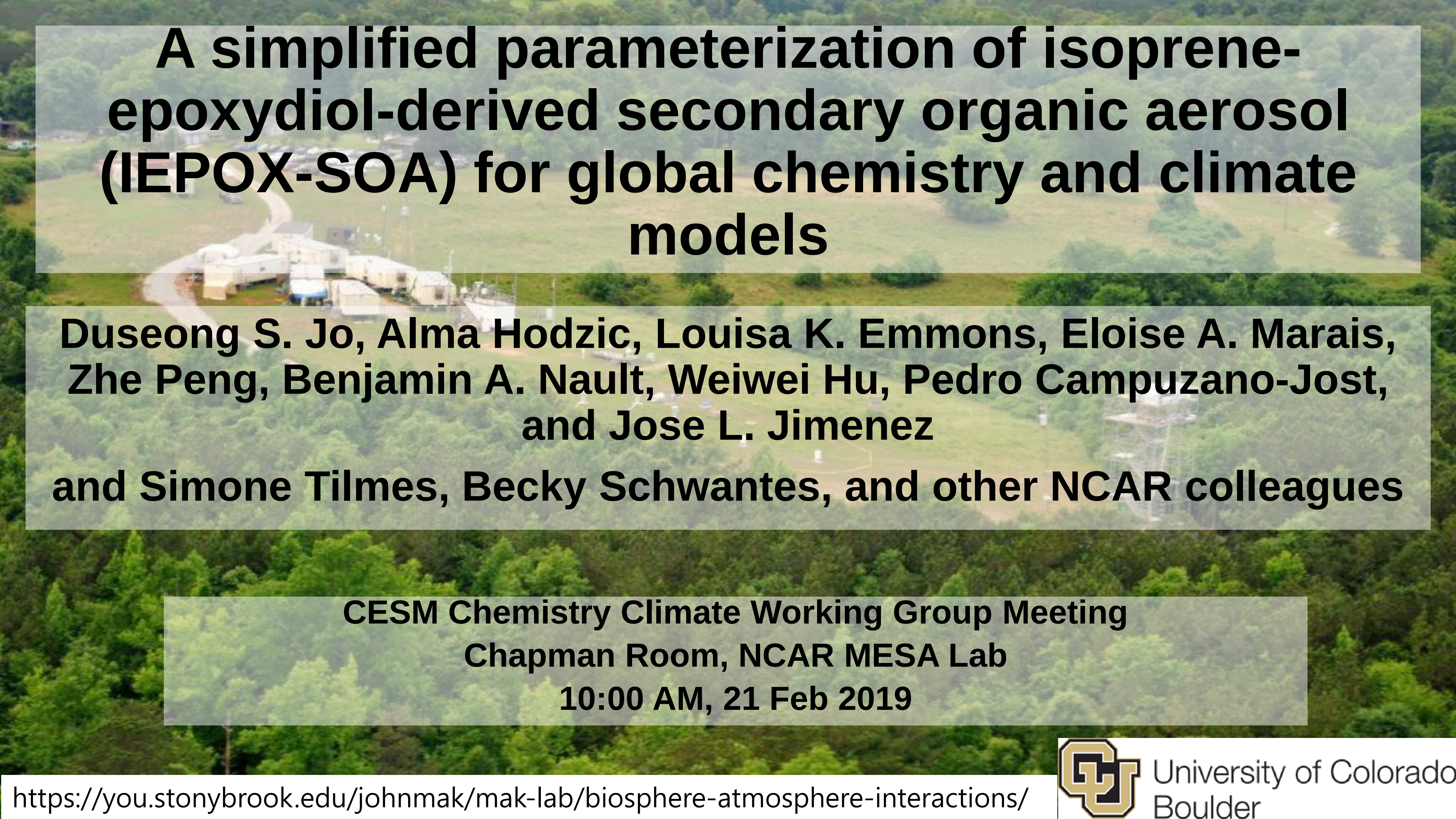

A simplified parameterization of isoprene-epoxydiol-derived secondary organic aerosol (IEPOX-SOA) for global chemistry and climate models

Duseong S. Jo, Alma Hodzic, Louisa K. Emmons, Eloise A. Marais, Zhe Peng, Benjamin A. Nault, Weiwei Hu, Pedro Campuzano-Jost, and Jose L. Jimenez

and Simone Tilmes, Becky Schwantes, and other NCAR colleagues

CESM Chemistry Climate Working Group Meeting
Chapman Room, NCAR MESA Lab
10:00 AM, 21 Feb 2019

https://you.stonybrook.edu/johnmak/mak-lab/biosphere-atmosphere-interactions/

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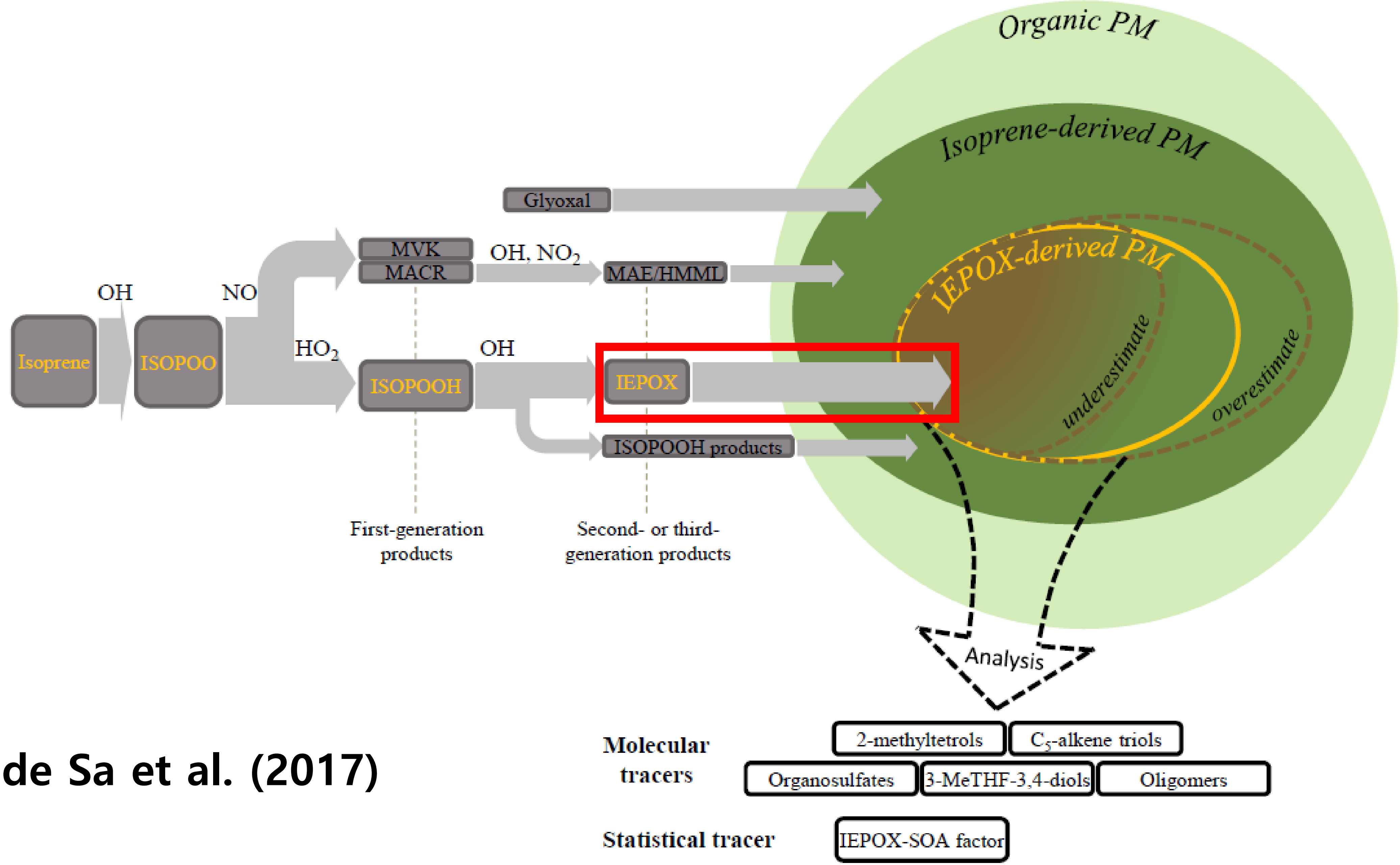
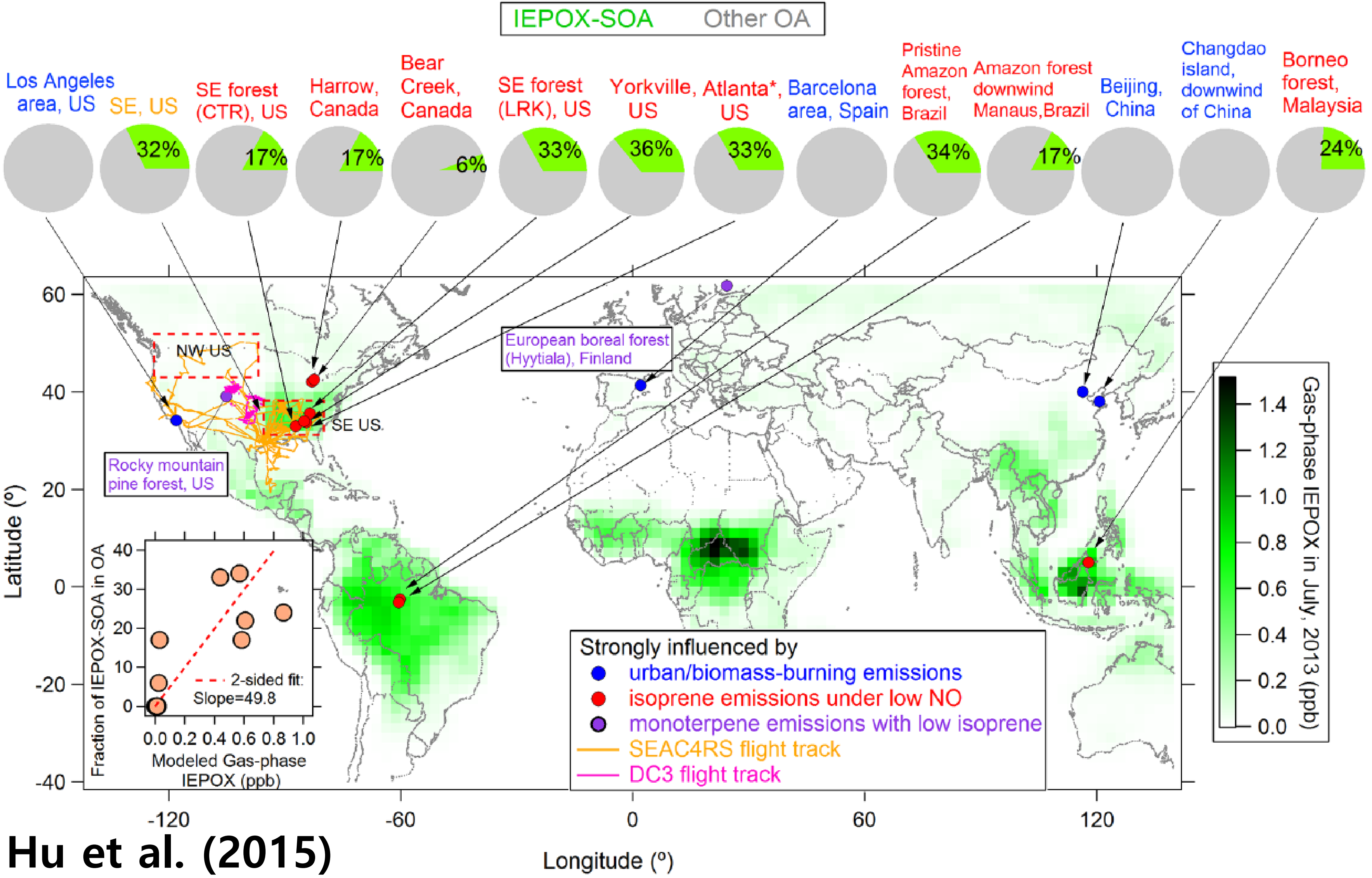
IEPOX-SOA : main source of isoprene-derived aerosol



de Sa et al. (2017)

IEPOX-SOA fractions of OA : up to 36%



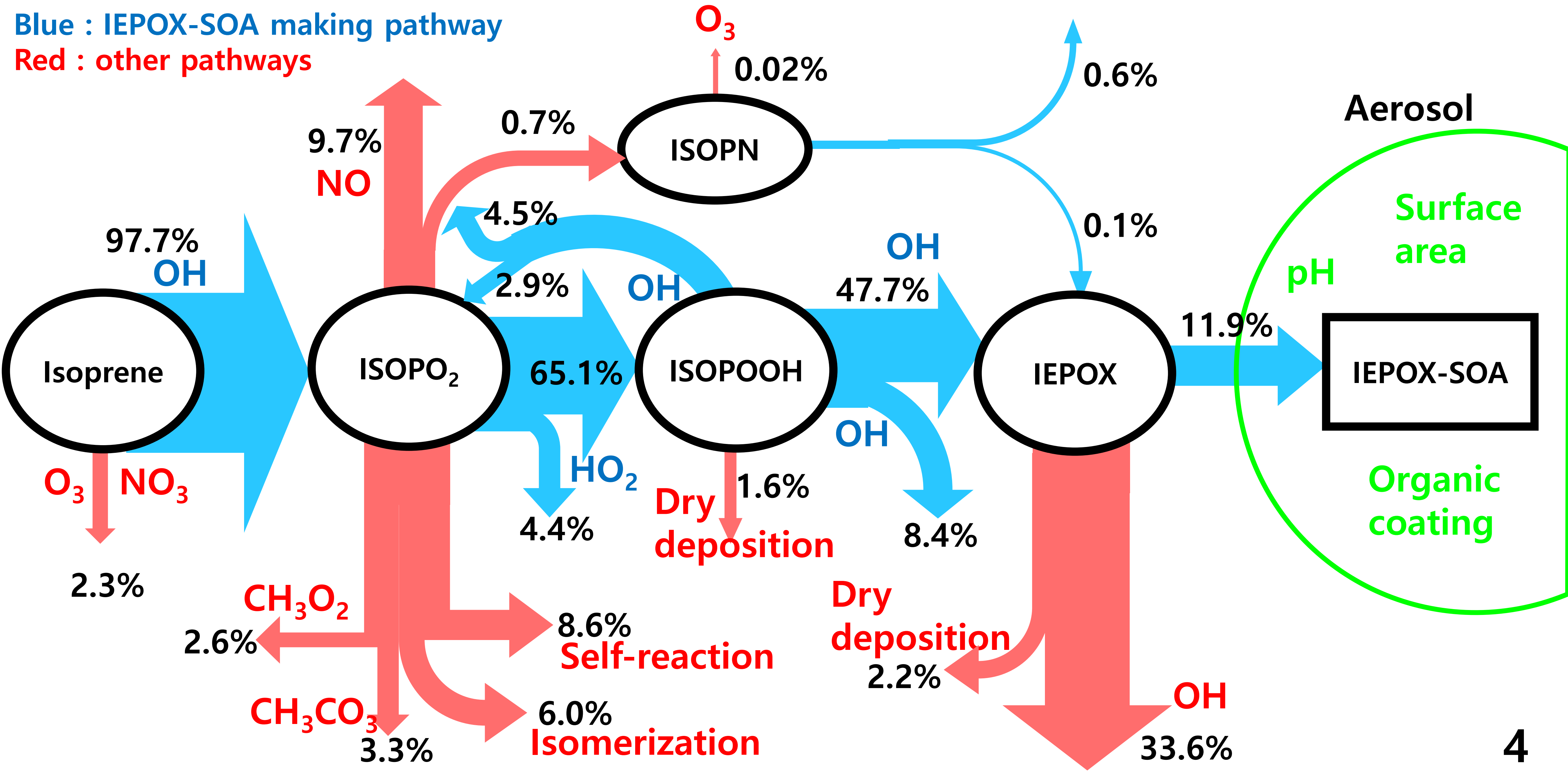
Hu et al. (2015)

