio at 10 mbar for Jan. 2 in Southern Hemisphere with 1-2-1 latitude smoothing. Greenwich meridian is marked at 4° intervals from 0° to 84°S with dashed circles at 30°S and 60°S. Contour spacing is 0.5 ppmv.

Very early stage in the 1990s

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 97, NO. D2, PAGES 2569–2588, FEBRUARY 20, 1992

1992

Toward the Four Dimensional Assimilation of Stratospheric Chemical Constituents

Method: Nudging

JOHN AUSTIN[1]

Department of Atmospheric Sciences, University of Washington, Seattle

A model to assimilate stratospheric chemical constituents is proposed. The chemical transport model used is two dimensional on an isentropic surface and solves the photochemical equations using an extended family approach. Thirty-day integrations are performed at the three isentropic surfaces given by the potential temperature values 600 K, 850 K and 1400 K starting on January 1, 1979. During the integrations, Limb Infrared Monitor of the Stratosphere (LIMS) satellite data are assimilated into the model and the results are compared with independently mapped (map archive tape (MAT)) data. The assimilation results are found to be in good agreement with the independent analyses at all three levels. Preliminary assimilations revealed significant biases in modeled HNO_3 at 850 K and in O_3 at 1400 K. However, by changing the adjustable parameters of the assimilation model the HNO_3 bias was successfully eliminated. The O_3 bias was easily eliminated by the addition of an extra source term. The comparisons reveal possible minor weaknesses in the MAT analyses. First, the chemical constituents appear to be occasionally in error in the MAT data during rapidly changing dynamical events such as stratospheric warmings. Second, the temporal continuity is sometimes lacking in the MAT analyses, leading to rapidly changing concentrations which cannot be understood on the basis of conventionally understood photochemistry. On the other hand, the assimilation model used here does not produce very satisfactory analyses when the chemical data are very noisy. The differences between the assimilated and MAT analyses are quite small and are generally less than data errors. Although the assimilation model is here applied to LIMS data, the method is generally applicable to any data source and could be especially useful for analyzing the large volume of data from the Upper Atmosphere Research Satellite.

Very early stage in the 1990s

1995

Q. J. R. Meteorol. Soc. (1995), **121**, pp. 1681–1704

Lagrangian four-dimensional variational data assimilation of chemical species

By M. FISHER*[1] and D. J. LARY[2]

[1]*Meteorological Office, UK*
[2]*Cambridge University, UK*

(Received 15 March 1994; revised 16 December 1994)

SUMMARY

For the first time, the method of four-dimensional variational data assimilation is applied to the analysis of
tions with a numerical model to analyse simultaneously
ethod is able to exploit information which is not available
se can be made of asynoptic observations even for species
produced. A Lagrangian approach is adopted, allowing a
ly reduces the computational expense of the method.

1996

Q. J. R. Meteorol. Soc. (1996), **122**, pp. 1545–1571

On four-dimensional variational assimilation of ozone data in weather-prediction models

By LARS PETER RIISHØJGAARD*

Danish Meteorological Institute, Denmark

(Received 6 December 1994; revised 9 February 1996)

SUMMARY

Routinely made satellite observations of total ozone contain information about the dynamical state of the atmosphere in the regions where the ozone gradients are strong. It is argued that four-dimensional variational assimilation (4D-VAR) of these data with a meteorological model may be a way of extracting this information in order to use it for determining the initial condition of the model. In the first part of this paper the problem of assimilating ozone data in a variational context is discussed. In the second part a series of simple experiments is presented in which ozone pseudo-observations are assimilated with a barotropic vorticity-equation model. The aim of these experiments is to examine whether the atmospheric flow at a given level near the tropopause can be reconstructed by a 4D-VAR scheme using a series of simulated observations of passive tracer mixing ratios. Both data produced by the assimilating model itself and data generated by a more realistic three-dimensional model have been tested. It is found that when started from a purely zonal flow field, 4D-VAR can to a large extent reconstruct the flow field, using only observations of the mixing ratio of the tracer. The quality of the result depends on the resolution of the model and on the choice of the length of the assimilation window.

Method: 4D-Var

But models are very poor…


After 10-year advancements
in computer and model
performance...

Progress in the 2000s

Atmos. Chem. Phys., 7, 5695–5710, 2007
www.atmos-chem-phys.net/7/5695/2007/

2007

Atmospheric Chemistry and Physics

Evaluating model performance of an ensemble-based chemical data assimilation system during INTEX-B field mission

Method: EnKF

A. F. Arellano Jr.[1], K. Raeder[2], J. L. Anderson[2], P. G. Hess[1], L. K. Emmons[1], D. P. Edwards[1], G. G. Pfister[1], T. L. Campos[1], and G. W. Sachse[3]

[1]Atmospheric Chemistry Division, Earth and Sun Systems Laboratory, National Center for Atmospheric Research, PO Box 3000, Boulder, Colorado 80307-3000, USA
[2]Institute for Mathematics Applied to Geosciences, Computational and Information Systems Laboratory, National Center for Atmospheric Research, PO Box 3000, Boulder, Colorado, 80307-3000, USA
[3]Chemistry and Dynamics Branch, NASA Langley Research Center, Hampton, Virginia, 23681-2199, USA

Received: 1 June 2007 – Published in Atmos. Chem. Phys. Discuss.: 5 July 2007
Revised: 30 October 2007 – Accepted: 31 October 2007 – Published: 16 November 2007

Abstract. We present a global chemical data assimilation system using a global atmosphere model, the Community Atmosphere Model (CAM3) with simplified chemistry and the Data Assimilation Research Testbed (DART) assimilation package. DART is a community software facility for assimilation studies using the ensemble Kalman filter approach. Here, we apply the assimilation system to constrain global tropospheric carbon monoxide (CO) by assimilating meteorological observations of temperature and horizontal wind velocity and satellite CO retrievals from the Measurement of Pollution in the Troposphere (MOPITT) satellite instrument.

1 Introduction

The availabi… …r global and long-term measurements of tropospheric chemi… …from space offers an opportunity t… composition t… predictions fr… tral to this inte… that is reasona… surements of various scales and of various chemical species. Such a system is useful as a tool in providing initial condi-

Very early work of the chemical data assimilation using EnKF (NCAR DART package)

Progress in the 2000s

Atmos. Chem. Phys., 7, 5695–5710, 2007
www.atmos-chem-phys.net/7/5695/2007/

2007

Atmospheric Chemistry and Physics

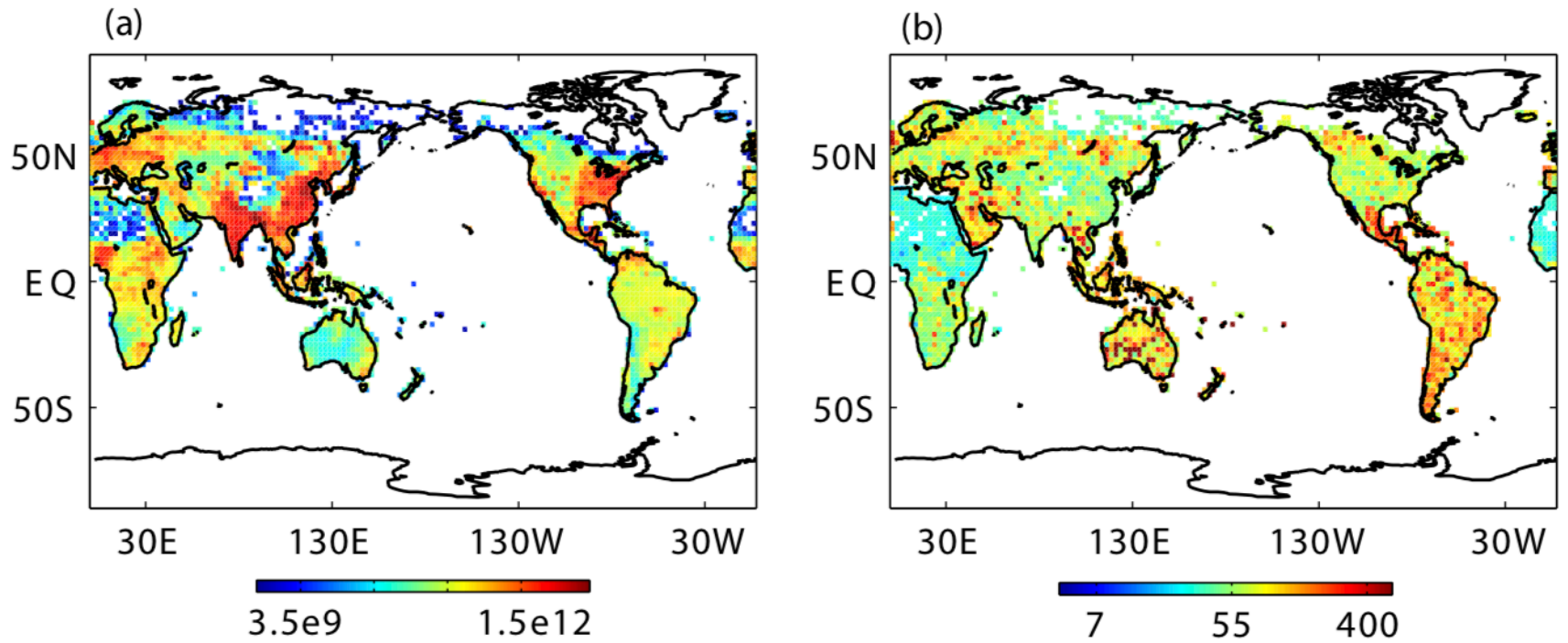


Fig. 2. Ensemble-spread of CAM3 total surface CO emissions for the month of April 2006 in molecules/cm^2/s **(a)**, and in percentage % relative to ensemble mean emissions **(b)**.

EnKF

mical
nKF
)

Progress in the 2000s

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 114, D13205, doi:10.1029/2008JD011115, 2009

2009

Aerosol analysis and forecast in the European Centre for Medium-Range Weather Forecasts Integrated Forecast System: 2. Data assimilation

Method: 4D-Var

A. Benedetti,[1] J.-J. Morcrette,[1] O. Boucher,[2] A. Dethof,[1] R. J. Engelen,[1] M. Fisher,[1] H. Flentje,[3] N. Huneeus,[4] L. Jones,[1] J. W. Kaiser,[1] S. Kinne,[5] A. Mangold,[6] M. Razinger,[1] A. J. Simmons,[1] and M. Suttie[1]

Received 5 September 2008; revised 30 April 2009; accepted 6 May 2009; published 11 July 2009.

[1] This study presents the new aerosol assimilation system, developed at the European Centre for Medium-Range Weather Forecasts, for the Global and regional Earth-system Monitoring using Satellite and in-situ data (GEMS) project. The aerosol modeling and analysis system is fully integrated in the operational four-dimensional assimilation apparatus. Its purpose is to produce osol forecasts and reanalyses of aerosol fields using optical depth data from satelli sors. This paper is the second of a series which describes the GEMS aero t. It focuses on the theoretical architecture and practical implementation of th assimilation system. It also provides a discussion of the background err rvations errors for the aerosol fields, and presents a subset of hich has been run for 2003 and 2004 using data from Spectroradiometer on the Aqua and Terra satellites. how that despite some compromises that have been rds to the choice of control variable and error killful in drawing to the observations and in improving the forecasts of aerosol optical depth.