Schematic diagram of IEPOX-SOA chemistry

For SOAS condition

Blue : IEPOX-SOA making pathway

Red : other pathways



O_3 0.02%

0.6%

Aerosol

9.7% NO

0.7%

ISOPN

4.5%

0.1%

Surface area

97.7% OH

2.9%

OH

OH 47.7%

pH

Isoprene

$ISOPO_2$

65.1%

ISOPOOH

IEPOX

11.9%

IEPOX-SOA

OH

O_3

NO_3

HO_2

Dry deposition 1.6%

Organic coating

4.4%

8.4%

2.3%

CH_3O_2 2.6%

8.6% Self-reaction

Dry deposition 2.2%

CH_3CO_3 3.3%

6.0% Isomerization

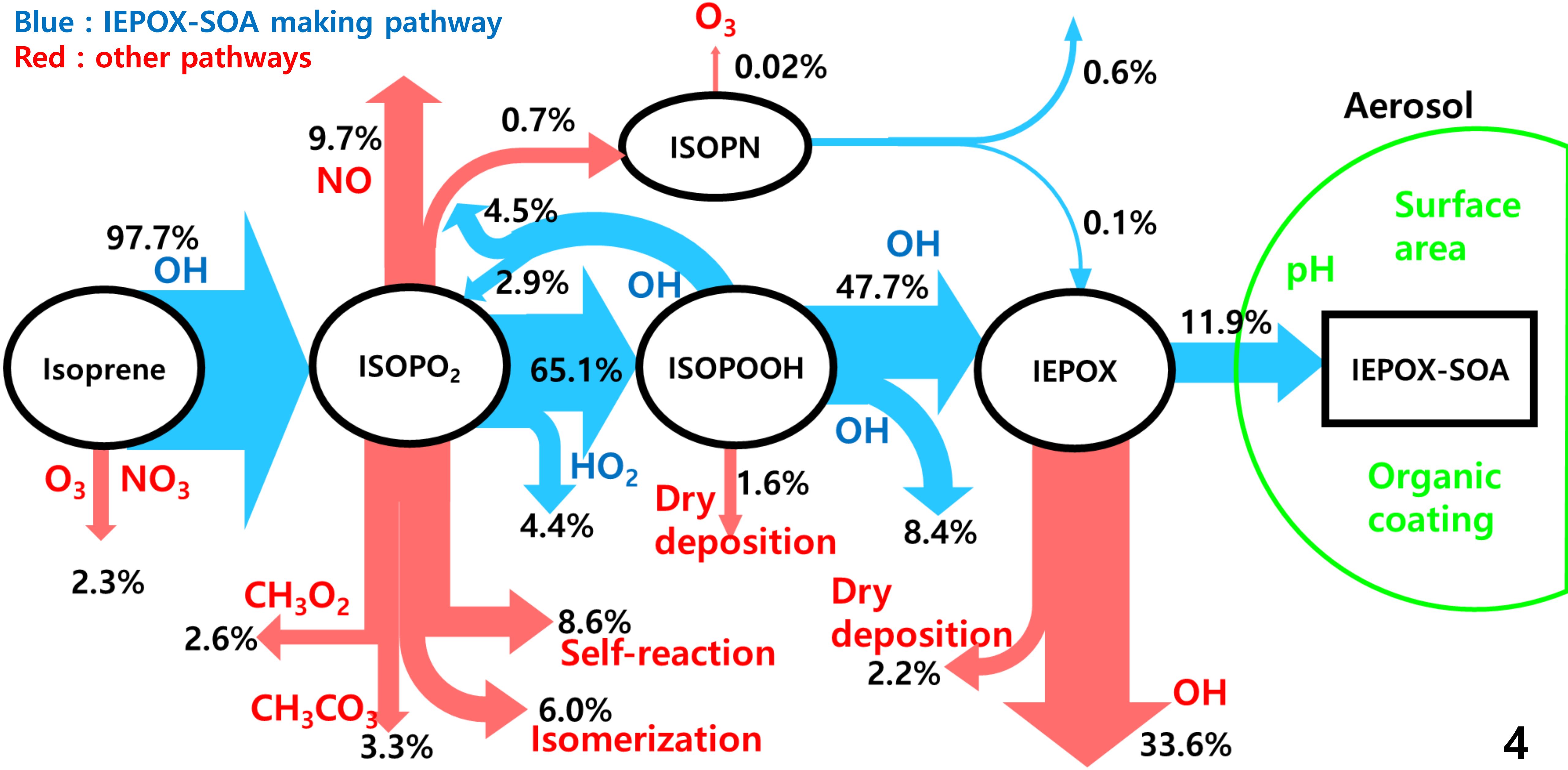
OH 33.6%

Schematic diagram of IEPOX-SOA chemistry

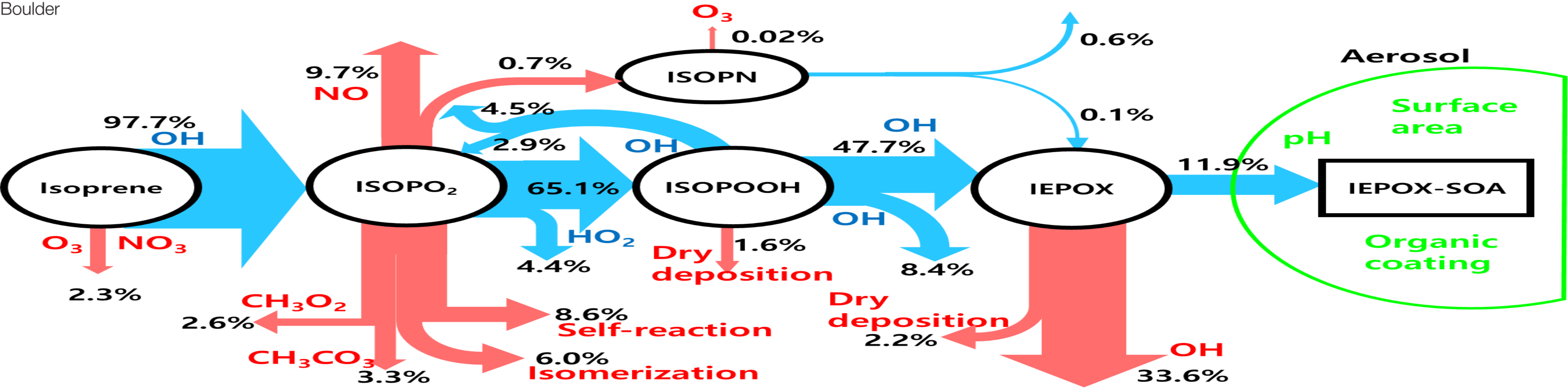
For SOAS condition

Blue : IEPOX-SOA making pathway

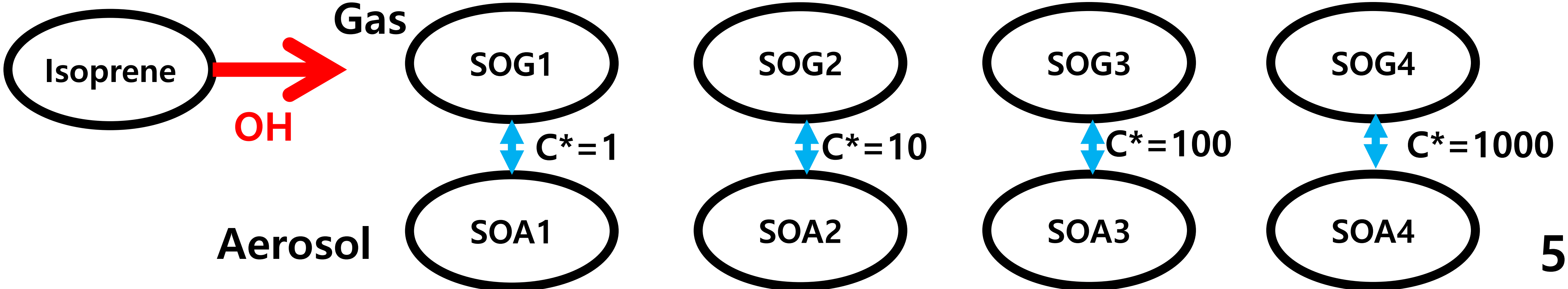
Red : other pathways



Schematic diagram of IEPOX-SOA chemistry

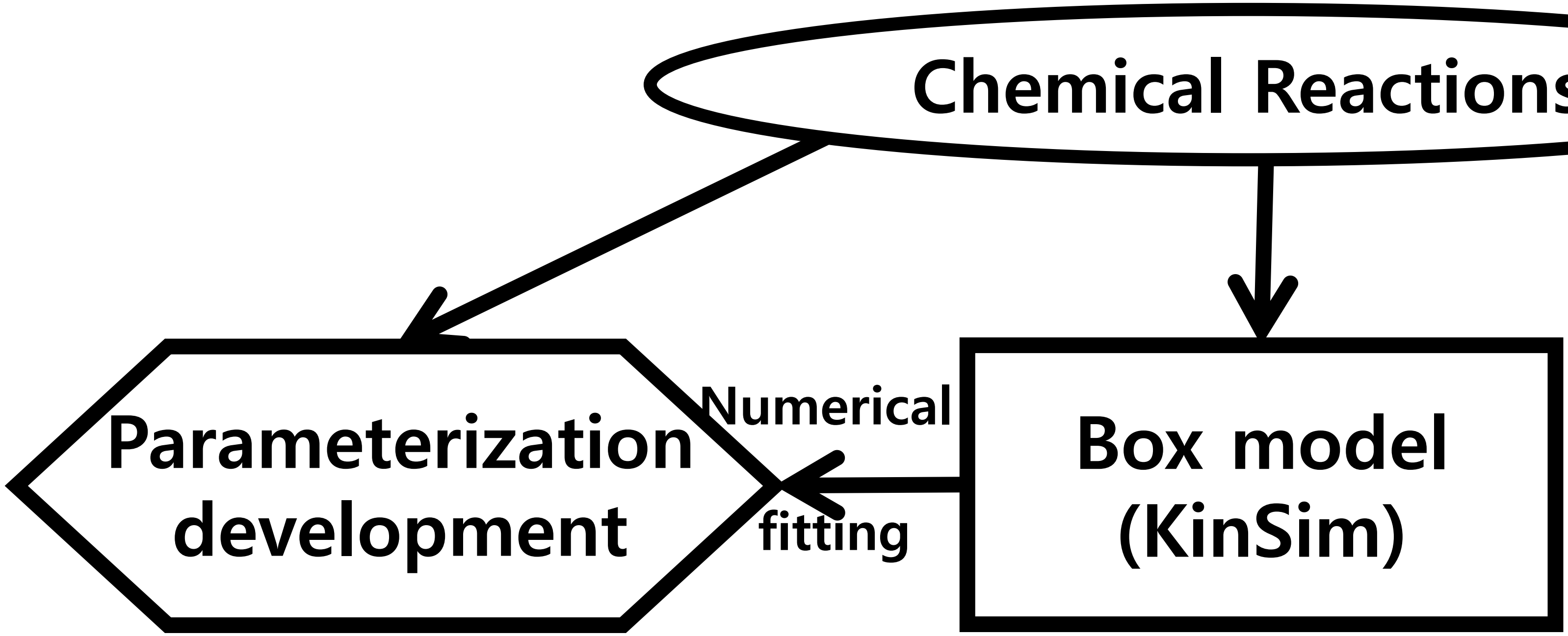


Chemistry models usually calculate isoprene-derived SOA using a simplified partitioning approach such as the Volatility basis set (VBS) approach



University
of Colorado
Boulder

Objective : Develop a parameterization of IEPOX-SOA without an additional heavy computational cost



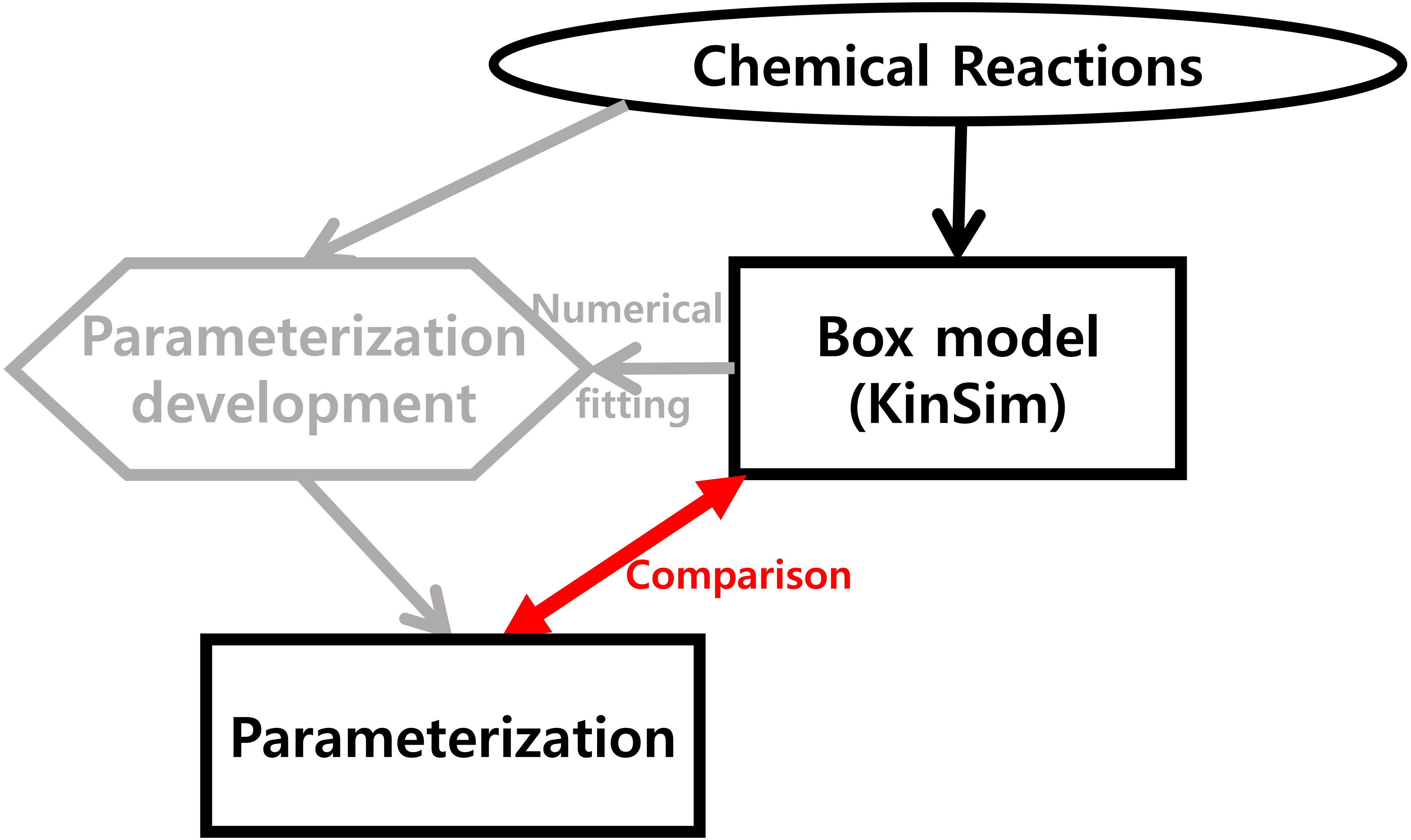
Chemical Reactions

Parameterization development

Numerical fitting

Box model (KinSim)

Objective : Develop a parameterization of IEPOX-SOA without an additional heavy computational cost



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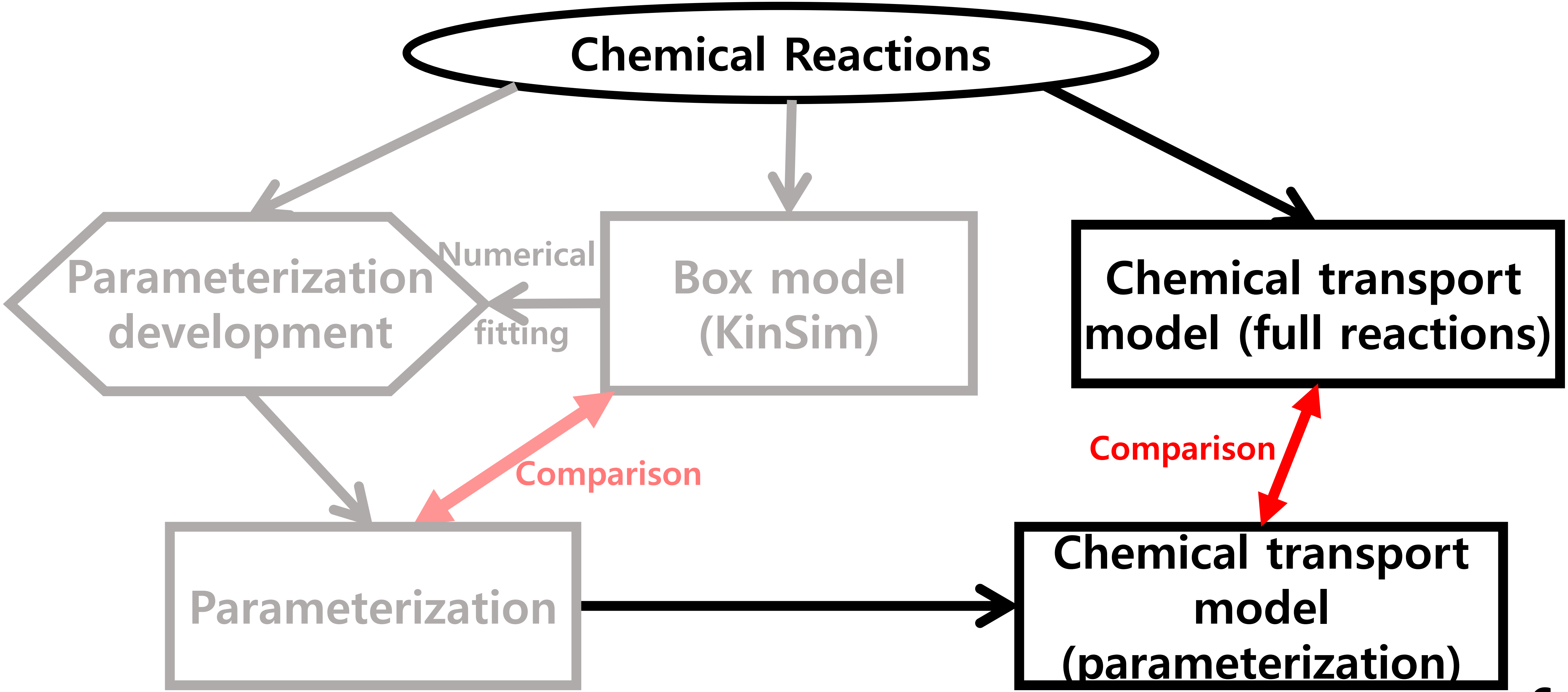


Chemical Reactions

Parameterization development

Numerical fitting

Box model (KinSim)

Chemical transport model (full reactions)

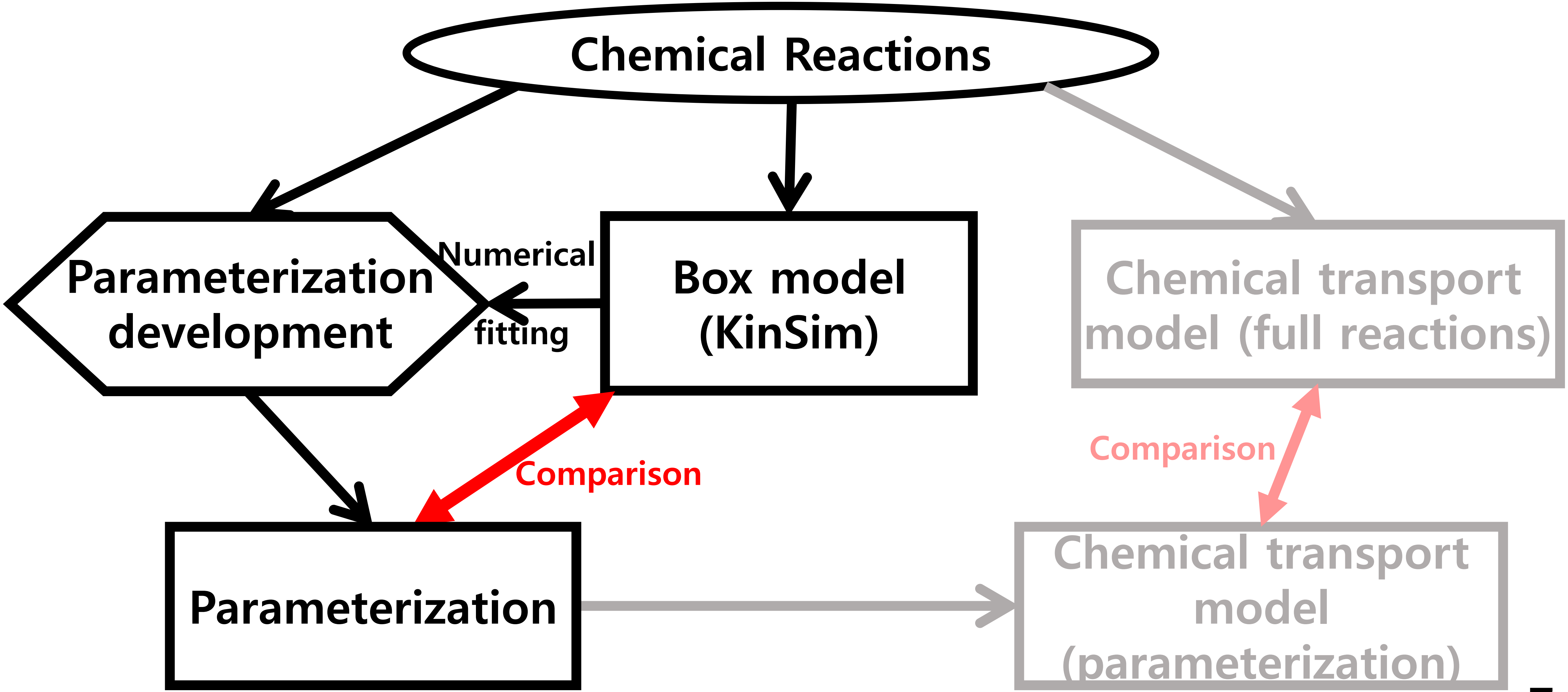
Comparison

Comparison

Parameterization

Chemical transport model (parameterization)

Objective : Develop a parameterization of IEPOX-SOA without an additional heavy computational cost



Chemical Reactions

Parameterization development

Numerical fitting

Box model (KinSim)

Chemical transport model (full reactions)

Comparison

Comparison

Parameterization

Chemical transport model (parameterization)

Reactions

#	Reactions	Reaction rate
1	ISOP	50/T)
2	ISOP	970/T)
3	ISOP	50/T)
4	ISOPC	300/T)
5	ISOPC	50/T)
6	ISOPC	
7	ISOPC	
8	ISOPC	
9	ISOPC	694/T)
10	ISOPC	00/T)
11	ISOPC	90/T)
12	ISOPC	5
13	ISOPN	80/T)
14	ISOPN	80/T)
15	ISOPN	
16	ISOPN	
17	IEPOX	00/T)
18	IEPOX	
19	ISOPC	depth]
20	IEPOX	depth]

Geoscientific Model Development
An interactive open-access journal of the European Geosciences Union

https://doi.org/10.5194/gmd-2019-9

Development and technical paper

05 Feb 2019

A simplified parameterization of isoprene-epoxydiol-derived secondary organic aerosol (IEPOX-SOA) for global chemistry and climate models

Review status
This discussion paper is a preprint. It is a manuscript under review for the journal Geoscientific Model Development (GMD).