Their chemistry forecast model is based on the ECMWF operational NWP model.

LETKF for aerosol data assimilation

Atmos. Chem. Phys., 10, 39–49, 2010
www.atmos-chem-phys.net/10/39/2010/

2010

Atmospheric Chemistry and Physics

Data assimilation of CALIPSO aerosol observations

Method: LETKF

T. T. Sekiyama[1], **T. Y. Tanaka**[1], **A. Shimizu**[2], **and T. Miyoshi**[3,*]

[1]Meteorological Research Institute, Tsukuba, Japan
[2]National Institute for Environmental Studies, Tsukuba, Japan
[3]Japan Meteorological Agency, Tokyo, Japan
[*]now at: Department of Atmospheric and Oceanic Science, University of Maryland, College Park, Maryland, USA

Received: 17 December 2008 – Published in Atmos. Chem. Phys. Discuss.: 4 March 2009
Revised: 1 December 2009 – Accepted: 4 December 2009 – Published: 5 January 2010

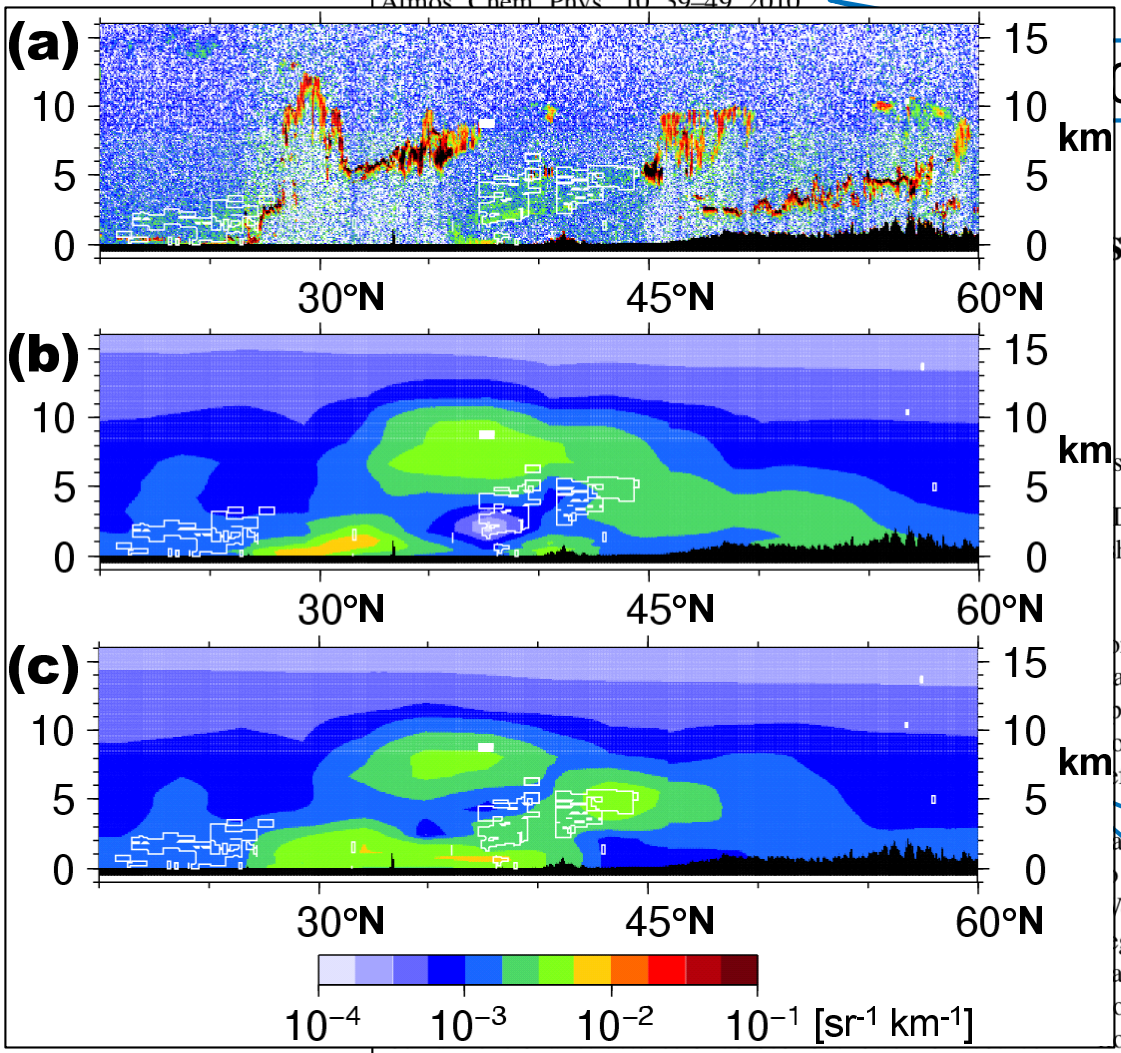
Abstract. We have developed an advanced data assimilation system for a global aerosol model with a four-dimensional ensemble Kalman filter in which the Level 1B data from the Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO) were successfully assimilated for the first time, to the best of the authors' knowledge. A one-month data assimilation cycle experiment for dust, sulfate, and sea-salt aerosols was performed in May 2007. The results were validated via two independent observations: 1) the ground-based lidar network in East Asia, managed by the National Institute for Environmental Studies of Japan, and 2) weather reports of aeolian dust events in Japan. Detailed four-dimensional structures of aerosol outflows from source regions over oceans and continents for various particle types and sizes were well reproduced. The intensity of dust emission at each grid point was also corrected by this data assimilation system. These results are valuable for the comprehensive analysis of aerosol behavior as well as aerosol forecasting.

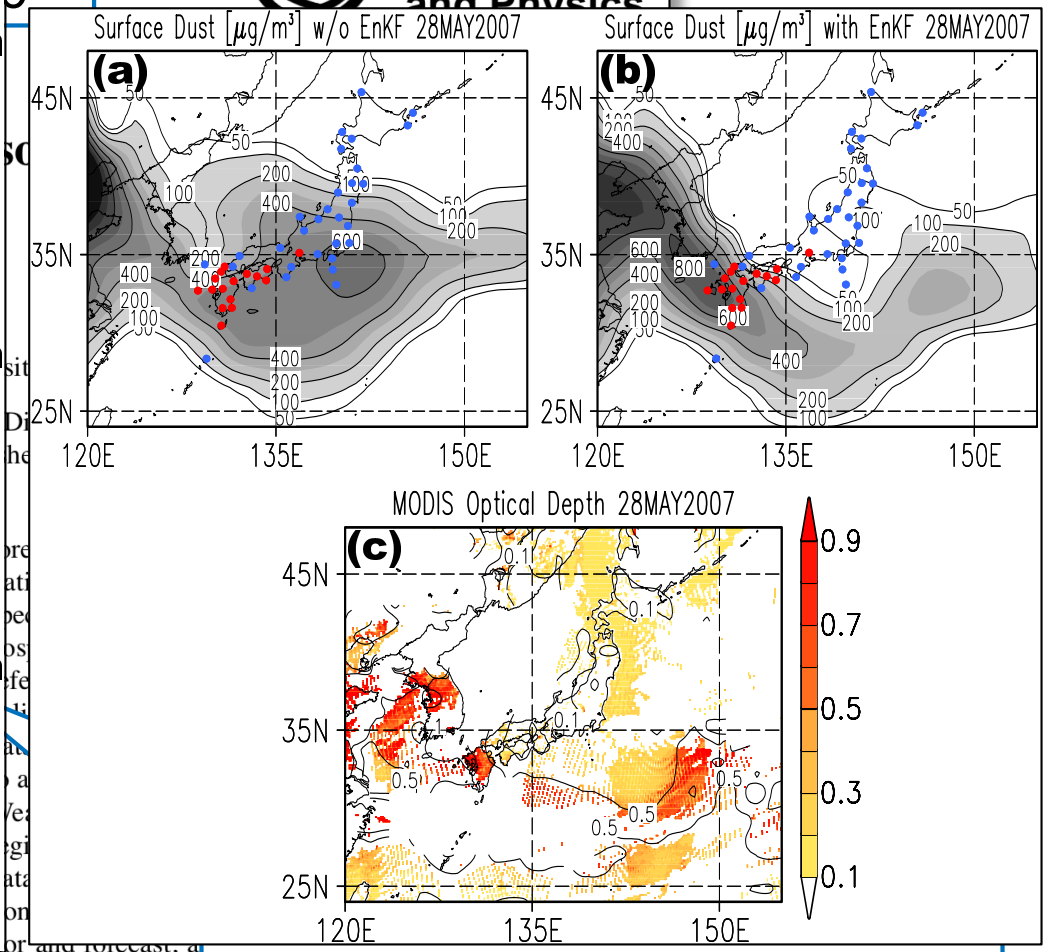
forecasts (cf. Kalnay, 2003). Additionally, some data assimilation analyses have been applied to atmospheric chemical species (e.g., stratospheric ozone by Geer et al., 2006; tropospheric carbon monoxide by Arellano et al., 2007, and references therein). Compared with the long history and

The first paper on chemical data assimilation using satellite LIDAR observations.

One of the first works for atmospheric chemistry using LETKF.

LETKF for aerosol data assimilation





Atmospheric Chemistry and Physics

regions over oceans and continents for various particle types and sizes were well reproduced. The intensity of dust emission at each grid point was also corrected by this data assimilation system. These results are valuable for the comprehensive analysis of aerosol behavior as well as aerosol forecasting.

black-carbon aeros
servations used in
optical depth data
Spectro-radiometer
satellites. Zhang et
simulation system
observations, to improve Naval Research Laboratory (NRL)

One of the first works for atmospheric chemistry using LETKF.

Status quo of atmospheric chemistry data assimilation

contribution to environment and health issues

LETKF for complicated ozone chemistry

Atmos. Chem. Phys., 12, 9545–9579, 2012
www.atmos-chem-phys.net/12/9545/2012/
doi:10.5194/acp-12-9545-2012

2012

Atmospheric Chemistry and Physics

Method: LETKF

Simultaneous assimilation of satellite NO_2, O_3, CO, and HNO_3 data for the analysis of tropospheric chemical composition and emissions

K. Miyazaki[1,2], H. J. Eskes[1], K. Sudo[2,3], M. Takigawa[2], M. van Weele[1], and K. F. Boersma[1,4]

[1]Royal Netherlands Meteorological Institute (KNMI), Wilhelminalaan 10, 3732 GK, De Bilt, The Netherlands
[2]Japan Agency for Marine-Earth Science and Technology, Yokohama, Japan
[3]Graduate School of Environmental Studies, Nagoya University, Nagoya, Japan
[4]Eindhoven University of Technology, Fluid Dynamics Lab, Eindhoven, The Netherlands

Correspondence to: K. Miyazaki (miyazaki@knmi.nl)

Received: 22 May 2012 – Published in Atmos. Chem. Phys. Discuss.:
Revised: 3 October 2012 – Accepted: 4 October 2012 – Published: 22

Abstract. We have developed an advanced chemical data assimilation system to combine observations of chemical compounds from multiple satellites. NO_2, O_3, CO, and HNO_3 measurements from the Ozone Monitoring Instrument (OMI), Tropospheric Emission Spectrometer (TES), Measurement of Pollution in the Troposphere (MOPITT), relat
The simultaneous adjustment of the emissions and concentrations is a powerful approach to correcting the tropospheric ozone budget and profile analyses.