Duseong S. Jo[1,2], **Alma Hodzic**[3,4], **Louisa K. Emmons**[3], **Eloise A. Marais**[5], **Zhe Peng**[1,2], **Benjamin A. Nault**[1,2], **Weiwei Hu**[1,2], **Pedro Campuzano-Jost**[1,2], **and Jose L. Jimenez**[1,2]

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[2]Department of Chemistry, University of Colorado, Boulder, CO, USA
[3]Atmospheric Chemistry Observations and Modeling Lab., National Center for Atmospheric Research, Boulder, CO, USA
[4]Laboratoire d'Aérologie, Université de Toulouse, CNRS, UPS, Toulouse, France
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Received: 12 Jan 2019 – Accepted for review: 04 Feb 2019 – Discussion started: 05 Feb 2019

Abstract. Secondary organic aerosol derived from isoprene epoxydiols (IEPOX-SOA) is thought to contribute the dominant fraction of total isoprene SOA, but the current volatility-based lumped SOA parameterizations are not appropriate to represent the reactive uptake of IEPOX onto acidified aerosols. A full explicit modelling of this chemistry is however computationally expensive owing to the many species and reactions tracked, which makes it difficult to include it in chemistry climate models for long-term studies. Here we present three simplified parameterizations for IEPOX-SOA simulation, based on an approximate analytical/fitting solution of the IEPOX-SOA yield and formation timescale. The yield and timescale can then be directly calculated using the global model fields of oxidants, NO, aerosol pH and other key properties, and dry deposition rates. The advantage of the proposed parameterizations is that they do not require the simulation of the intermediates while retaining the key physico-chemical dependencies. We have implemented the new parameterizations into the GEOS-Chem v11-02-rc chemical transport model, which has two empirical treatments for isoprene SOA (the volatility basis set (VBS) approach and a fixed 3 % yield parameterization) and compared all of them to the case with detailed full chemistry. The best parameterization (PAR3) captures the

Reactions

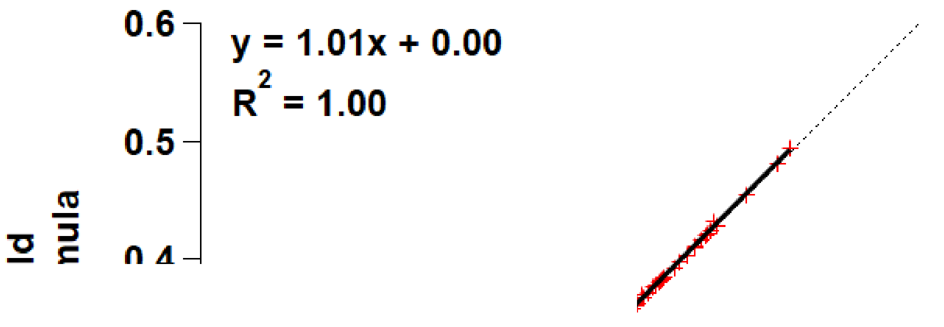
#	Reactions	Reaction rate
1	ISOP + OH -> 1.0 $ISOPO_2$	3.1E-11 exp(350/T)
2	ISOP + O_3 -> other products	1.00E-14 exp(-1970/T)
3	ISOP + NO_3 -> other products	3.3E-12 exp(-450/T)
4	$ISOPO_2$ + HO_2 -> 0.937 ISOPOOH	2.12E-13 exp(1300/T)
5	$ISOPO_2$ + NO -> 0.023 ISOPND + 0.047ISOPNB	2.7E-12 exp(350/T)
6	$ISOPO_2$ + CH_3O_2 -> other products	2.00E-12
7	$ISOPO_2$ + $ISOPO_2$ -> other products	2.30E-12
8	$ISOPO_2$ + CH_3CO_3 -> other products	1.40E-11
9	$ISOPO_2$ -> other products	4.07E+08 exp(-7694/T)
10	ISOPOOH + OH -> 0.387 $ISOPO_2$	4.75E-12 exp(200/T)
11	ISOPOOH + OH -> 0.850 IEPOX	1.9E-11 exp(390/T)
16	ISOPNB + O_3 -> other products	[illegible]E-18
17	IEPOX + OH -> other products	4.42e-11 exp(-400/T)
18	IEPOX -> IEPOX-SOA	Calculated
19	ISOPOOH dry deposition	2.5 cm s^{-1} / [PBL depth]
20	IEPOX dry deposition	2.5 cm s^{-1} / [PBL depth]

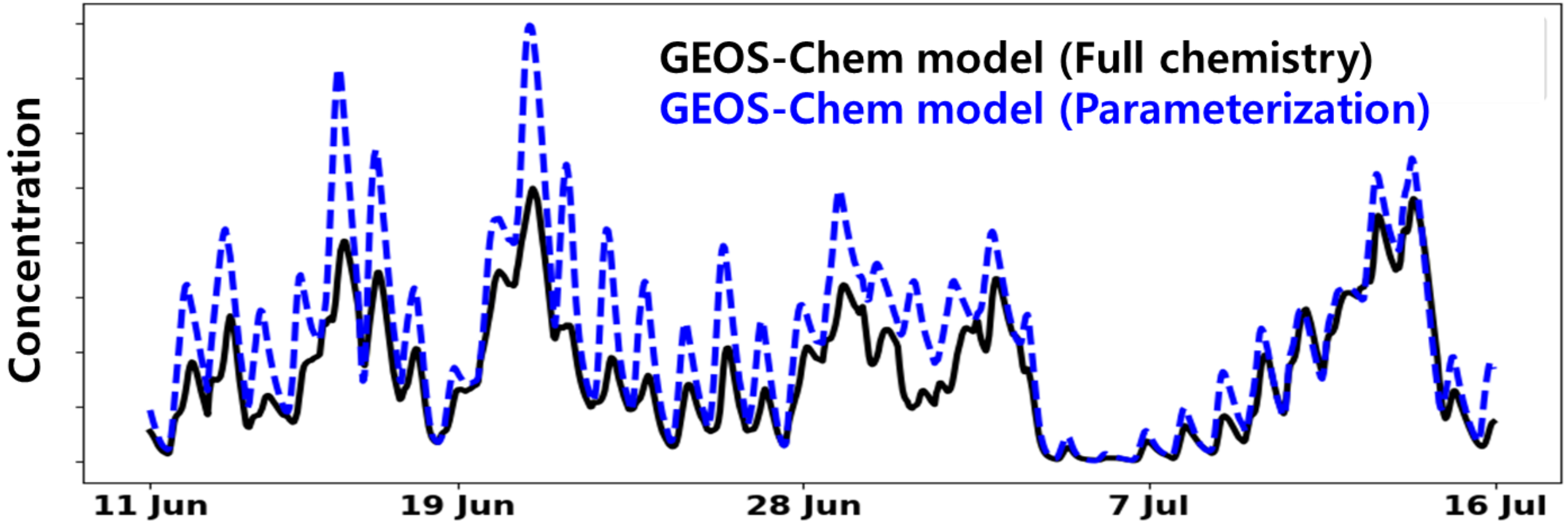
$$f_{Isoprene \rightarrow ISOPO_2} = \frac{k_1 \times [OH]}{k_1 \times [OH] + k_2 \times [O_3] + k_3 \times [NO_3]}$$

$$\text{IEPOX-SOA}_{PAR} = Y_{\text{IEPOX-SOA}} \times E_{Isoprene}$$

$$Y_{\text{IEPOX-SOA}} = f(OH, O_3, NO_3, HO_2, NO, CH_3O_2, CH_3CO_3, pH, \text{Aerosol surface area}, \text{organic coating})$$

#	Species	Values
1	NO [ppt]	1, 5, 10, 50, 100, 500, 1000, 5000, 10^4, 5×10^4, 10^5, 5×10^5, 10^6
2	OH [molecules cm^{-3}]	10^4, 5×10^4, 10^5, 5×10^5, 10^6, 2×10^6, 3×10^6, 4×10^6, 5×10^6
3	HO_2 [ppt]	1, 2, 5, 10, 20, 50, 100
4	pH [	
5	Aero	
6	O_3 [	
7	NO_3	
8	CH_3	
9	CH_3	
10	Aero	
11	Orga	
12	Temperature [K]	288, 293, 298, 303, 308, 313, 318
13	Planetary boundary layer height [m]	100, 200, 500, 1000, 1500, 2000, 2500, 3000, 3500, 4000
14	Photolysis rate of ISOPOOH [s^{-1}]	10^{-7}, 5×10^{-7}, 10^{-6}, 5×10^{-6}, 10^{-5}, 2×10^{-5}



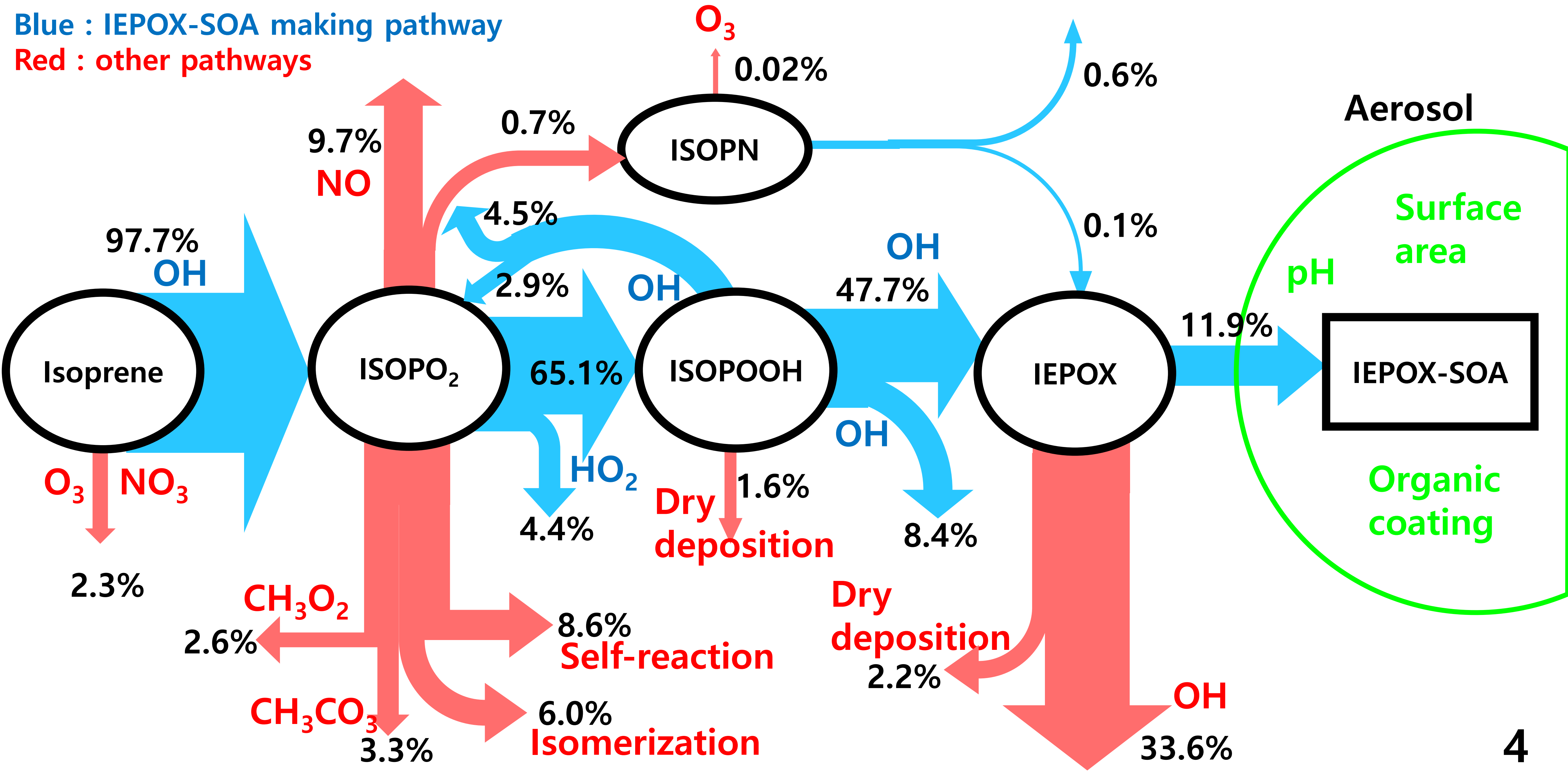


Schematic diagram of IEPOX-SOA chemistry

For SOAS condition

Blue : IEPOX-SOA making pathway

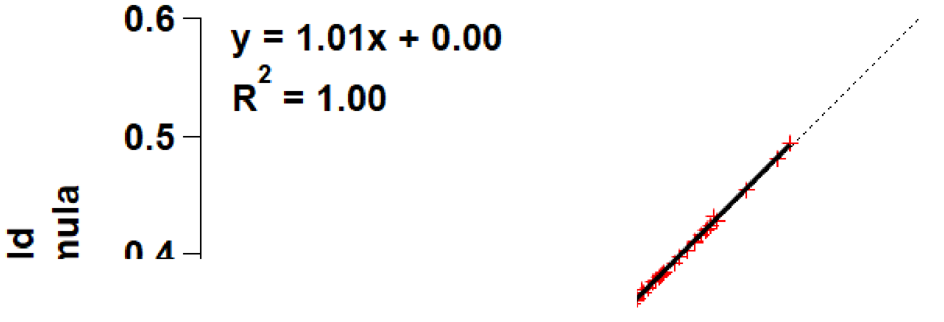
Red : other pathways

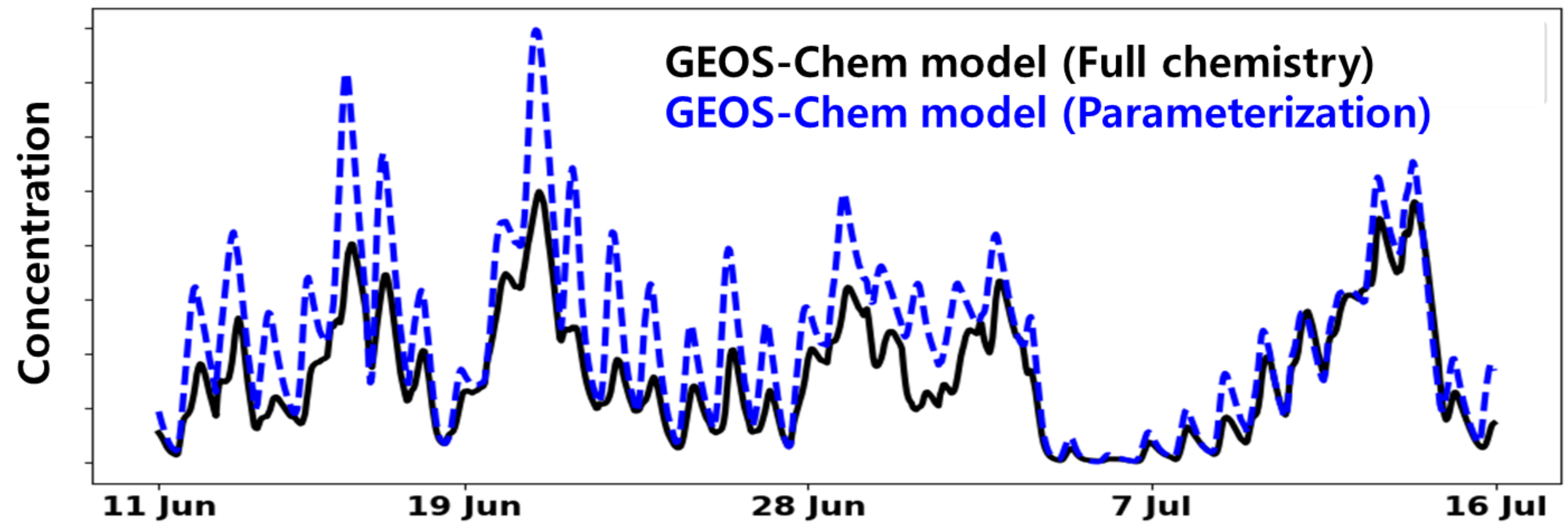


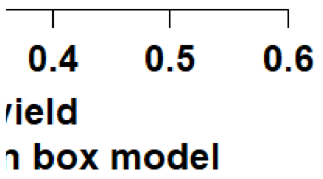
$\text{IEPOX-SOA}_{\text{PAR}} = Y_{\text{IEPOX-SOA}} \times E_{\text{Isoprene}}$

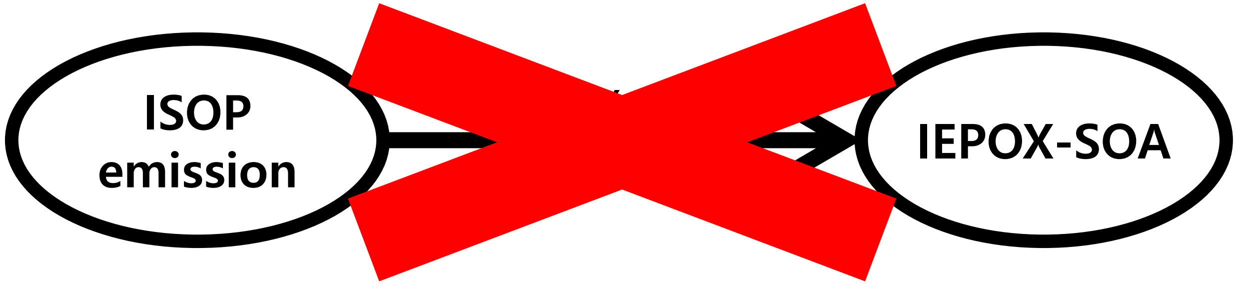
$Y_{\text{IEPOX-SOA}} = f(OH, O_3, NO_3, HO_2, NO, CH_3O_2, CH_3CO_3, \text{pH}, \text{Aerosol surface area}, \text{organic coating})$

#	Species	Values
1	NO [ppt]	1, 5, 10, 50, 100, 500, 1000, 5000, 10^4, 5×10^4, 10^5, 5×10^5, 10^6
2	OH [molecules cm^{-3}]	10^4, 5×10^4, 10^5, 5×10^5, 10^6, 2×10^6, 3×10^6, 4×10^6, 5×10^6
3	HO_2 [ppt]	1, 2, 5, 10, 20, 50, 100
4	pH [	
5	Aer	
6	O_3 [	
7	NO_3	
8	CH_3	
9	CH_3	
10	Aer	
11	Org	
12	Temperature [K]	288, 293, 298, 303, 308, 313, 318
13	Planetary boundary layer height [m]	100, 200, 500, 1000, 1500, 2000, 2500, 3000, 3500, 4000
14	Photolysis rate of ISOPOOH [s^{-1}]	10^{-7}, 5×10^{-7}, 10^{-6}, 5×10^{-6}, 10^{-5}, 2×10^{-5}



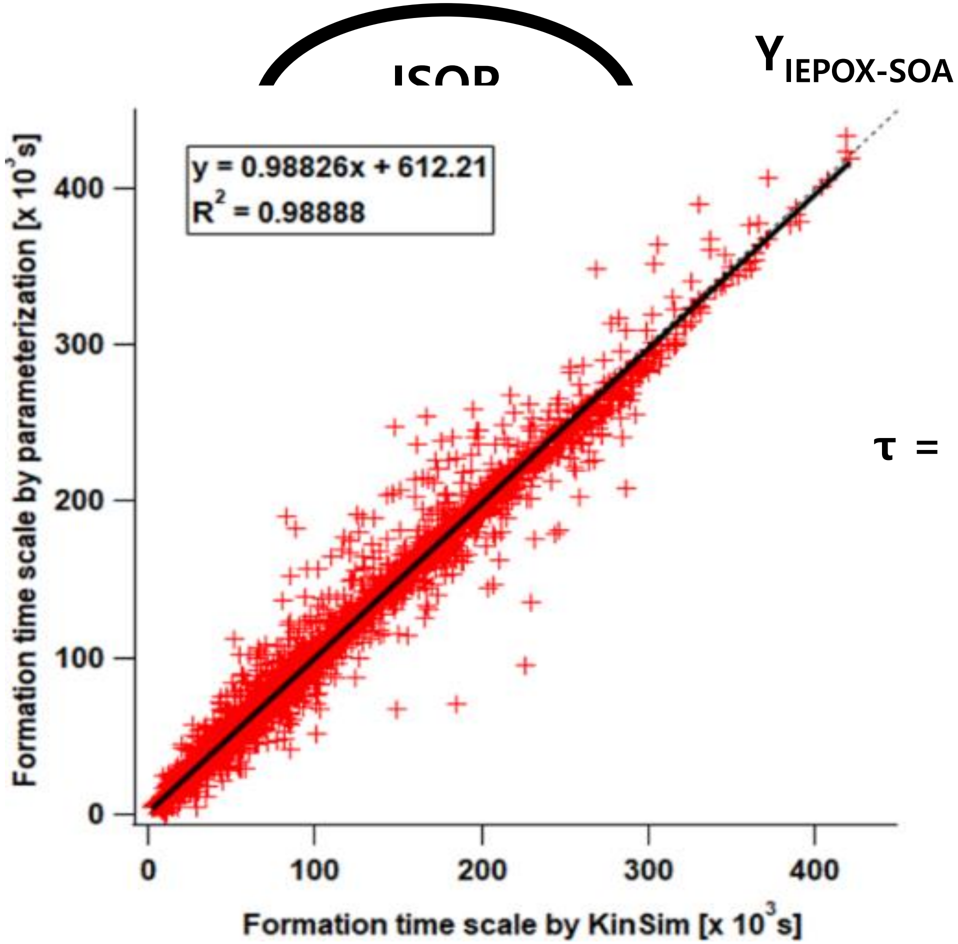


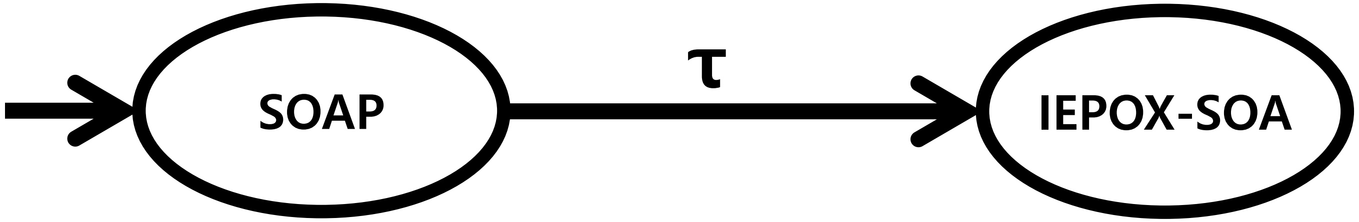




ISOP emission

IEPOX-SOA





SOAP

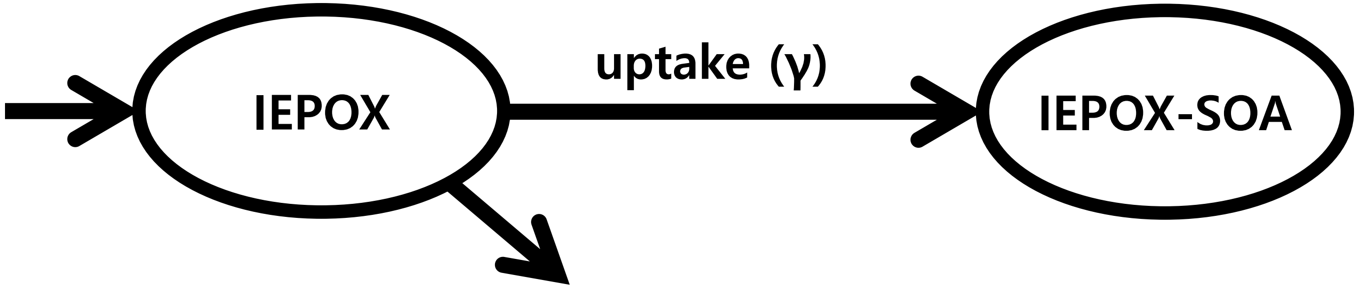
τ

IEPOX-SOA

g time in the first order kinetic equation

$$\Delta t) = \text{IEPOX-SOA}(t) + \{1 - \exp(-\frac{\Delta t}{\tau})\} \times \text{SOAP}(t)$$

$$\tau = f(L_{ISOP}, L_{ISOPOOH}, L_{IEPOX}, L_{ISOPN}, NO, HO_2)$$



IEPOX

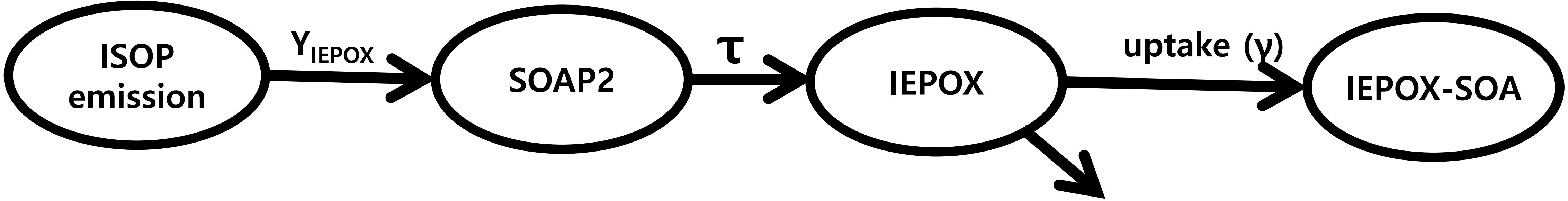
uptake (γ)

IEPOX-SOA

- Chemical loss by OH
- Dry deposition

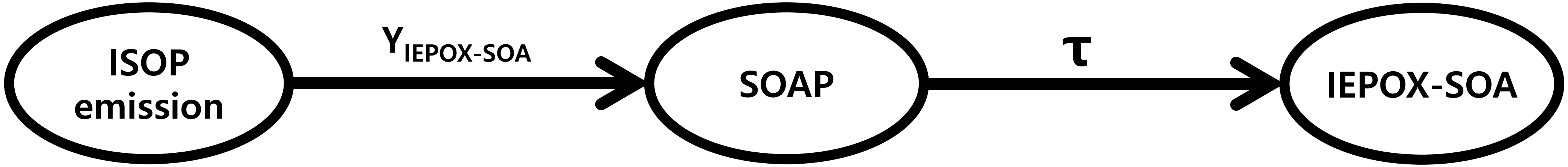
University of Colorado Boulder

PAR3



- Chemical loss by OH
- Dry deposition

PAR1

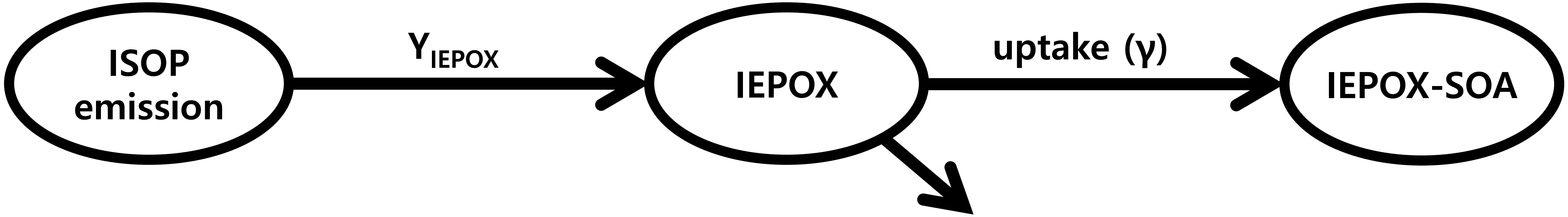


τ : E-folding time in the first order kinetic equation

$$\text{IEPOX-SOA}(t+\Delta t) = \text{IEPOX-SOA}(t) + \{1 - \exp(-\frac{\Delta t}{\tau})\} \times \text{SOAP}(t)$$