Probably, this is the first paper on the multiple chemical data assimilation to demonstrate the correlation between chemical constituents.

LETKF for complicated ozone chemistry

Atmos. Chem. Phys., 12, 9545–9579, 2012
www.atmos-chem-phys.net/12/9545/2012/

2012

Atmospheric

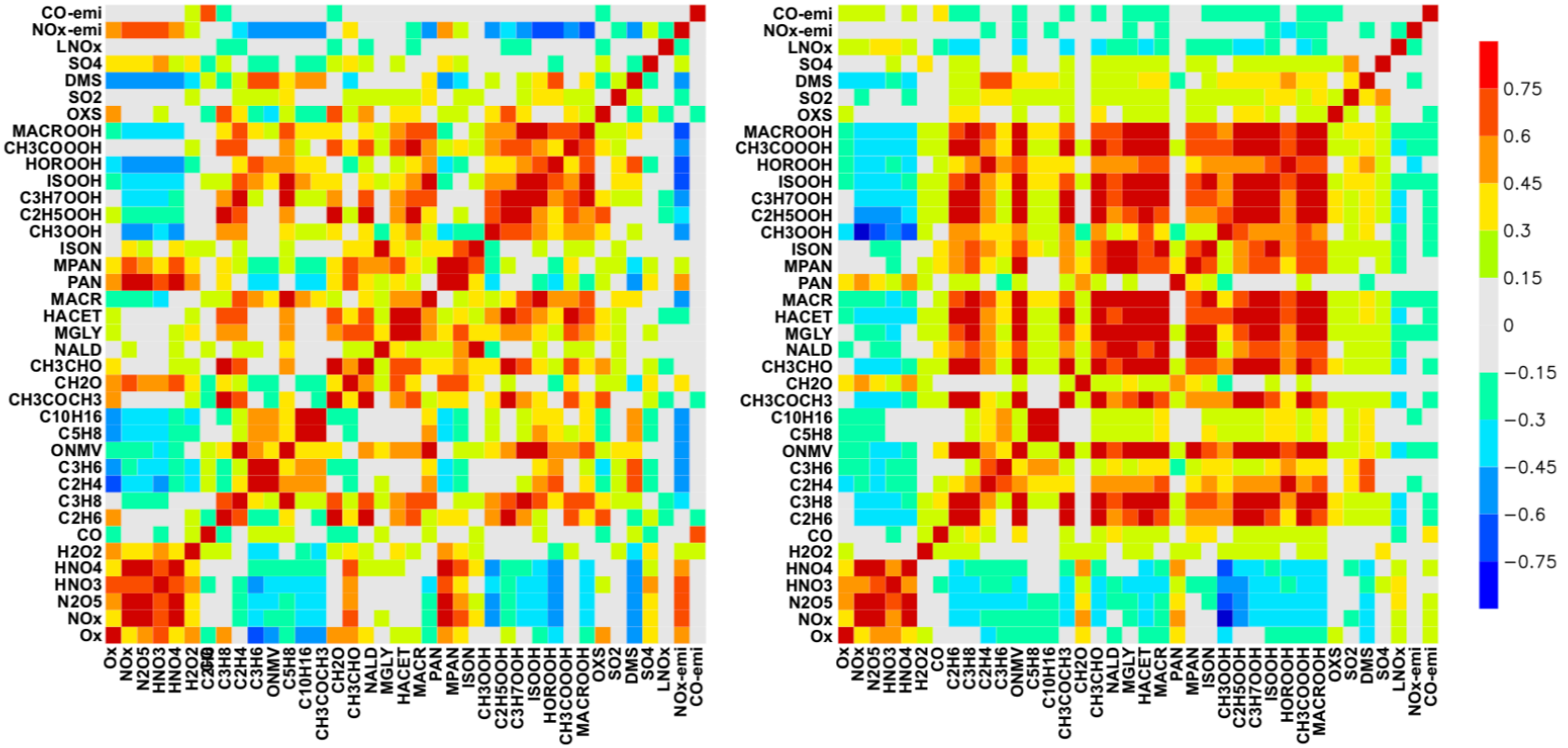


Fig. 3. Correlations between species in the background error covariance matrix, estimated from the LETKF ensemble at 950 hPa (left) and 500 hPa (right) averaged over 15–20 July 2007. The global mean of the covariance estimated for each grid point is plotted. The matrix includes concentrations of all the predicted species, surface NO_x emission (NO_x-emi.), surface CO emissions (CO-emi.), and lightning NO_x sources (LNO_x). O_x is the sum of O_3 and $O(^1D)$, and NO_x is the sum of NO, NO_2, and NO_3. The red (blue) colour represents positive (negative) correlations.

ment (OMI), Tropospheric Emission Spectrometer (TES), Measurement of Pollution in the Troposphere (MOPITT),

ozone budget and profile analyses.

LETKF for CO_2 flux estimation (OSSE)

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 116, D09110, doi:10.1029/2010JD014673, 2011

2011

"Variable localization" in an ensemble Kalman filter: Application to the carbon cycle data assimilation

Method: LETKF

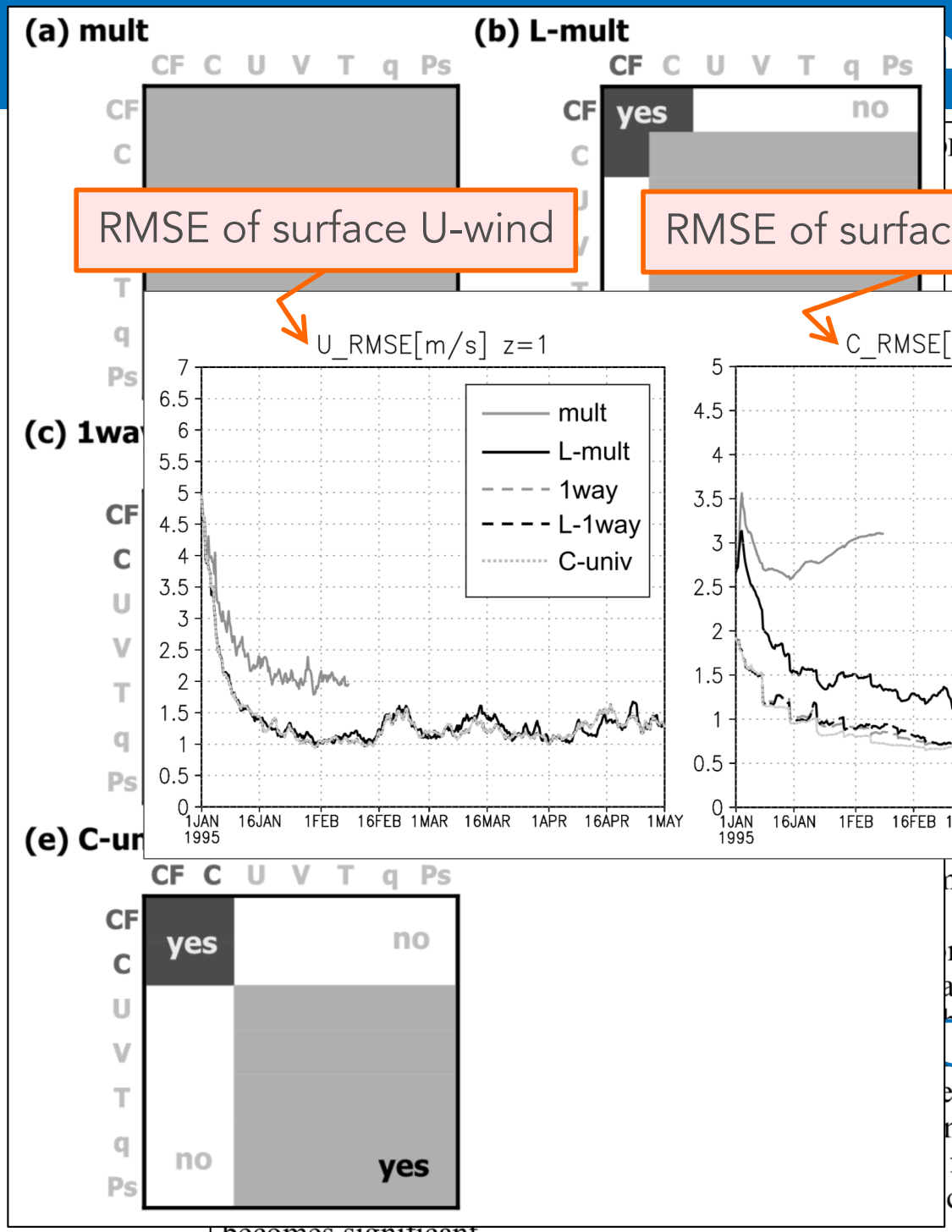
Ji-Sun Kang,[1] Eugenia Kalnay,[1] Junjie Liu,[2] Inez Fung,[2] Takemasa Miyoshi,[1] and Kayo Ide[1]

Received 28 June 2010; revised 17 February 2011; accepted 24 February 2011; published 12 May 2011.

[1] In ensemble Kalman filter, space localization is used to reduce the impact of long-distance sampling errors in the ensemble estimation of the forecast error covariance. When two variables are not physically correlated, their error covariance is still estimated by the ensemble and, therefore, it is dominated by sampling errors. We introduce a "variable localization" method, zeroing out such covariances between unrelated variables to the problem of assimilating carbon dioxide concentrations into a dynamical model using the local ensemble transform Kalman filter (LETKF) in an observing system simulation experiments (OSSE) framework. A system where meteorological and carbon variables are simultaneously assimilated is used to estimate surface carbon fluxes that are not directly observed. A range of covariance structures are explored for the LETKF, with emphasis on configurations allowing nonzero error covariance between carbon variables and the wind field, which affects transport of atmo... CO_2 and the other meteorological variables. Such variable l... the background error covariance among prognostic va... related, thus reducing sampling errors. Results from the ide... that the performance in the estimation of surface carbon flu... localization is much better than that using a standard full ... relative improvement increases when the surface fluxes chan... becomes significant.

Though this is OSSE, they assimilate both concentration and meteorological observations using the variable localization.

(OSSE)



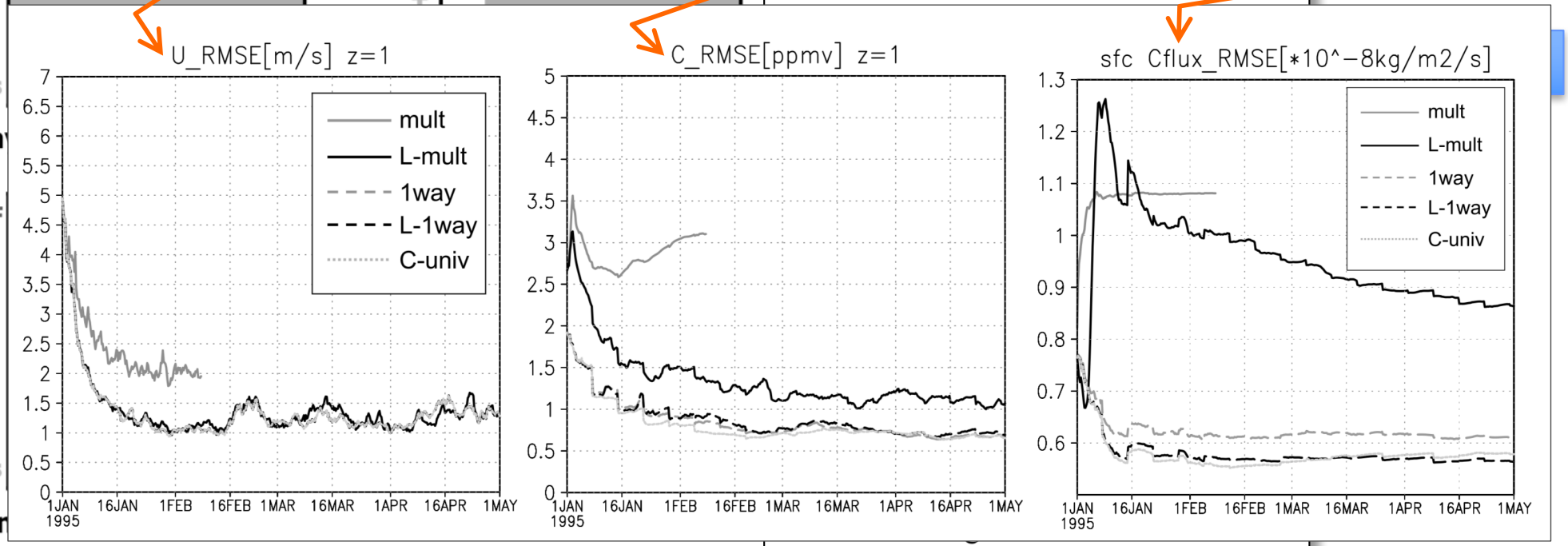
L. 116, D09110, doi:10.1029/2010JD014673, 2011

2011

RMSE of surface U-wind

RMSE of surface CO_2 Conc

RMSE of CO2 surface flux

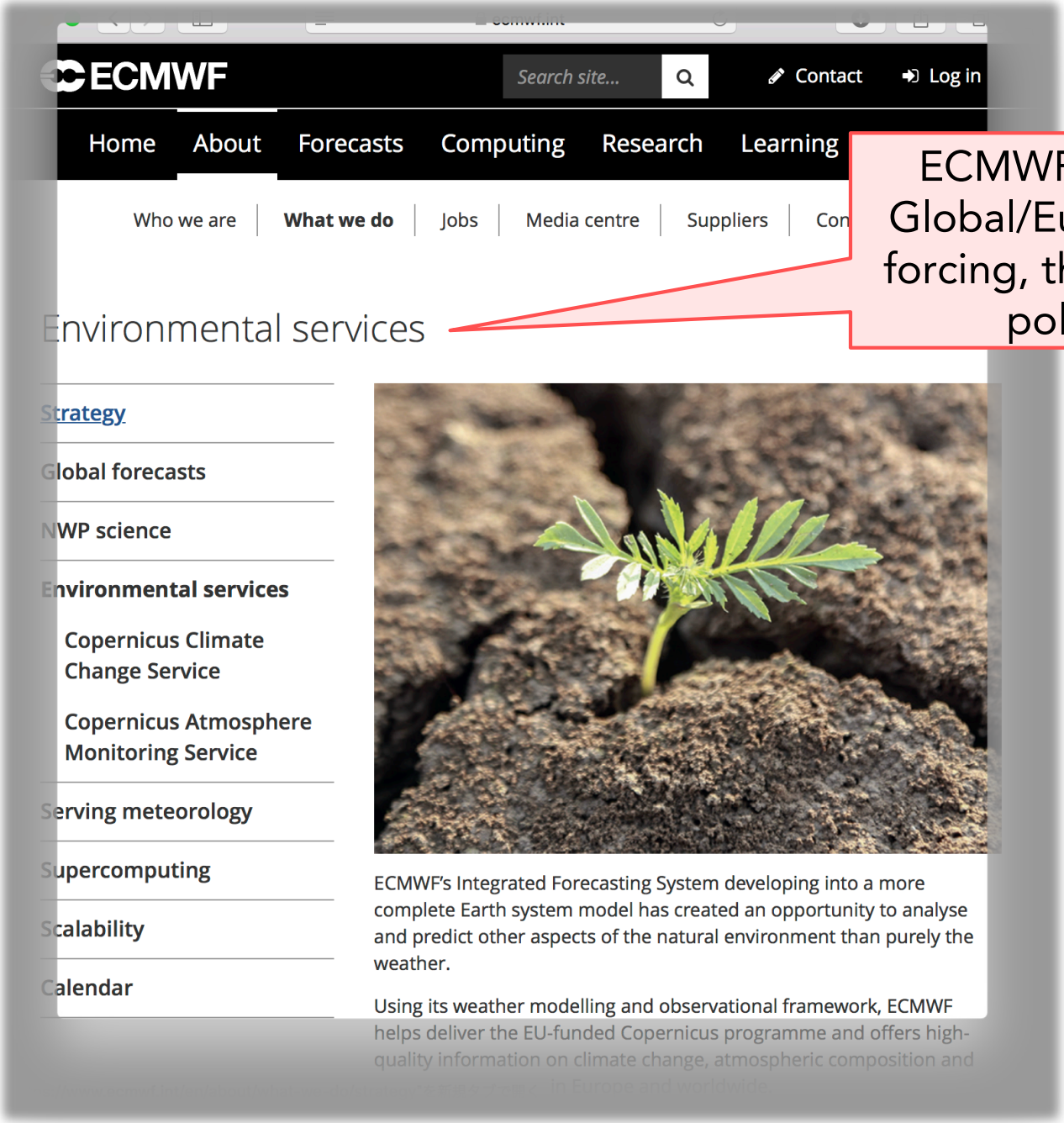


nate surface carbon fluxes that are
are explored for the LETKF,
r covariance between carbon

becomes significant.

Though this is OSSE, they assimilate both concentration and meteorological observations using the variable localization.

Operational products of ECMWF

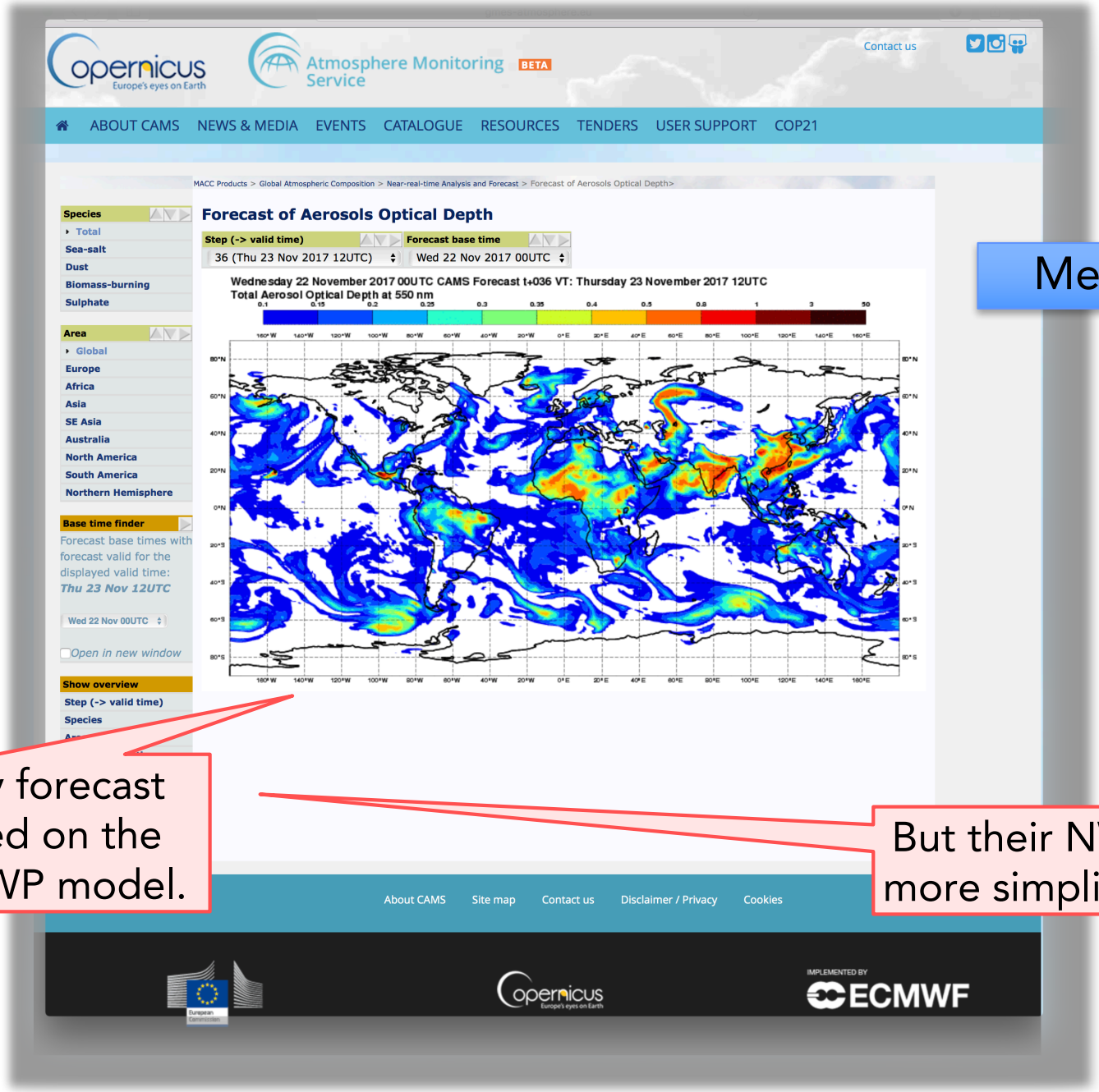


ECMWF provides information on Global/European air quality, climate forcing, the ozone layer and UV, and pollutant surface fluxes.

The air quality service is now officially one of the ECMWF's compulsory jobs.

ECMWF has been developing a data assimilation system of atmospheric chemistry for decades.

Operational products of ECMWF



Method: 4D-Var

The chemistry forecast model is based on the operational NWP model.

But their NWP model has more simplified chemistry.

Operational products of NOAA

U.S. Department of Commerce / National Oceanic & Atmospheric Administration / NOAA Research

Earth System Research Laboratory
Global Monitoring Division

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Carbon Tracker is a global CO_2 flux/concentration estimation service.