$$\tau = f(L_{ISOP}, L_{ISOPOOH}, L_{IEPOX}, L_{ISOPN}, NO, HO_2)$$

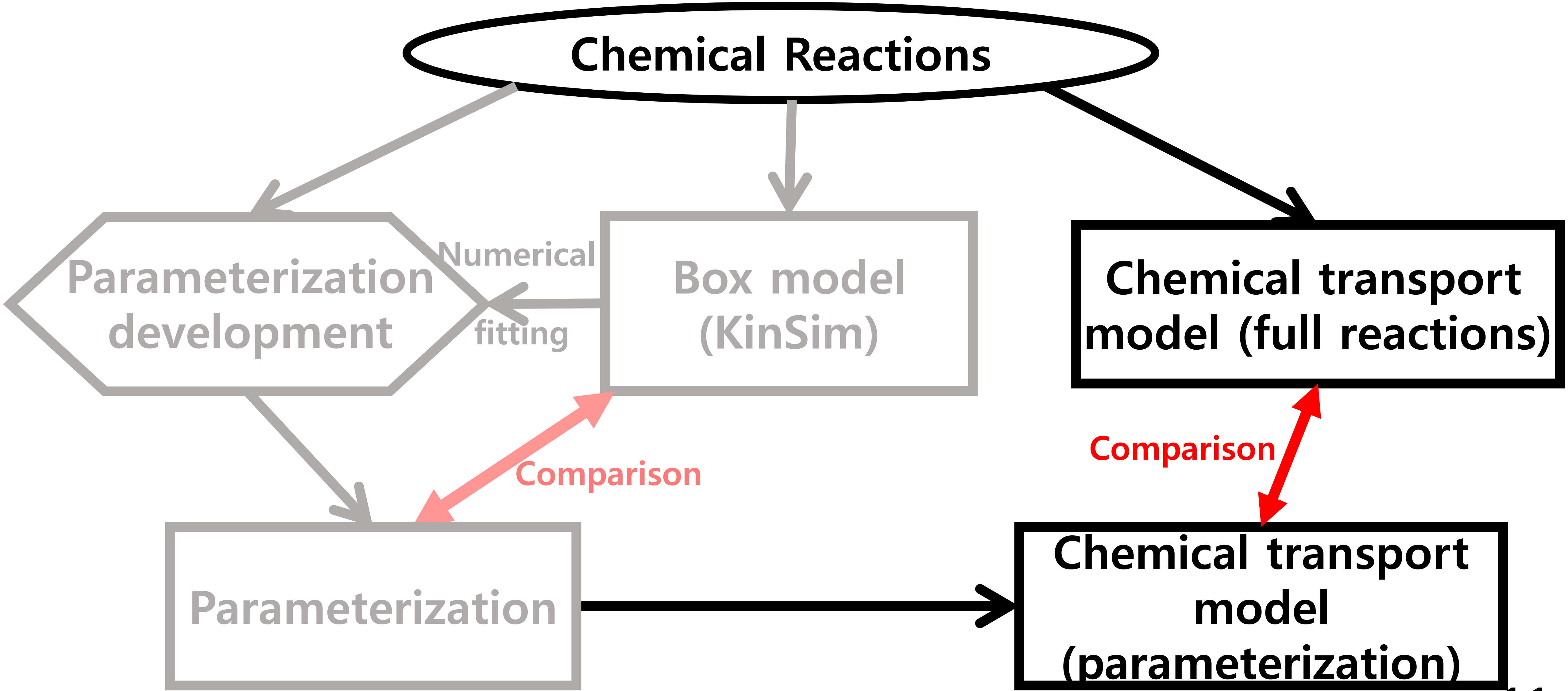
PAR2



- Chemical loss by OH
- Dry deposition

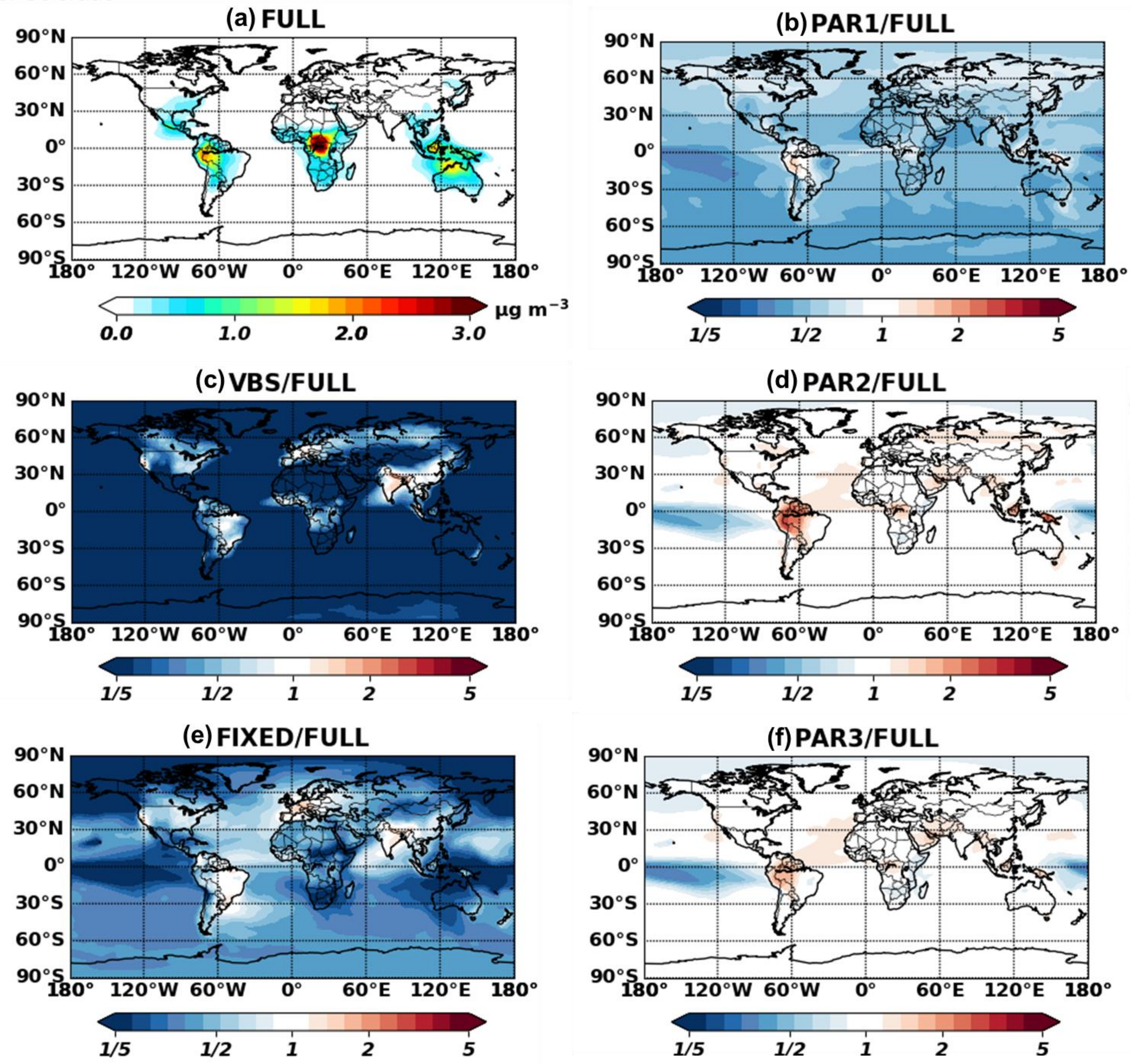
University of Colorado Boulder

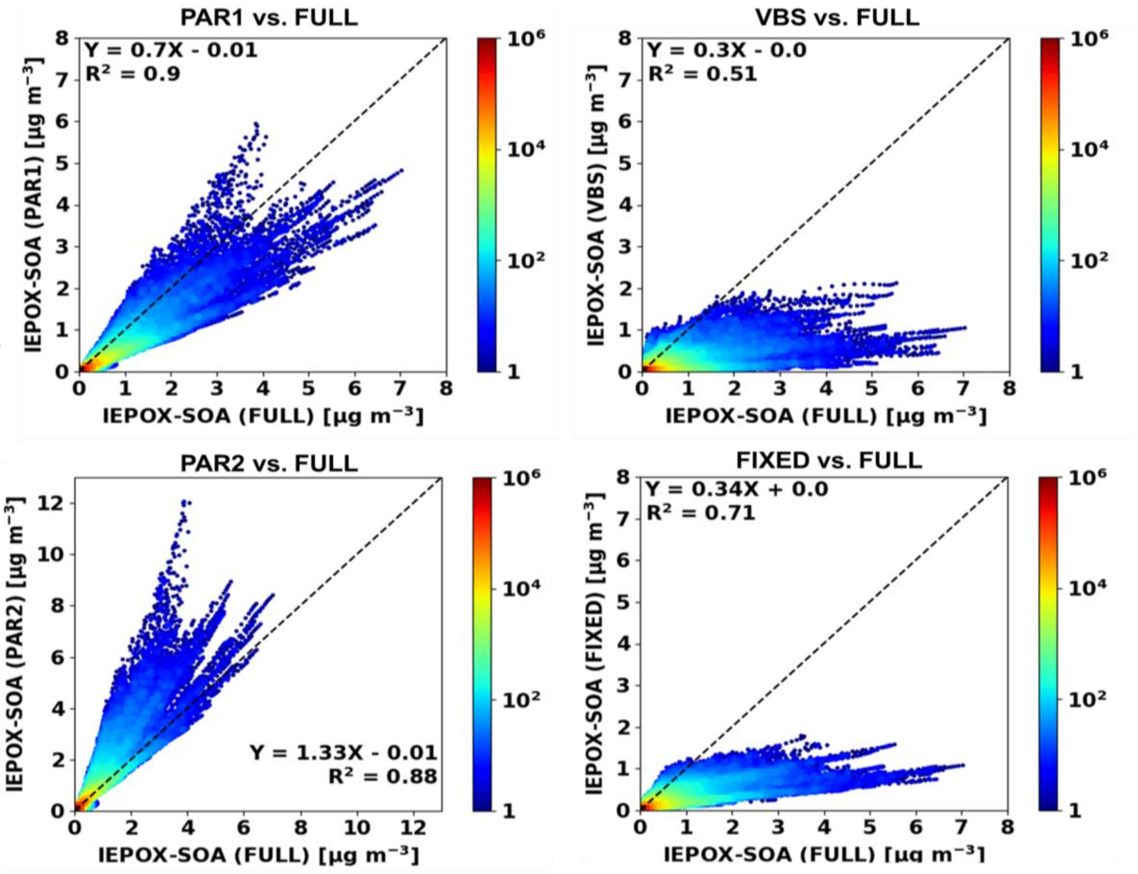
Objective : Develop a parameterization of IEPOX-SOA without an additional heavy computational cost

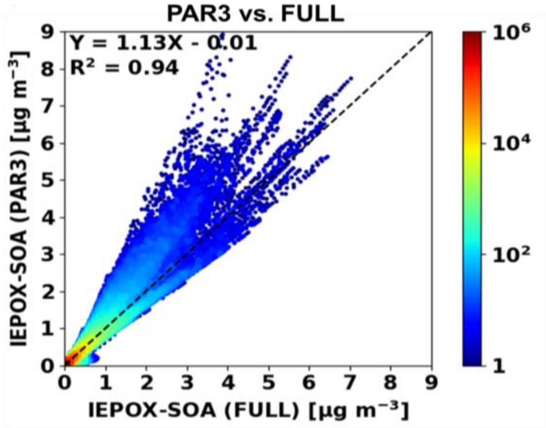


University of Colorado

Annual mean IEPOX-SOA surface maps and scatterplots for troposphere

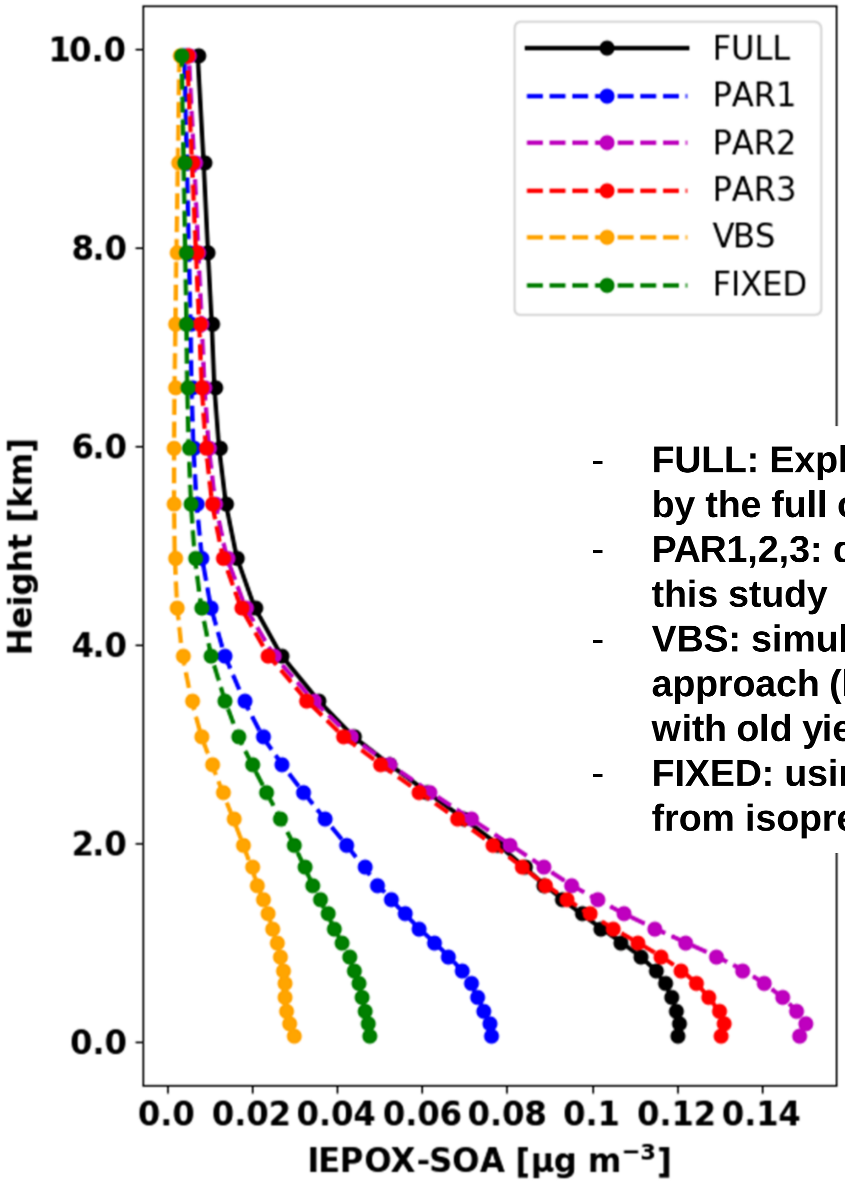






- **FULL: Explicitly simulated by the full of reactions**
- **PAR1,2,3: developed by this study**
- **VBS: simulated by VBS approach (like CESM2 but with old yields)**
- **FIXED: using a fixed yield from isoprene emissions**

Vertical profiles



- FULL: Explicitly simulated by the full of reactions
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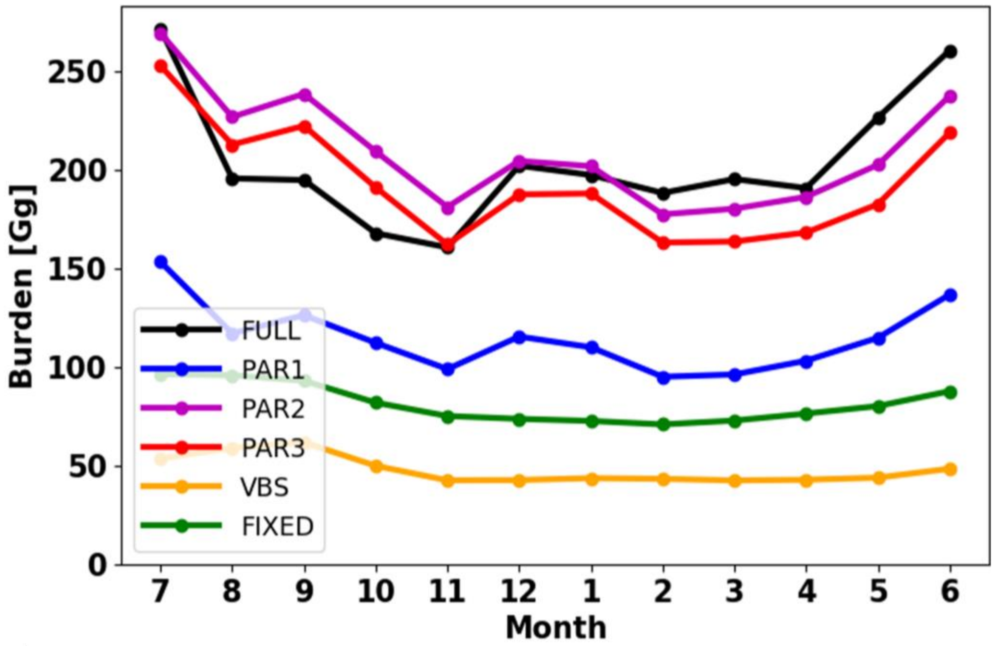
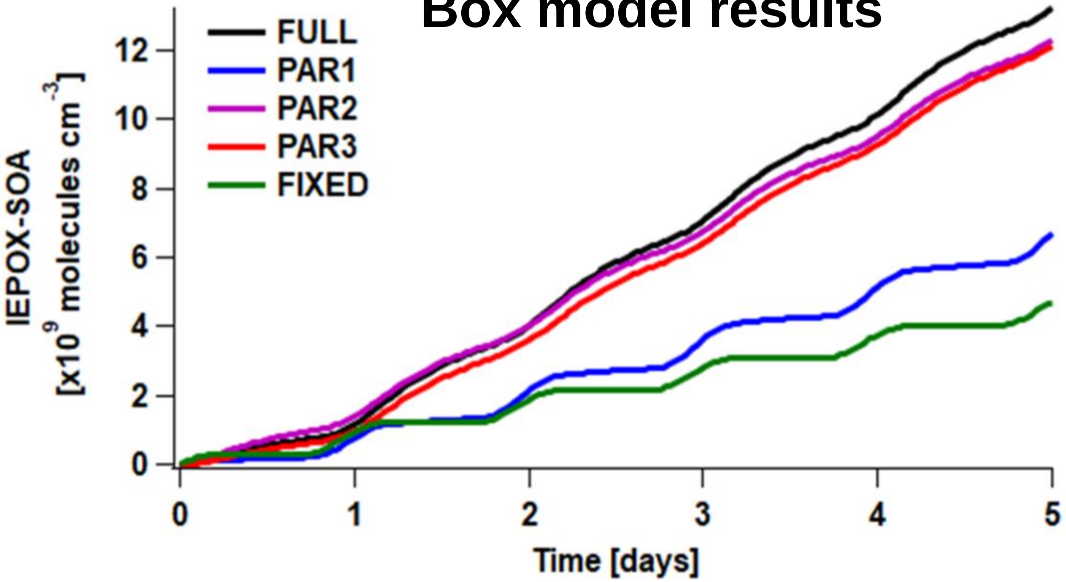
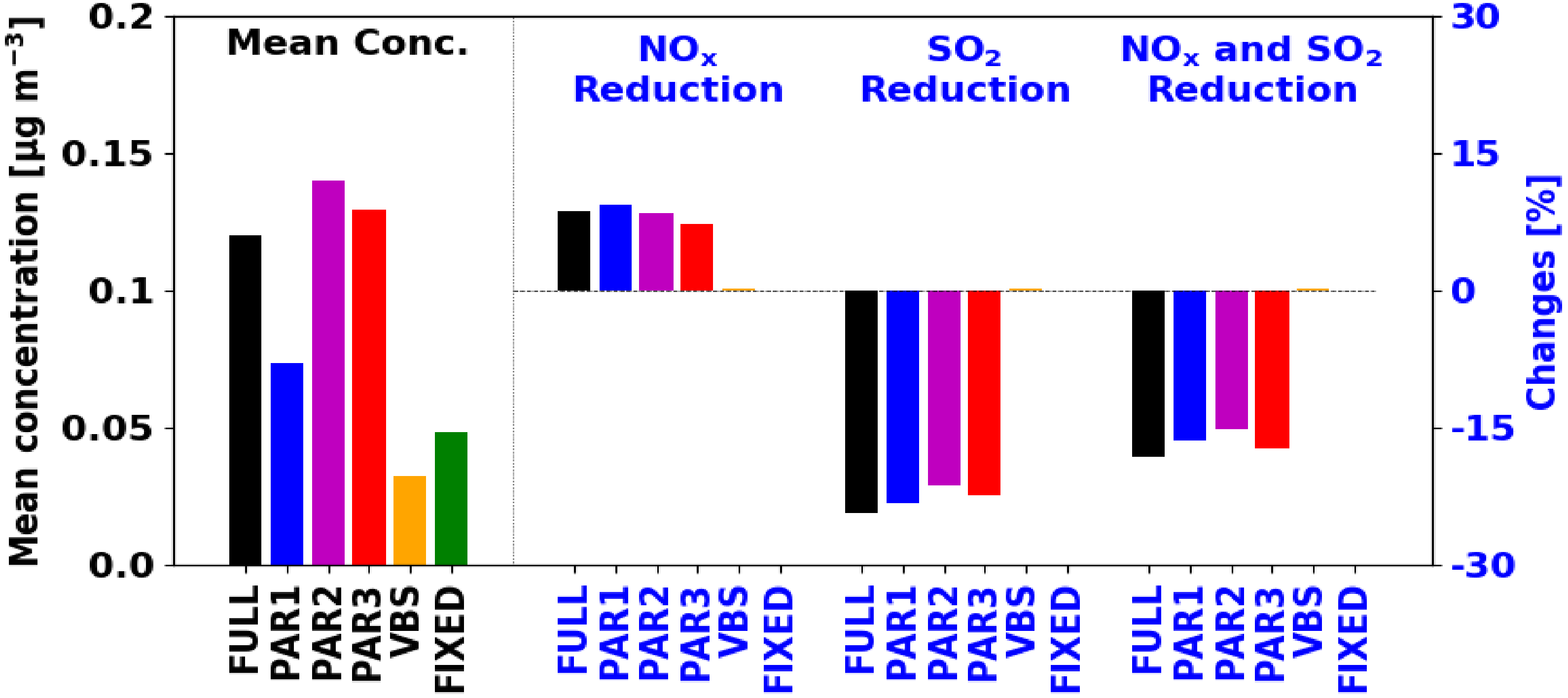
Burdens



Box model results



Sensitivity to emission changes and computational time



- FULL: Explicitly simulated by the full of reactions
- PAR1,2,3: developed by this study
- VBS: simulated by VBS approach (like CESM2 but with old yields)
- FIXED: using a fixed yield from isoprene emissions

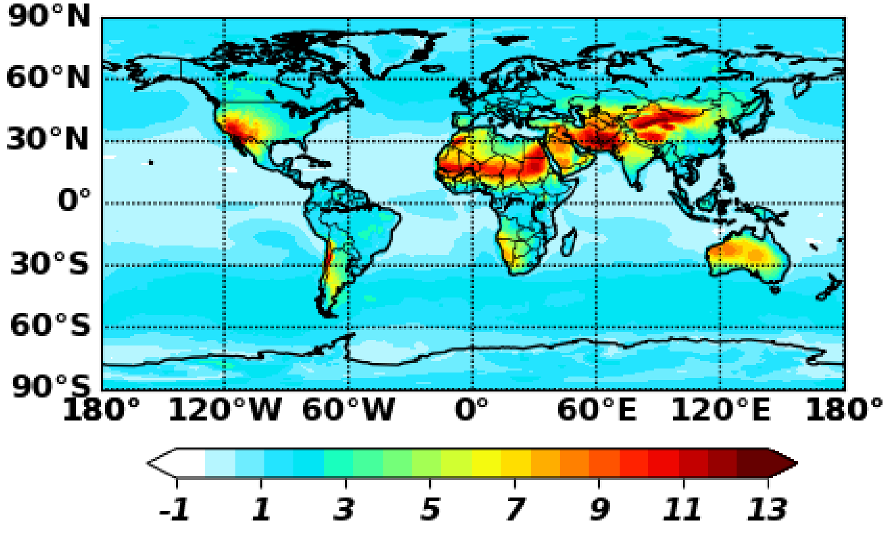
Unit: [s]	Chemistry	Transport	Dry deposition	Wet deposition	Total
FULL	559	172	30	380	1141
VBS	7	120	20	253	400
PAR1	47	34	7	84	172
PAR2	13	34	7	84	138
PAR3	48	52	7	127	234
FIXED	1	34	2	42	80