Method: EnKF

- FAQ
- Documentation
- Tutorial
- Collaborators
- Versions

Results

- Evaluation
- Fluxes
- Observations
- Mole Fractions
- Download

Resources

- Usage Policy
- E-mail List
- Contact Us
- CT on YouTube
- Glossary
- References

CarbonTracker CT2016

CarbonTracker is a CO_2 measurement and modeling system developed by NOAA to keep track of sources (emissions to the atmosphere) and sinks (removal from the atmosphere) of carbon dioxide around the world. CarbonTracker uses atmospheric CO_2 observations from a host of collaborators and simulated atmospheric transport to estimate these surface fluxes of CO_2. The current release of CarbonTracker, CT2016, provides global estimates of surface-atmosphere fluxes of CO_2 from January 2000 through December 2015.

What is CarbonTracker?

CarbonTracker is a global model of atmospheric carbon dioxide with a focus on North America, designed to keep track of CO_2 uptake and release at the Earth's surface over time. [read more]

Who needs CarbonTracker?

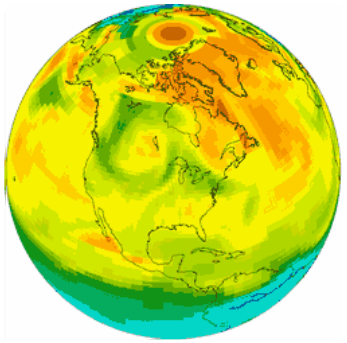
Policy makers, industry, scientists, and the public need CarbonTracker information to make informed decisions to limit greenhouse gas levels in the atmosphere. [read more]

What does CarbonTracker tell us?

North America is a source of CO_2 to the atmosphere. The natural uptake of CO_2 that occurs mostly east of the Rocky Mountains removes about a third of the CO_2 released by the use of fossil fuels. [read more]

What is new in this release of CarbonTracker? NEW!

This release of CarbonTracker ("CT2016") uses new hourly observations from GLOBALVIEW+ and refined first-guess flux models. [read more]



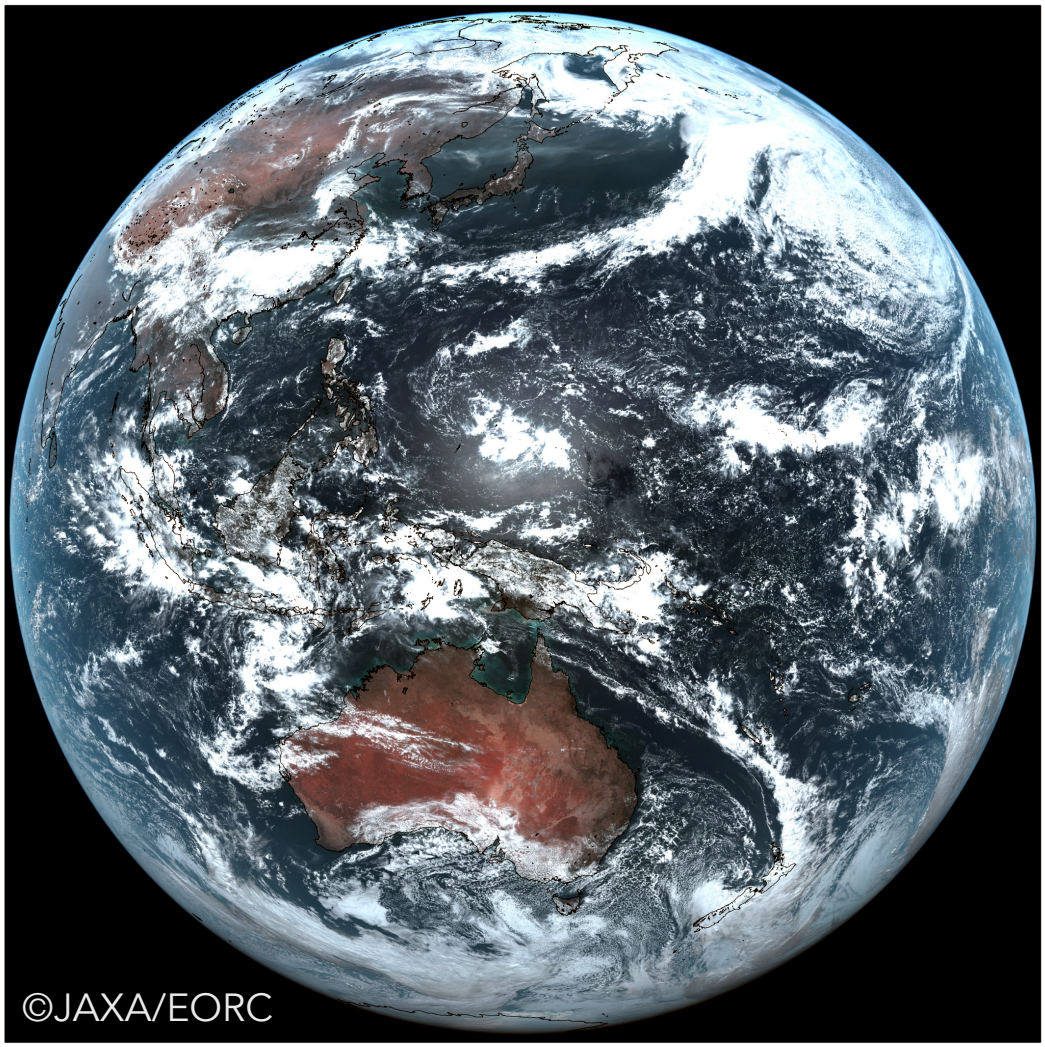
CarbonTracker CO_2 weather for June-July, 2008. *Warm colors show high atmospheric CO_2 concentrations, and cool colors show low concentrations. As the summer growing season takes hold, photosynthesis by forests and crops draws concentrations of CO_2 down, opposing the general increase from fossil fuel burning. The resulting high- and low-CO_2 air masses are then moved around by weather systems to form the patterns shown here. [More on CO_2 weather]*


Observation technology is
developing day by day.

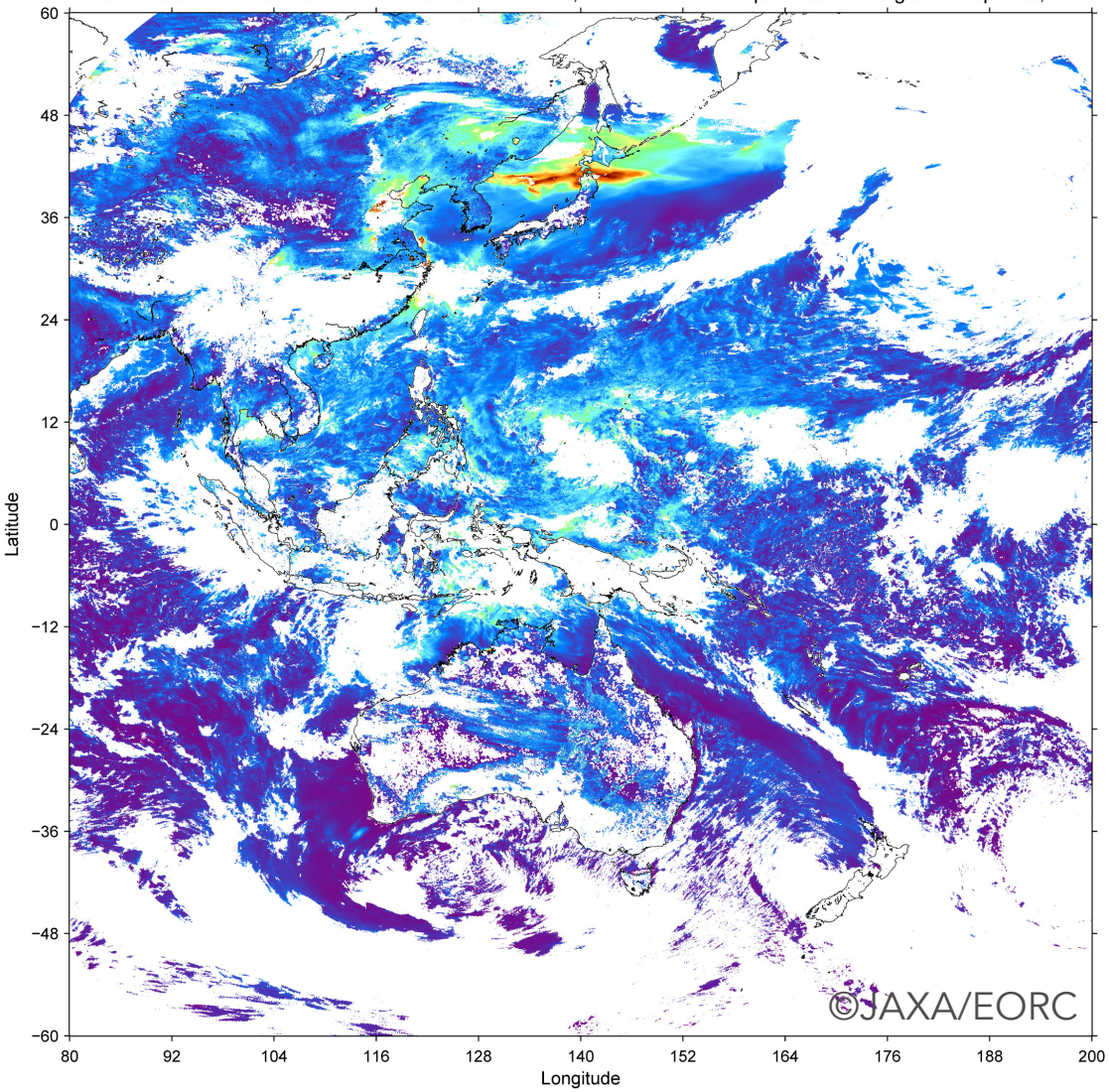
Himawari-8 aerosol product (since 2015)

- The latest geostationary RGB imager compatible with GOES-R's

HS−H08−20150427−0230−S21−FLDK.02750−02750.nc, Himawari−8 AHI standard map data, albedo−06



NC−H08−20150427−0600−R06OC−FLDK.02401−02401.nc, Himawari−8 AHI equal latitude−longitude map data, AOT−



Himawari-8 aerosol product in the near future

Method: LETKF

86 SOLA, 2016, Vol. 12, 86−90, doi:10.2151/sola.2016-020

Data Assimilation of Himawari-8 Aerosol Observations: Asian Dust Forecast in June 2015

Geophysical Research Letters

RESEARCH LETTER
10.1002/2016GL069298

Key Points:
- Next-generation geostationary meteorological satellite Himawari-8 launched on 7 October 2014
- Himawari-8 provides full-disk aerosol optical properties at 10 min intervals from geostationary orbit
- Promising results of aerosol assimilation experiment on Himawari-8 retrievals

Supporting Information:
- Supporting Information S1
- Figure S1
- Figure S2
- Figure S3
- Text S1
- Movie S1

Correspondence to:
K. Yumimoto,
yumimoto@mri-jma.go.jp

Citation:
Yumimoto, K., et al. (2016), Aerosol data

Aerosol data assimilation using data from Himawari-8, a next-generation geostationary meteorological satellite

K. Yumimoto[1], T.M. Nagao[2], M. Kikuchi[2], T.T Sekiyama[1], H. Murakami[2], T.Y. Tanaka[1], A. Ogi[3], H. Irie[4], P. Khatri[4,5], H. Okumura[6], K. Arai[6], I. Morino[7], O. Uchino[1,7], and T. Maki[1]

[1]Meteorological Research Institute, Japan Meteorological Agency, Tsukuba, Japan, [2]Earth Observation Research Center, Japan Aerospace Exploration Agency, Tsukuba, Japan, [3]Japan Meteorological Agency, Tokyo, Japan, [4]Center for Environmental Remote Sensing (CERes), Chiba University, Chiba, Japan, [5]Now at Center for Atmospheric and Oceanic Studies, Graduate School of Science, Tohoku University, Sendai, Japan, [6]Graduate School of Science and Engineering, Saga University, Saga, Japan, [7]National Institute for Environmental Studies, Tsukuba, Japan

Abstract Himawari-8, a next-generation geostationary meteorological satellite, was launched on 7 October 2014 and became operational on 7 July 2015. The advanced imager on board Himawari-8 is equipped with 16 observational bands (including three visible and three near-infrared bands) that enable retrieval of full-disk aerosol optical properties at 10 min intervals from geostationary (GEO) orbit. Here we show the first application of aerosol optical properties (AOPs) derived from Himawari-8 data to aerosol data assimilation. Validation of the assimilation experiment by comparison with independent observations demonstrated successful modeling of continental pollution that was not predicted by simulation without assimilation and reduced overestimates of dust front concentrations. These promising results suggest that AOPs derived from Himawari-8/9 and other planned GEO satellites will considerably improve forecasts of air quality, inverse modeling of emissions, and aerosol reanalysis through assimilation techniques.

Future of atmospheric chemistry data assimilation

integration with NWP

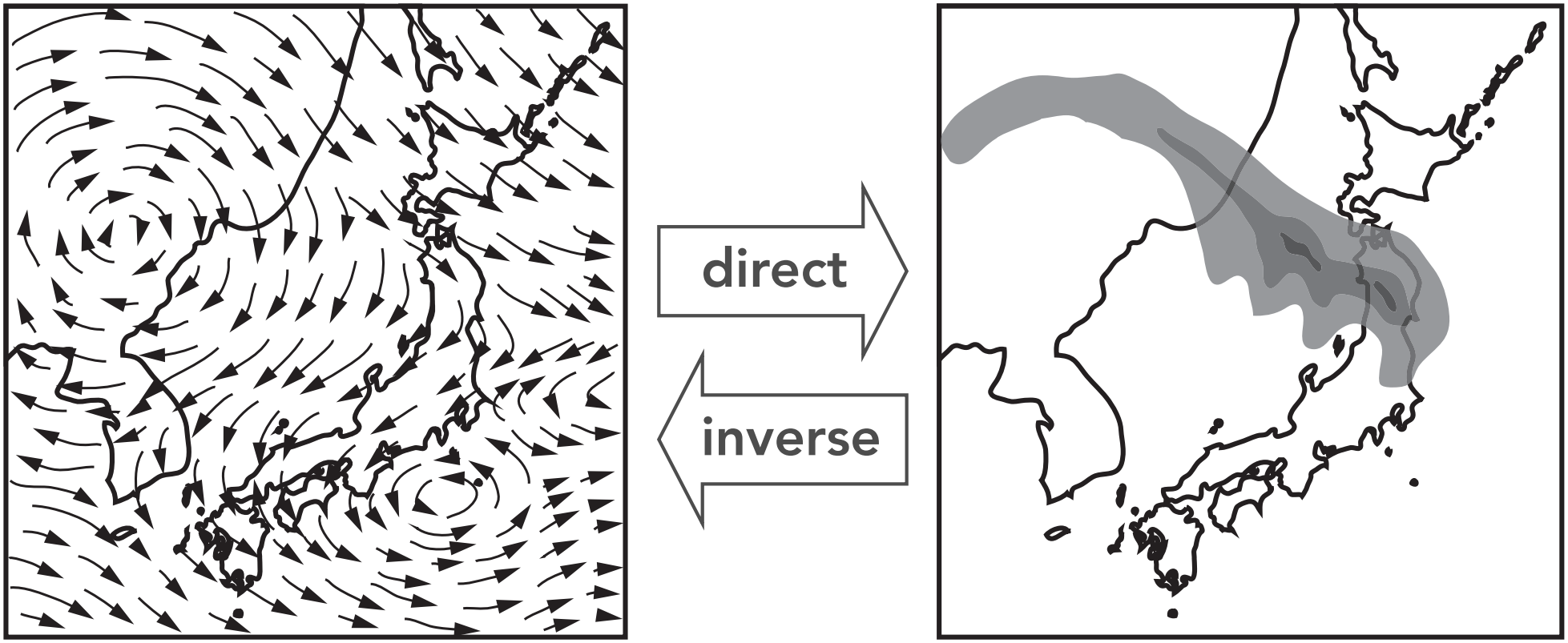
Integration of Atmospheric Chemistry with NWP

- Contribution to radiation (indirect interaction)
  - O_3, CO_2, aerosols,…
    - Model temperature through the radiation data assimilation
    - Improvement of radiative budget
- **Contribution to dynamics** (direct interaction)
  - **Constituents are tracers of advection**

    ➜ Wind fields could be inversely estimated.
    - **O_3 in the stratosphere**
    - **CO_2/CO/aerosols in the troposphere**

Integration of Atmospheric Chemistry with NWP

- Theoretically possible (e.g., many successful OSSEs), but not well-known for the real situations.



Wind Field

Concentration Distribution

Integration of Atmospheric Chemistry with NWP

GEOPHYSICAL RESEARCH LETTERS, VOL. 37, L17801, doi:10.1029/2010GL044416, 2010

Method: EnKF

Constraints on black carbon aerosol distribution from Measurement of Pollution in the Troposphere (MOPITT) CO

Avelino F. Arellano Jr.,[1,2] Peter G. Hess,[3] D. P. Edwards,[1] and D. Baumgardner[4]

Received 18 June 2010; revised 12 July 2010; accepted 26 July 2010; published 1 September 2010.

[1] We present an approach to constrain simulated atmospheric black carbon (BC) using carbon monoxide (CO) observations. The approach uses: (1) the Community Atmosphere Model with Chemistry to simulate the evolution of BC and CO within an ensemble of model simulations; (2) satellite CO retrievals from the MOPITT/Terra instrument to assimilate observed CO into these simulations; (3) the derived sensitivity of BC to CO within these simulations to correct the simulated BC distributions. We demonstrate the performance of this approach through model experiments with and without the BC corrections during the period coinciding with the Intercontinental Chemical Transport Experiment (INTEX-B). Our results show significant improvements (~50%) in median BC profiles using constraints from MOPITT, based on comparisons with INTEX-B measurements. We find that assimilating MOPITT CO provides considerable impact on simulated BC concentrations, especially over source regions. This approach offers an opportunity to augment our current ability to predict BC distributions.

bon and the large uncertainty in its emissions hinders our kn ledge of its importance to present radiative forcing.

[3] atly, direct measurements of BC are limited across a f surface stations and aircraft flights taken from a nu ific field campaigns. Indirect measurements of in the form of retrievals of aer gro rep tio det sur aer pre a c 20 sion inventories [e.g., *Bond et al.*, 2004]. The conventional approach maintains the model-derived relative aerosol fraction and vertical distributions in the assimilated distribu-

They indicated Carbon Monoxide data assimilation had a positive impact for Black Carbon aerosol simulation, but did not investigate the full potential of chemical and dynamical interaction.

* CO and BC have similar sources.

Integration of Atmospheric Chemistry with NWP

Atmos. Chem. Phys., 9, 4855–4867, 2009
www.atmos-chem-phys.net/9/4855/2009/

Atmospheric Chemistry and Physics

Method: 4D-Var

On the extraction of wind information from the assimilation of ozone profiles in Météo–France 4-D-Var operational NWP suite

N. Semane[1,2], V.-H. Peuch[1], S. Pradier[1], G. Desroziers[1], L. El Amraoui[1], P. Brousseau[1], S. Massart[3], B. Chapnik[1], and A. Peuch[4]

[1]CNRM-GAME, Météo-France and CNRS URA 1357, Toulouse, France
[2]CNRM, Direction de la Météorologie Nationale, Casablanca, Morocco
[3]CERFACS, Toulouse, France
[4]DP, Météo–France, Toulouse, France

Received: 24 June 2008 – Published in Atmos. Chem. Phys. Discuss.: 28 August 2008
Revised: 2 July 2009 – Accepted: 10 July 2009 – Published: 22 July 2009

Abstract. By applying four-dimensional variational data-assimilation (4-D-Var) to a combined ozone and dynamics Numerical Weather Prediction model (NWP), ozone observations generate wind increments through the ozone-dynamics coupling. The dynamical impact of Aura/MLS satellite ozone profiles is investigated using Météo-France operational *ARPEGE* NWP 4-D-Var assimilation system for a period of 3 months. A data-assimilation procedure has been designed and run on 6-h windows. The procedure includes: (1) 4-D-Var assimilating both ozone and operational NWP standard observations, (2) *ARPEGE* transporting ozone as a passive-tracer, (3) *MOCAGE*, the Météo–France chemistry

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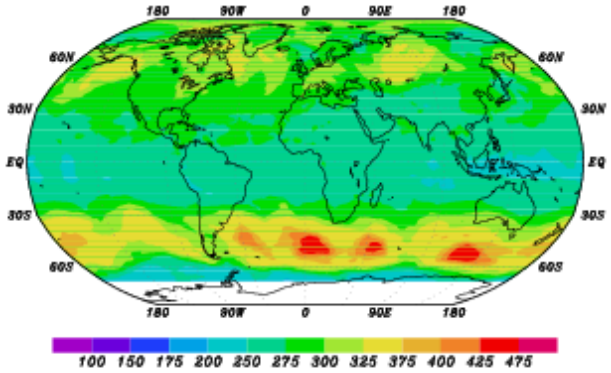
ing the 4-D-Var process, the evolution of the linearized forecast model and its adjoint act as an additional constraint (Andersson et al., 1994).

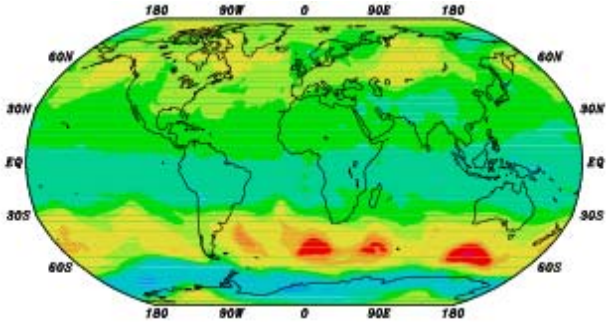
They found that the influence of the ozone assimilation on the wind analysis was positive in the lower stratosphere, but its improvement was small.