Moving from GEOS-Chem to CAM-chem for future simulations of SOA

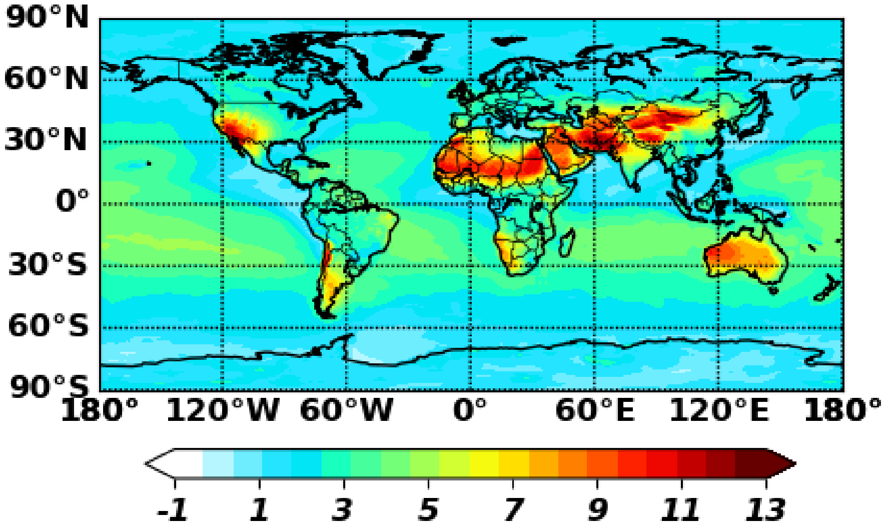
	GEOS-Chem	**CAM-chem**
Aerosol scheme	Bulk aerosol scheme	Modal aerosol scheme (MAM4: 4 modes)
Species	BC, POA, SOA, Sulfate, Nitrate, Ammonium, Sea salt, Dust	BC, POA, SOA, Sulfate, Sea salt, Dust, Number + Nitrate, Ammonium (MOSAIC)
Thermodynamics	ISORROPIA Ⅱ	MOSAIC
Mixing state	External	External(between modes) + Internal (within modes)
Condensation and coagulation	No	Yes
Aging of BC and POA	Fixed e-folding time scale (1.15 days)	Directly calculated
Time required for 1 year simulation	~ 5 days	~12 hours

Aerosol pH fields from CESM2.1 (MOSAIC)

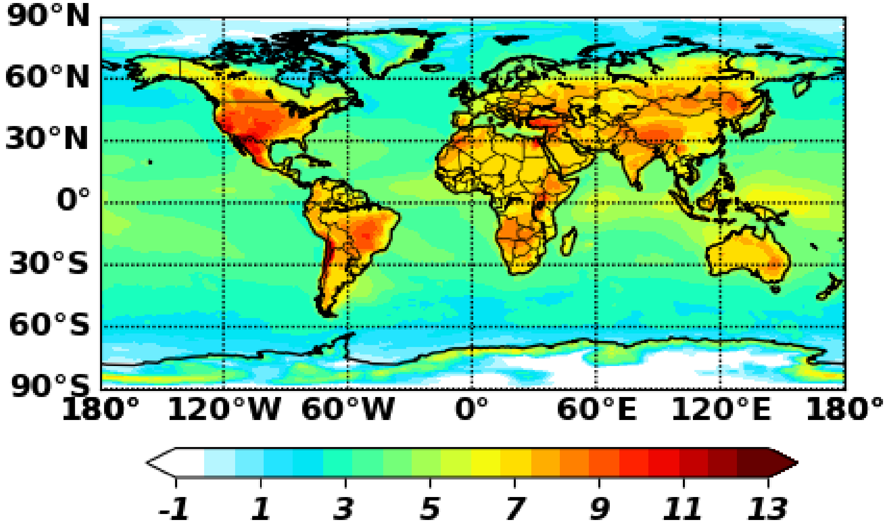
Aitken mode

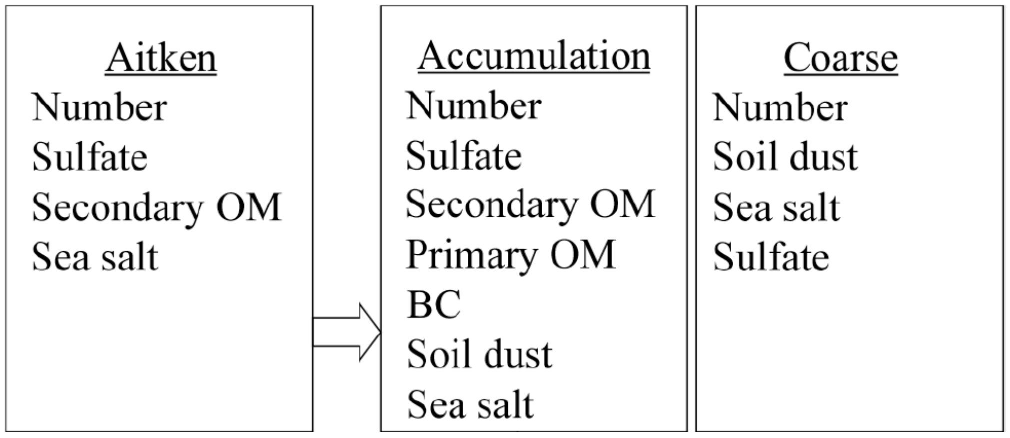


Accumulation mode



Coarse mode



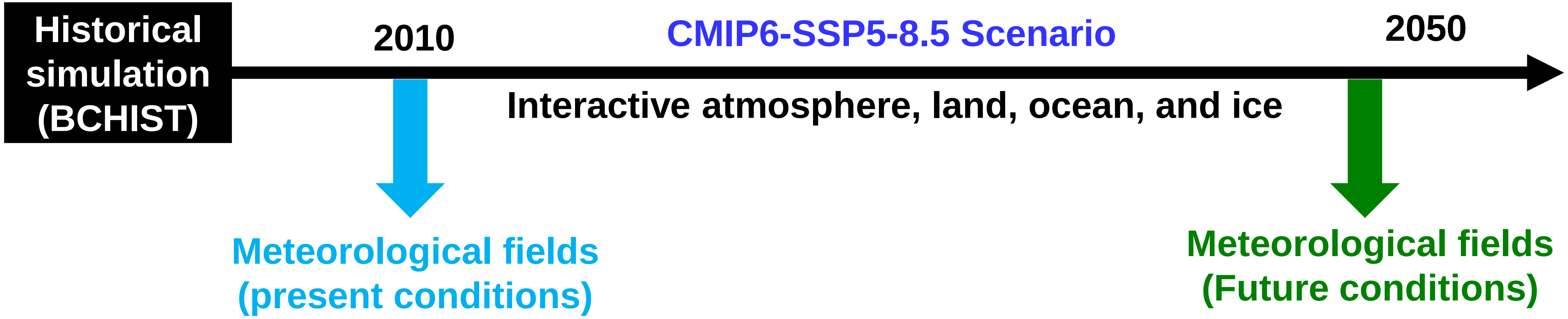


Aitken	Accumulation	Coarse
Number	Number	Number
Sulfate	Sulfate	Soil dust
Secondary OM	Secondary OM	Sea salt
Sea salt	Primary OM	Sulfate
	BC	
	Soil dust	
	Sea salt	

+ Ca^{2+}, Cl^-, NH_4^+, NO_3^-, CO_3^{2-} (MOSAIC)

Liu et al. (2016)

Evaluating SOA under Future Climate



Historical simulation (BCHIST)

2010

CMIP6-SSP5-8.5 Scenario

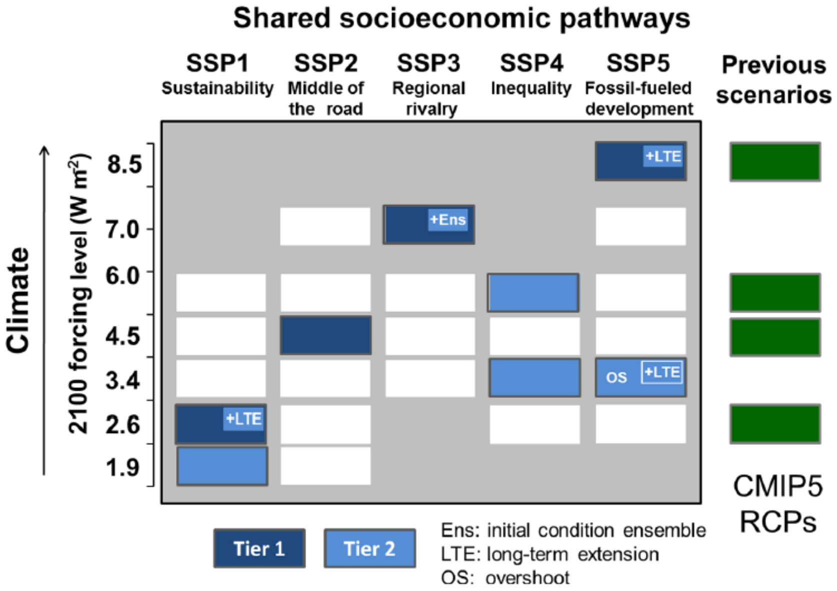
2050

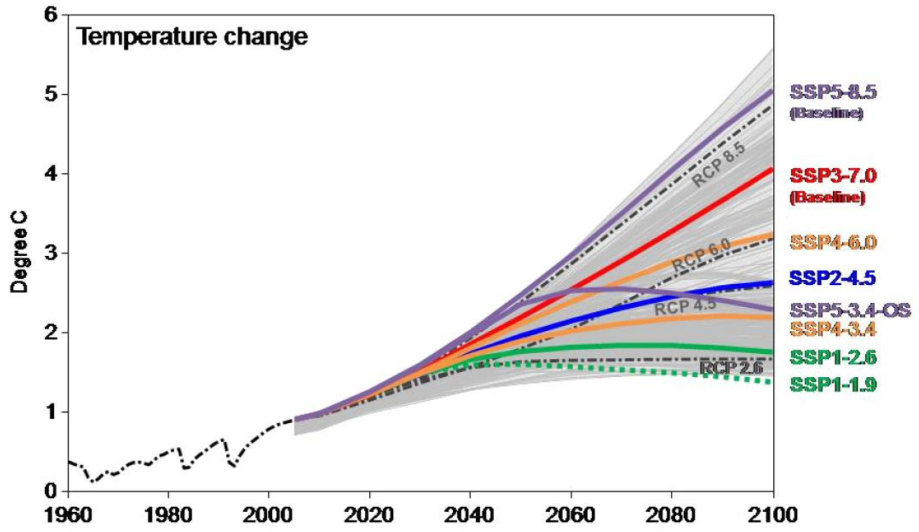
Interactive atmosphere, land, ocean, and ice

Meteorological fields (present conditions)

Meteorological fields (Future conditions)

Calculates secondary organic aerosol chemistry in present and future conditions

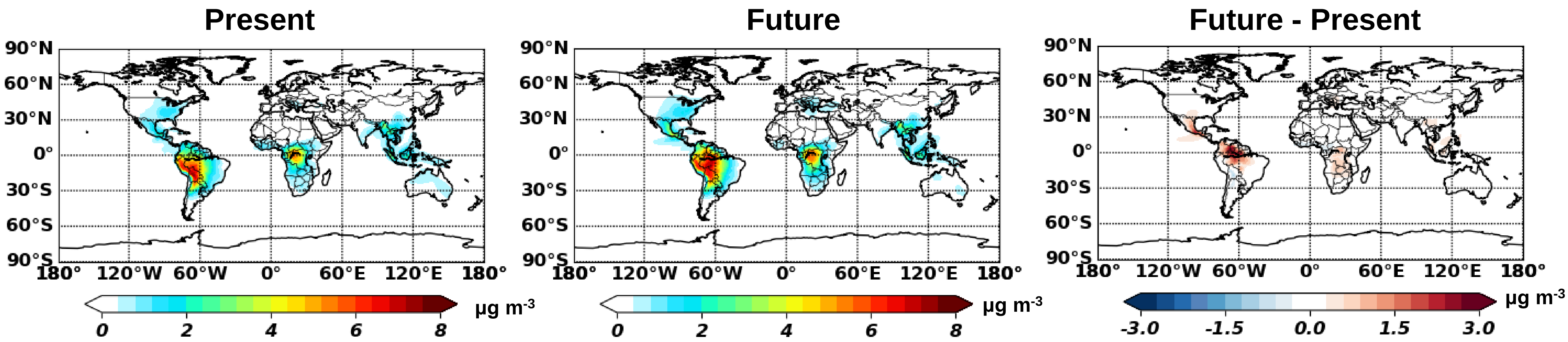




O'Neill et al. (2016)

IEPOX-SOA and Monoterpene SOA change in future climate

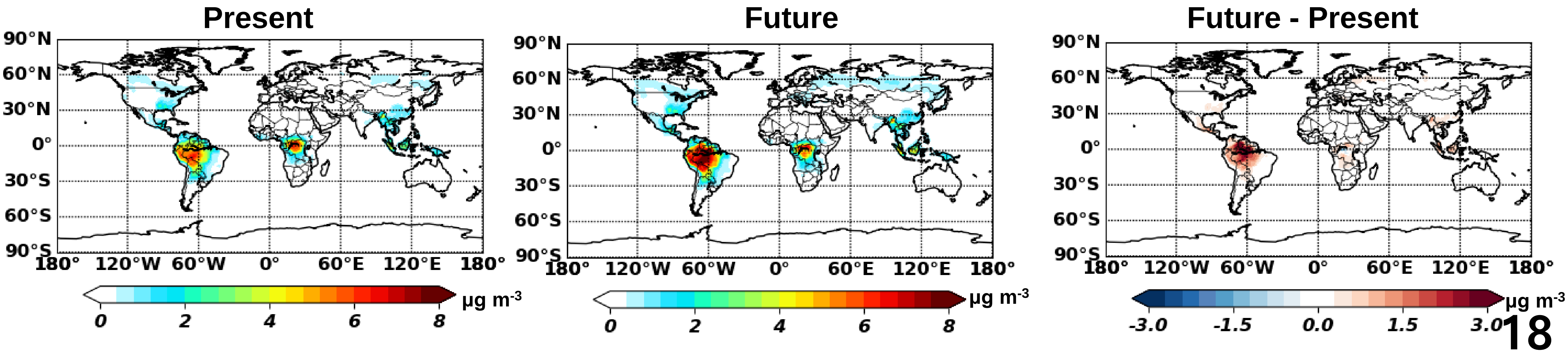
IEPOX-SOA


Present

Future

Future - Present

Monoterpene SOA

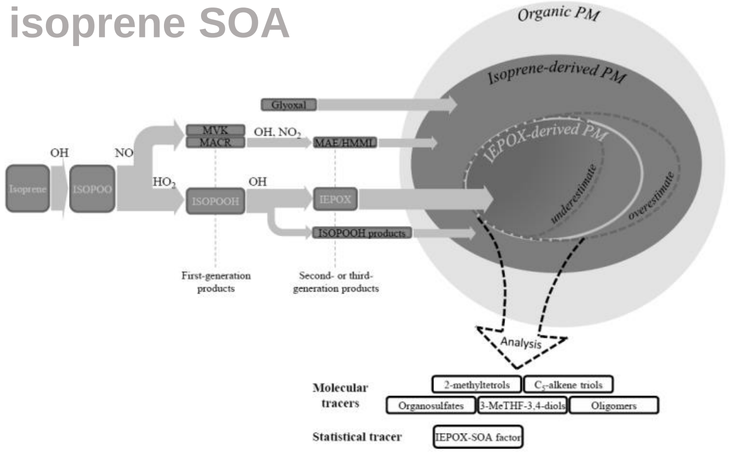

Present

Future

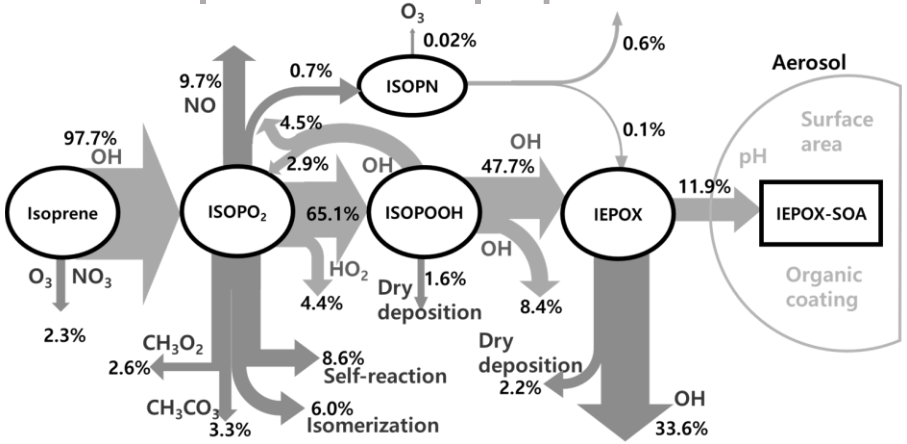
Future - Present

Summary

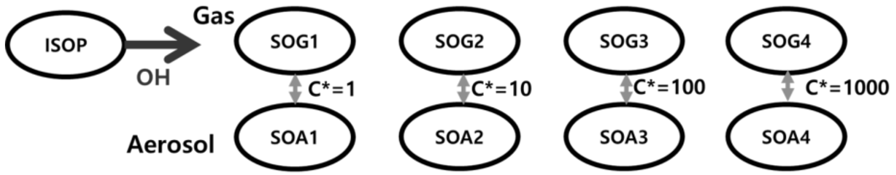
IEPOX-SOA is thought to contribute the dominant fraction of total isoprene SOA



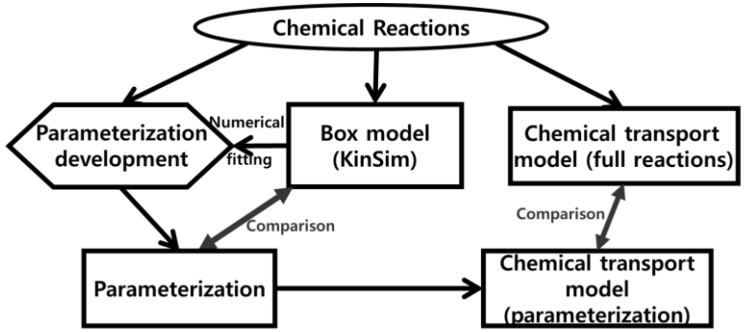
IEPOX-SOA formation depends on oxidants, aerosol pH and other properties



But current SOA parameterizations (e.g. VBS) used in chemistry models consider only simple chemistry such as VOC + OH



New IEPOX-SOA parameterizations retaining key physico-chemical dependencies were developed, and they captured the response to changes on emissions



Chemical Reactions

Parameterization development

Numerical fitting

Box model (KinSim)

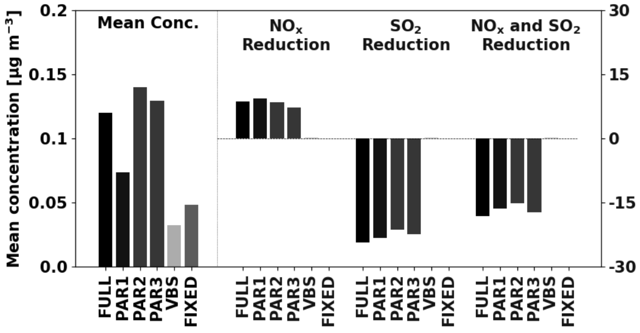
Chemical transport model (full reactions)

Comparison

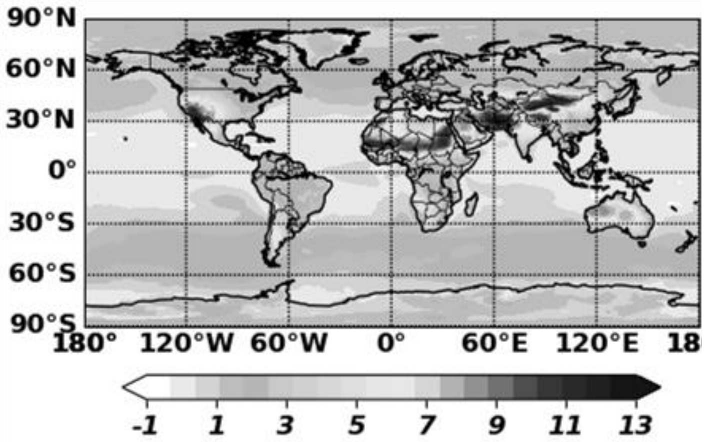
Comparison

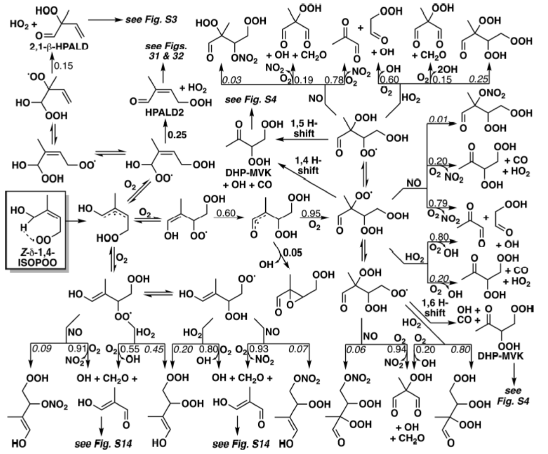
Parameterization

Chemical transport model (parameterization)



With a new MAM-MOSAIC framework and updated isoprene and monoterpene chemistry, CESM2.1 can be a best tool for investigating future SOA changes





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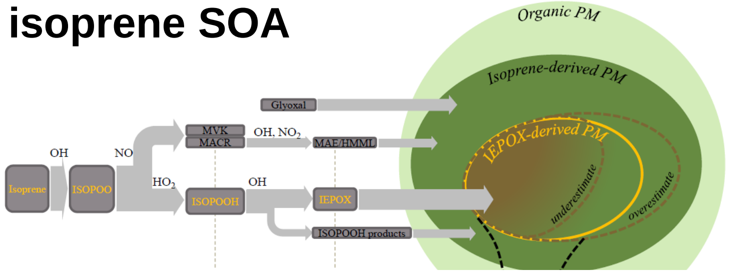
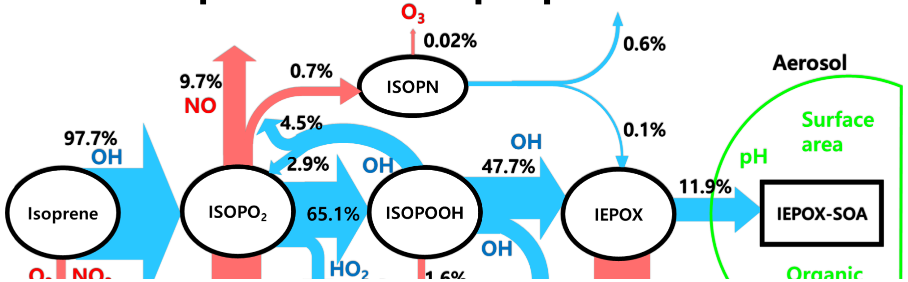
Summary

IEPOX-SOA is thought to contribute the dominant fraction of total isoprene SOA



IEPOX-SOA formation depends on oxidants, aerosol pH and other properties



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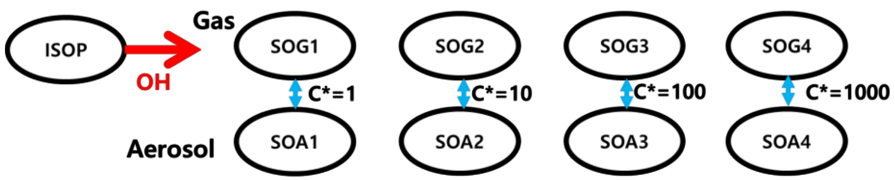
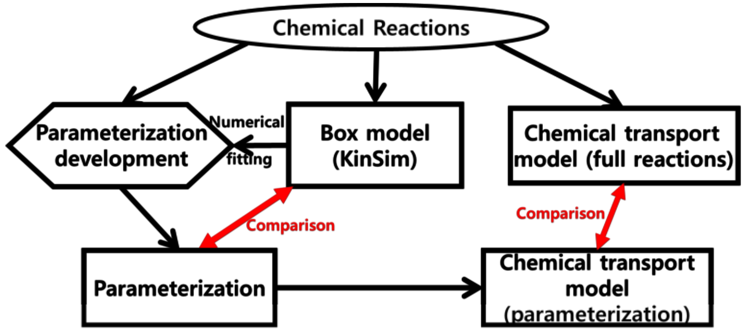
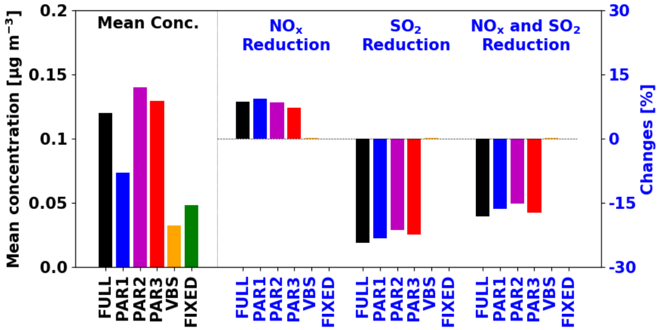


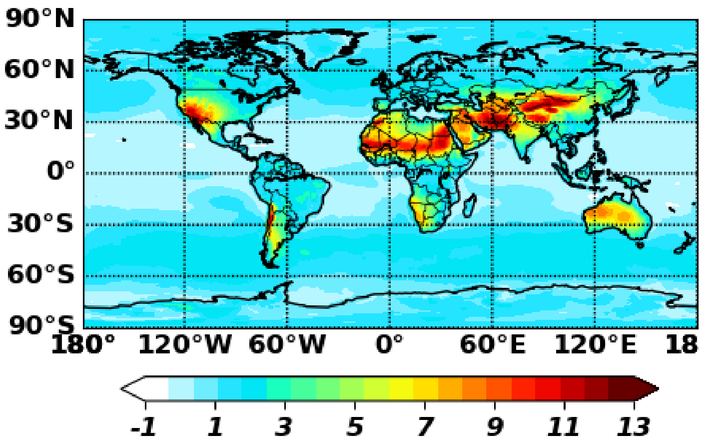
Thank you!

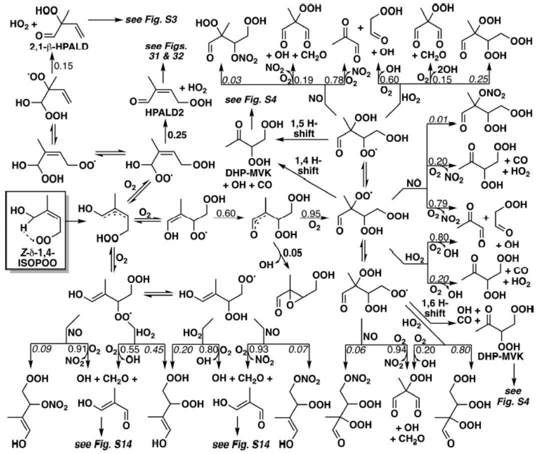
New IEPOX-SOA parameterizations retaining key physico-chemical dependencies were developed, and they captured the response to changes on emissions





With a new MAM-MOSAIC framework and updated isoprene and monoterpene chemistry, CESM2.1 can be a best tool for investigating future SOA changes





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Back-up slides

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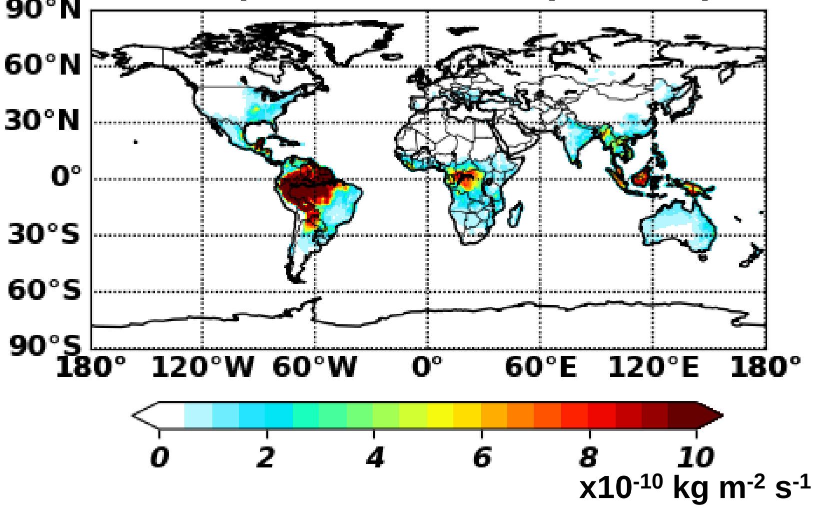
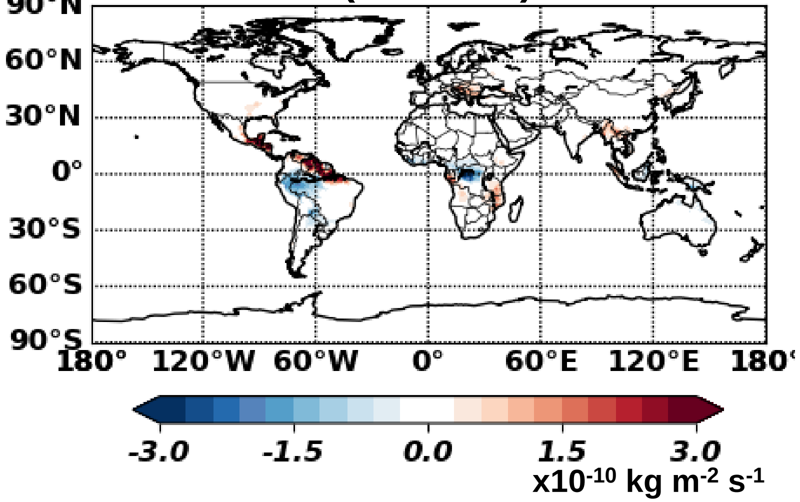
Isoprene emission change

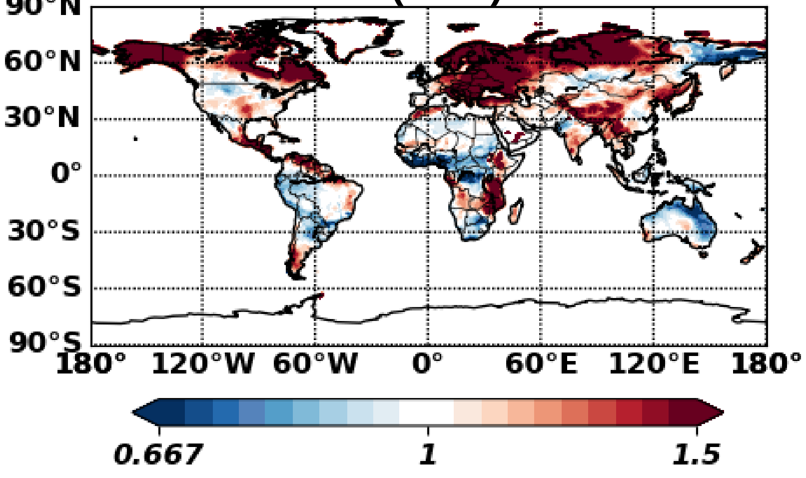
Isoprene emission (Present)



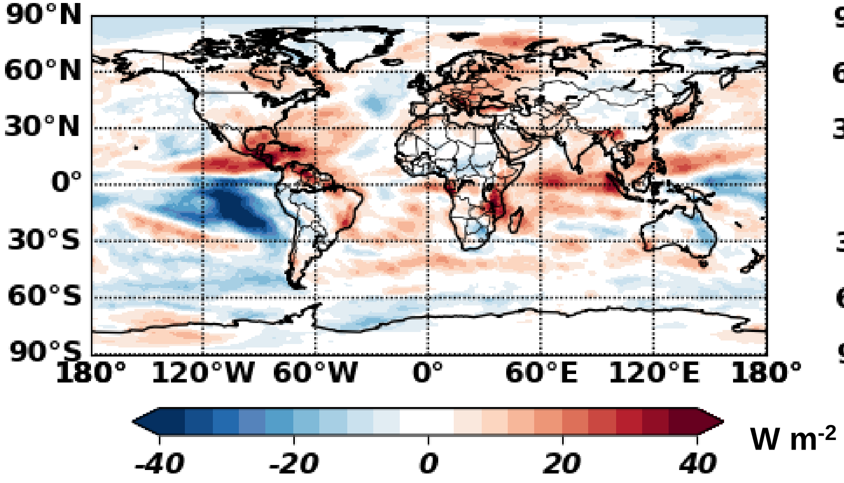
Isoprene emission change (absolute)



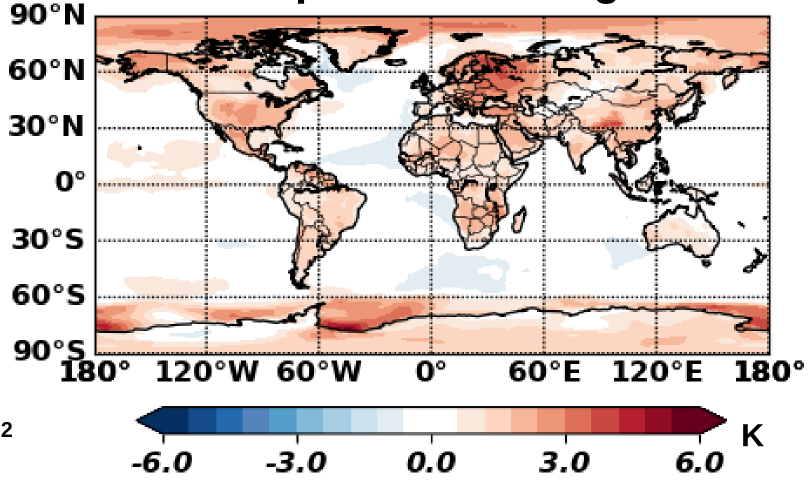
Isoprene emission change (ratio)



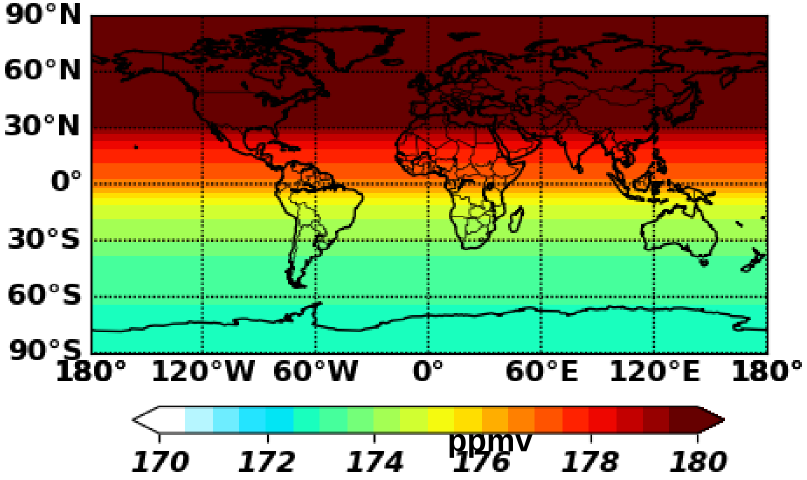
Downwelling solar flux change



Temperature Change



CO_2 Change



- Factors affecting isoprene emissions

→ light, temperature, leaf age, leaf area index, and CO_2

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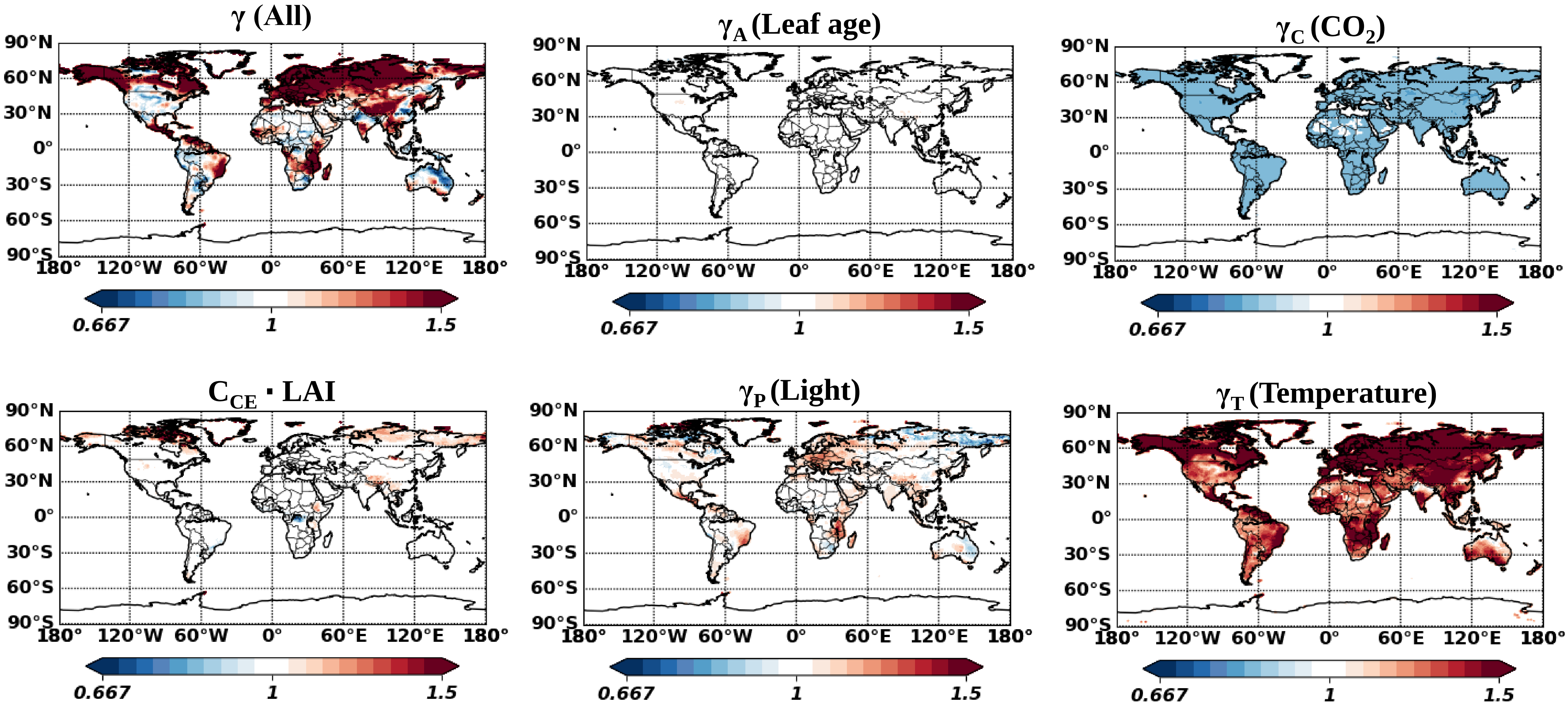
Gamma values change (2050/2010) for biogenic emissions

$$\gamma = C_{CE} \cdot LAI \cdot \gamma_p \cdot \gamma_T \cdot \gamma_A \cdot \gamma_{SM} \cdot \gamma_C$$