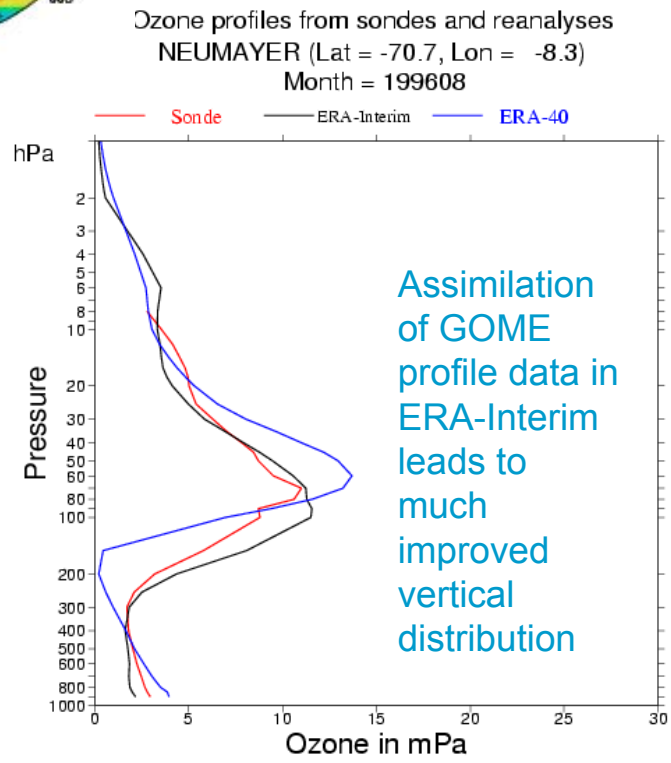
Ozone assimilation
Can ozone data be used to infer stratospheric winds?

Total ozone from TOMS
(August 1996)



ERA-Interim
(TOMS + SBUV + GOME)





- Ozone observations contain information about the flow
- 4D-Var should be able to extract this information, since it uses the forecast model as a dynamical constraint

- **How does this work in practise ?**

Assimilation of GOME profile data in ERA-Interim leads to much improved vertical distribution

Ozone assimilation
Can 4D-Var infer stratospheric winds from ozone data?

- The answer is: **Not yet.**

- Assimilation of ozone profile data causes large and unrealistic T/U/V increments near the stratopause to accommodate the observed discrepancies between background and data

- A large part of these discrepancies are due to biases (in both data and model)

- It is natural for 4D-Var to make adjustments to the flow where constraints are few:
  - Lack of wind observations
  - Large background uncertainties

- A short-term fix is to disable this feature for the assimilation of ozone and other trace gases (use the background flow for ozone transport during minimisation)

- Comprehensive ozone bias correction (as for radiances) will help.

What's wrong?

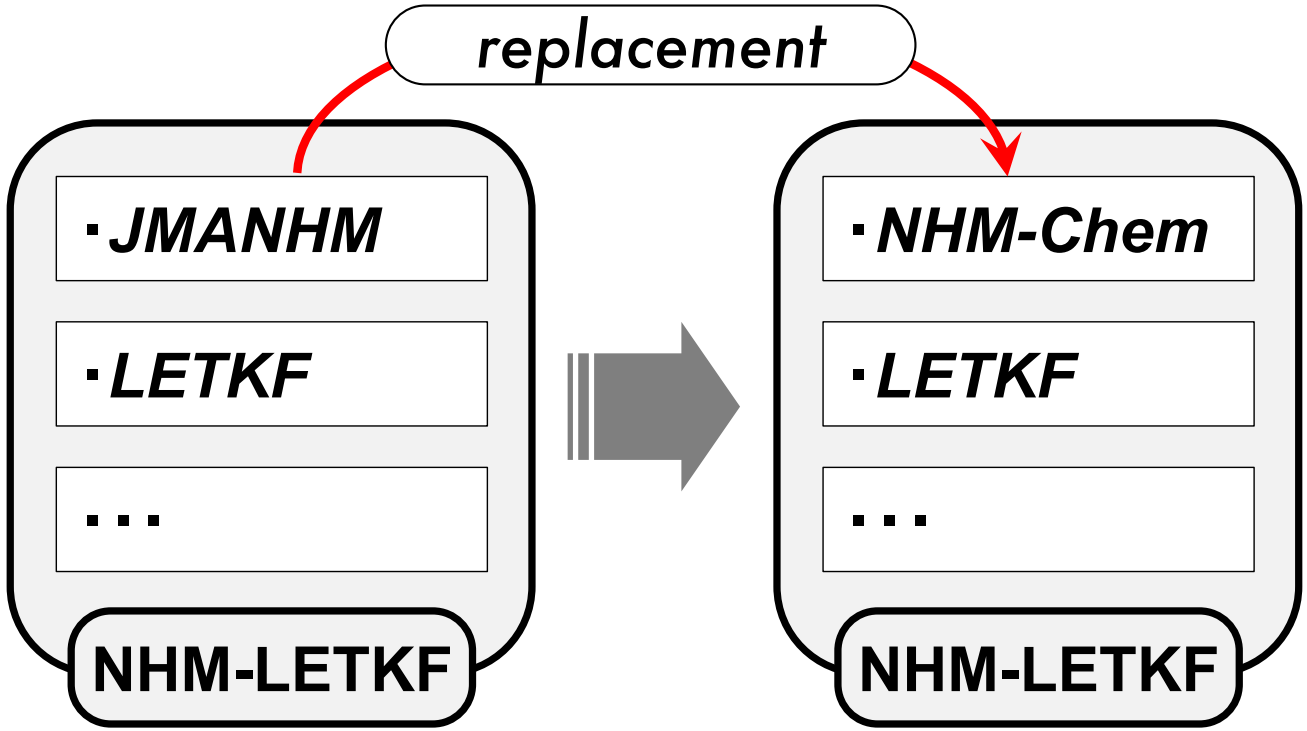
- Poor coverage of observation data
  - Yeah, chemical data often have a severe shortage, but we have many satellites for chemical constituents now.
- Low quality of observation data
  - Yeah, remote-sensing observations are often inaccurate, but NWP also has the same problems.
- Low quality of chemistry models
  - Yeah, but inert chemical constituents must be performed as accurate as water vaper in NWP models.
- Inaccuracy of error covariance
  - Hmm, between chemistry and dynamics...

I want to check the feasibility of the dynamical integration under the real condition.

Ideally, it will work.

- Coverage of observation data
  - Some ***plumes*** are closely chased from its source like volcanic ash.
- Quality of observation data
  - Constituents are sometimes measured with an extremely high accuracy like ***radioisotopes***.
- Quality of chemistry models
  - It's possible to use a ***perfectly inert*** constituent as a tracer like volcanic ash or radioisotopes.
- Accuracy of error covariance
  - If the error covariance does matter, the ***variable localization*** can be used?

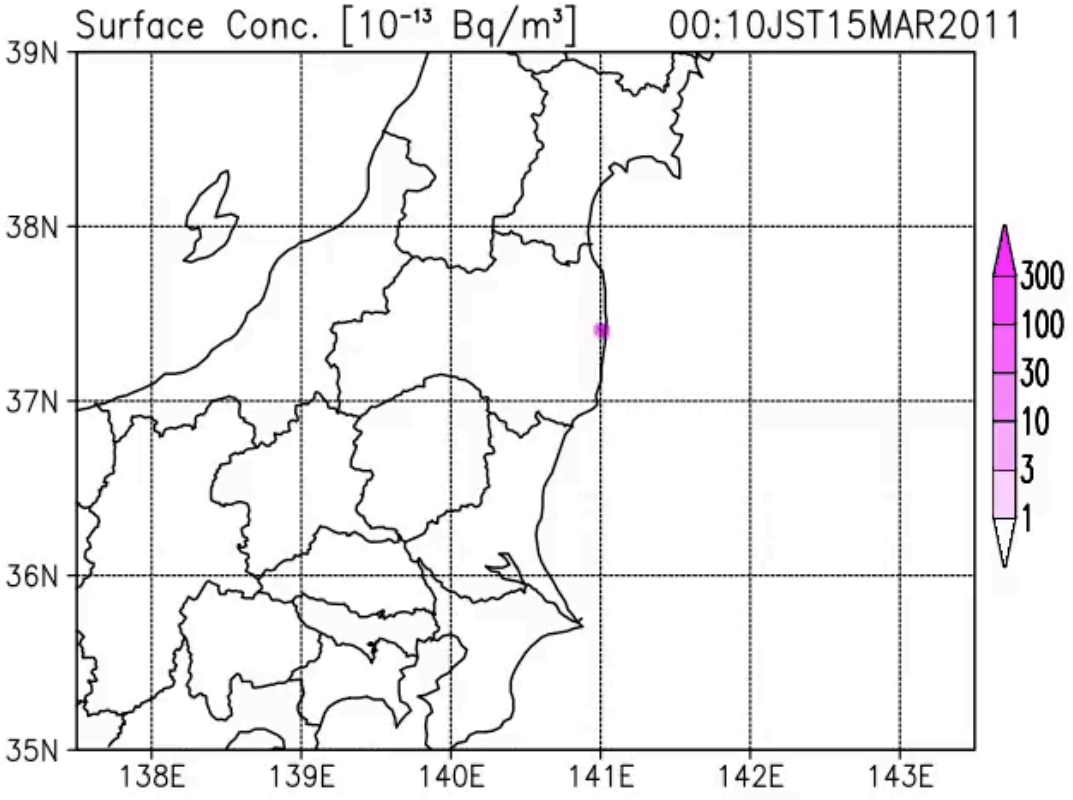
Wind+chemistry data assimilation (under construction)

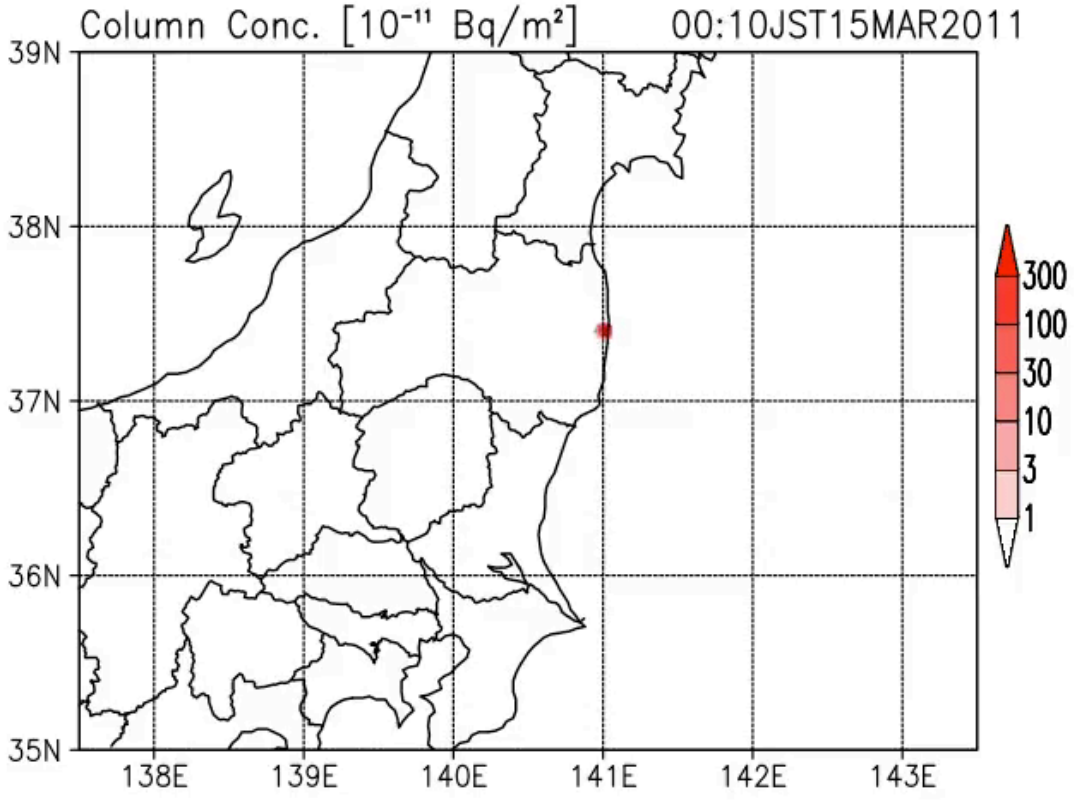


- I'll investigate the concentration-wind interaction in the troposphere especially in the PBL using NHM-Chem-LETKF.
- Hopefully, to use constituents from a simple emission source, chemically inert, and measured with high accuracy/frequency.
  - Ozone? Carbon dioxide? Mineral dust? Volcanic ash? Radioisotopes?

Fukushima radionuclide dispersion simulation

- Plumes of the Fukushima nuclear accident





MRI/JMA radionuclide dispersion model (NHM-Chem)

Fukushima radionuclide dispersion simulation

Journal of the Meteorological Society of Japan, Vol. 95, No. 6, pp. 447–454, 2017
DOI:10.2151/jmsj.2017-025

Method: LETKF

NOTES AND CORRESPONDENCE

The Impact of Surface Wind Data Assimilation on the Predictability of Near-Surface Plume Advection in the Case of the Fukushima Nuclear Accident

Tsuyoshi Thomas SEKIYAMA, Mizuo KAJINO, and Masaru KUNII

Meteorological Research Institute, Tsukuba, Japan

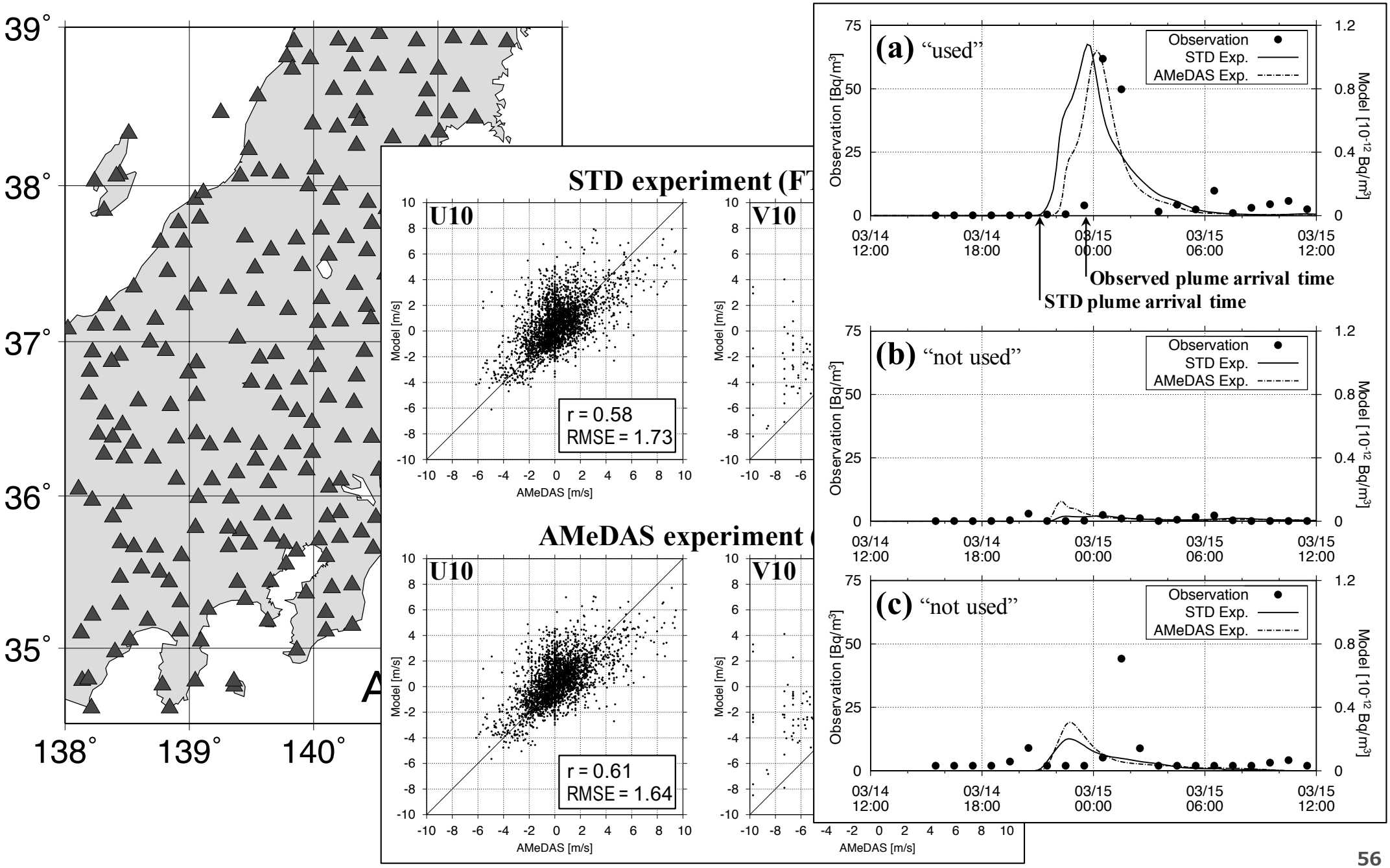
(Manuscript received 24 March 2017, in final form 4 August 2017)

Abstract

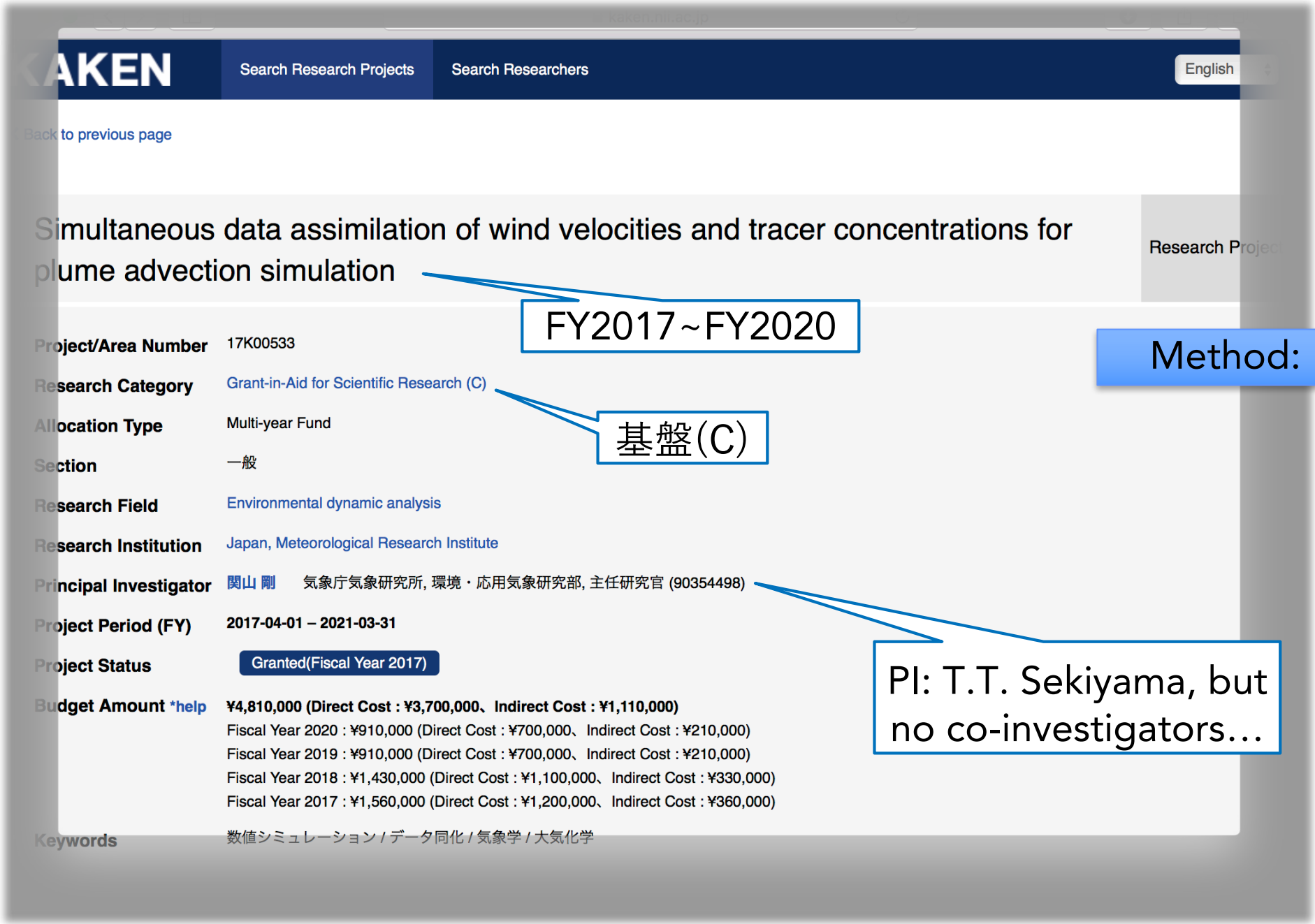
We investigated the predictability of plume advection in the troposphere and the impact of AMeDAS surface wind data assimilation by using radioactive cesium emitted by the Fukushima nuclear accident in March 2011 as an atmospheric tracer. We conducted two experiments for Japan for March 15, 2011 with a 3-km horizontal resolution, a non-hydrostatic weather forecast model and local ensemble transform Kalman filter system. The assimilated meteorological data were obtained from the Japan Meteorological Agency operational numerical weather prediction model. The standard archives do not contain land-surface wind data, so concentrations were examined for plume arrival times at 40 observation points for the standard experiment (assimilating only the standard meteorological data) was 72.8 min on average. In contrast, the mean error of the AMeDAS experiment (assimilating AMeDAS surface wind observations) was 72.8 min, which was significantly smaller than the standard experiment. This result indicates that the plume prediction has a reasonable accuracy for the environmental emergency response and the prediction can be significantly improved by the surface wind data assimilation.

This work was just published: NOT chemical BUT only meteorological data assimilation. We explored the importance of surface wind accuracy for the predictability of plume advection.

Fukushima radionuclide dispersion simulation



Integration of Dynamics in NWP and Tracer Models



Summary

- Data assimilation of atmospheric chemistry is the frontier of atmospheric science!
- Data assimilation of atmospheric chemistry has been used for environmental issues, e.g., chemical weather forecasts, chemical species emission estimation, etc.
- Data assimilation of atmospheric chemistry will be integrated with NWP, hopefully.

Thank you;-)