γ (All)

γ_A (Leaf age)

γ_C (CO_2)

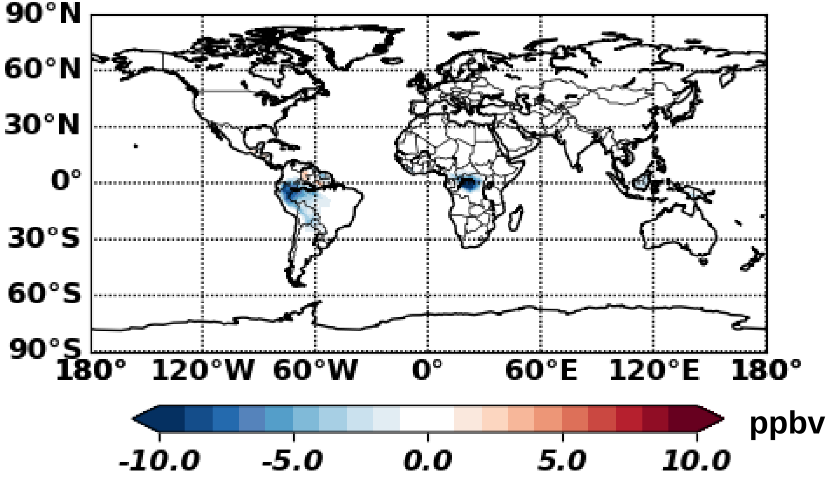
$C_{CE} \cdot LAI$

γ_P (Light)

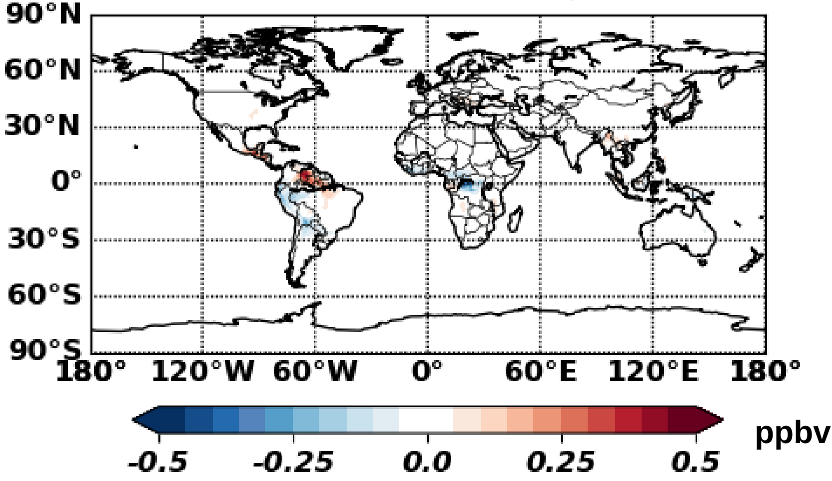
γ_T (Temperature)

Future changes of IEPOX-SOA precursors and oxidants

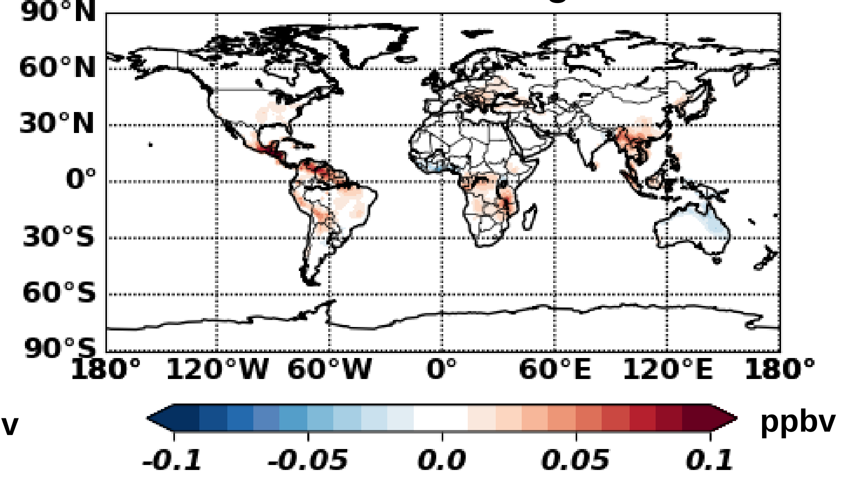
Isoprene change



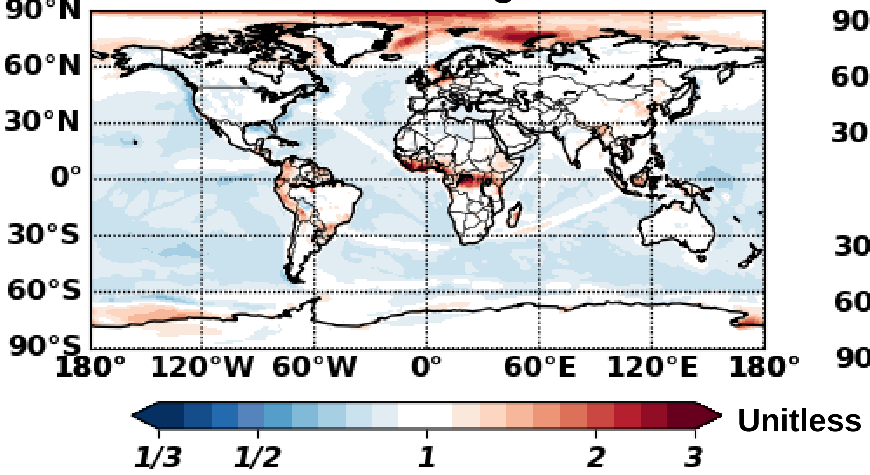
ISOPOOH change



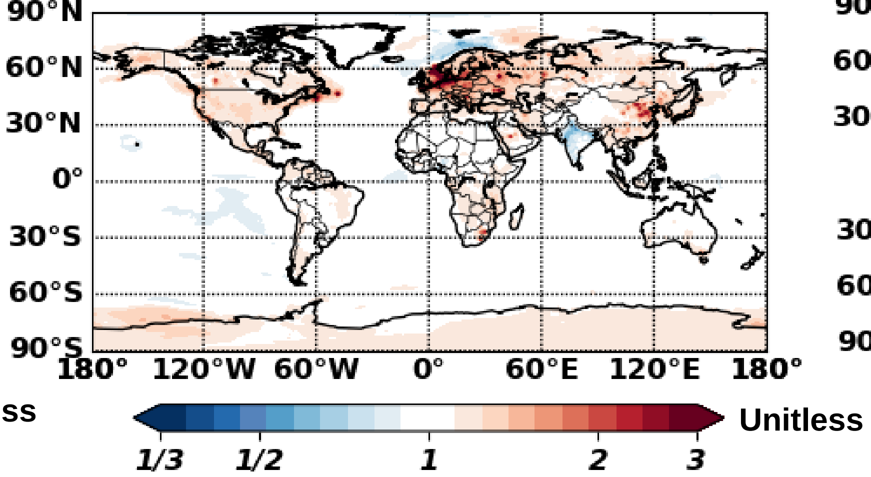
IEPOX change



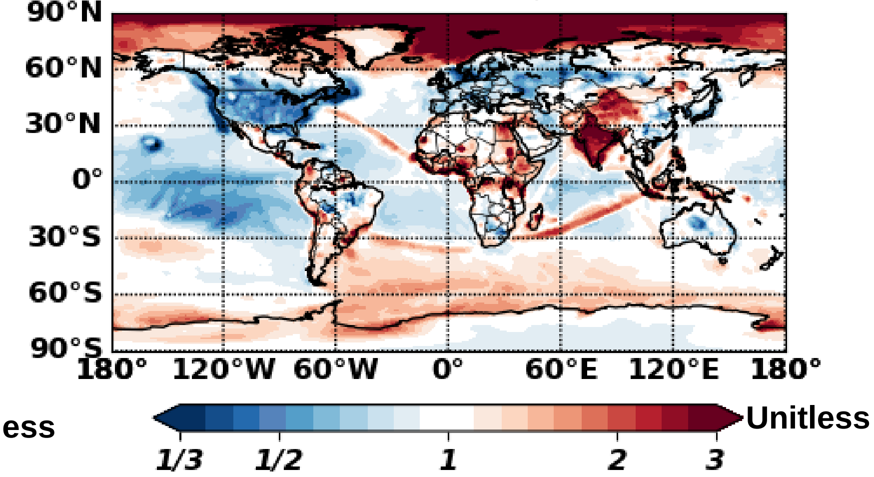
OH change



HO_2 change



NO change



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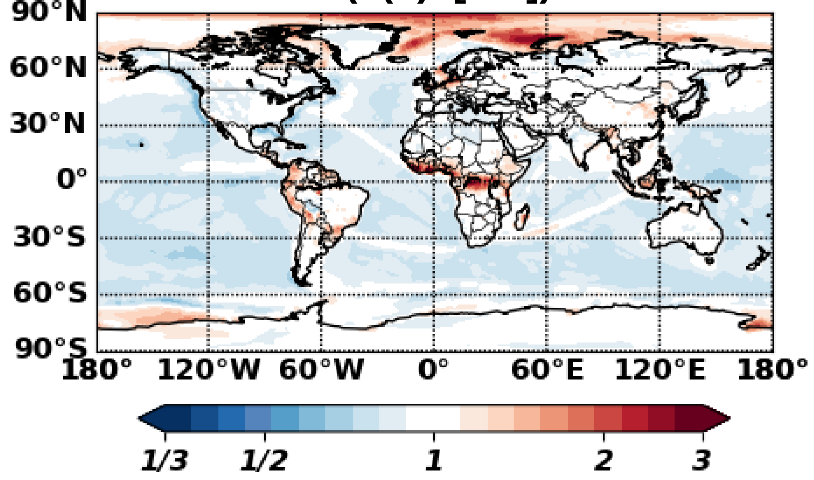
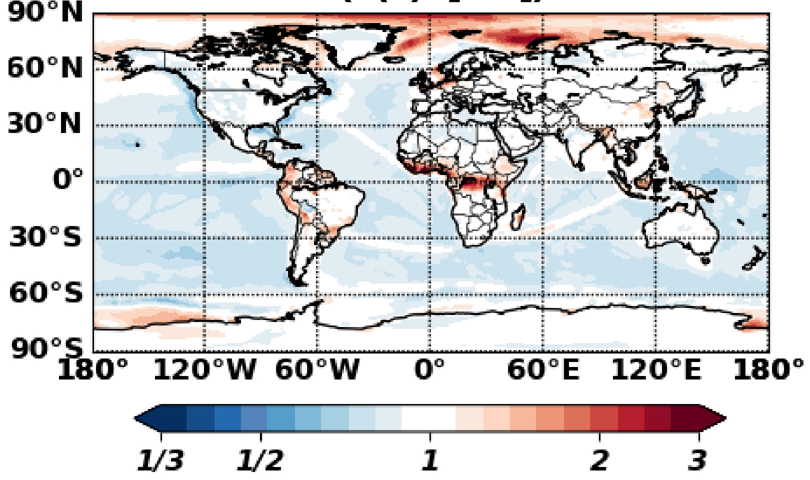
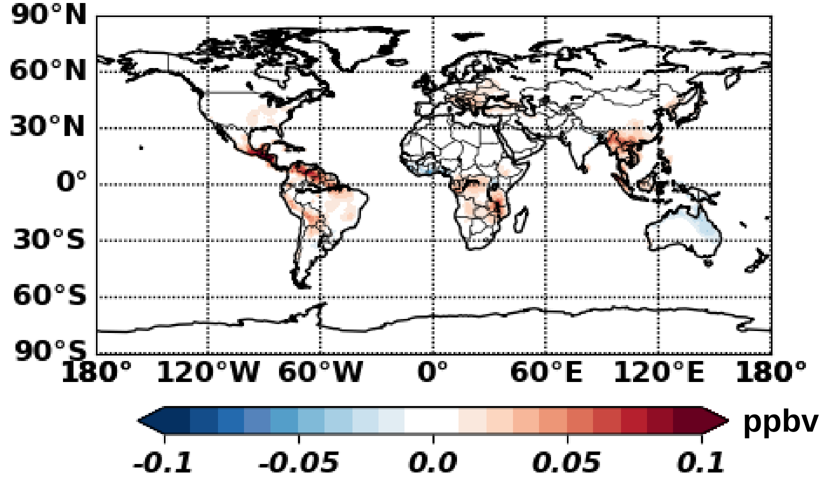
Future changes of chemical pathways affecting IEPOX-SOA (2050/2010)



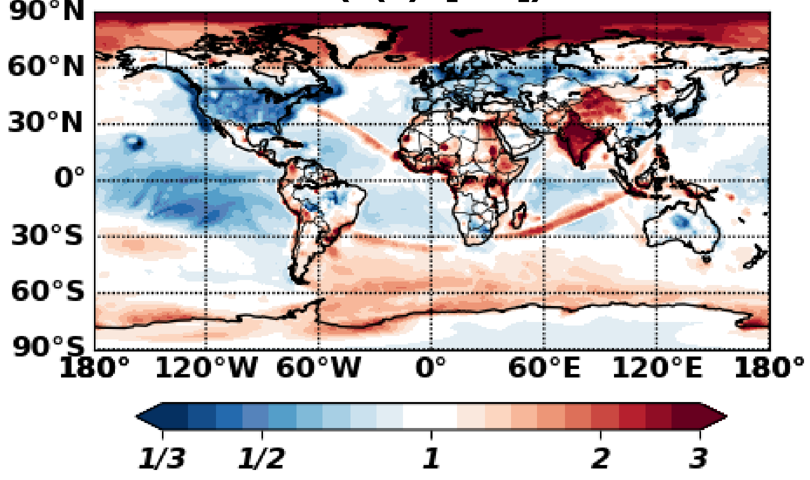
Isoprene + OH
(k(T)x[OH])



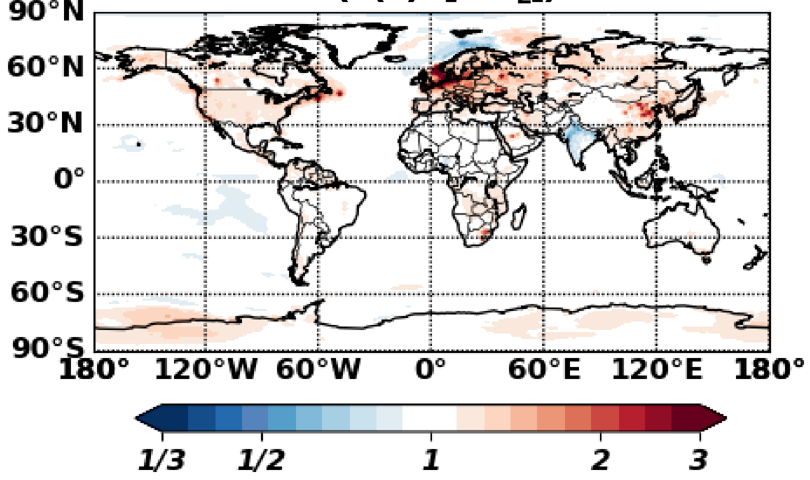
ISOPOOH + OH
(k(T)x[OH])



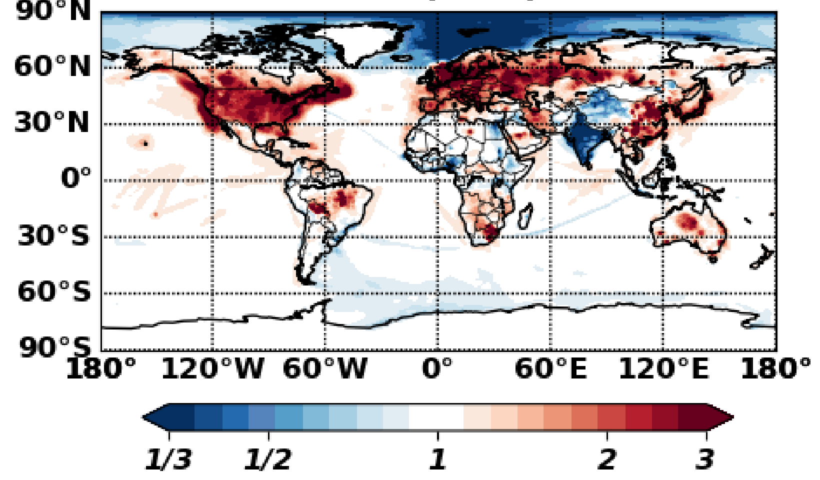
IEPOX change



(a) $ISOPO_2$ + NO
(k(T)x[NO])



(b) $ISOPO_2$ + HO_2
(k(T)x[HO_2])



b / (a + b)

Biogenic emission estimate algorithm

- Based on MEGANv2.1 (Guenther et al., 2012)

$$\gamma = C_{CE} \cdot LAI \cdot \gamma_p \cdot \gamma_T \cdot \gamma_A \cdot \gamma_{SM} \cdot \gamma_C$$

(1) C_{CE}: canopy environment coefficient. A value that results in **γ** = 1 for the standard conditions and is dependent on the canopy environment model being used. 0.3 is used for CESM2 land model

(2) LAI: Leaf Area Index

(3) γ_p: gamma for emission response to light (applied separately for the sunlit and shaded leaves)

$$\gamma_p = (1\text{-}LDF) + LDF \cdot \gamma_{p\_LDF}$$

LDF: light dependent fraction (1 for isoprene)

$$\gamma_{p\_LDF} = C_p \frac{\alpha \cdot PPFD}{\sqrt{1+\alpha^2 \cdot PPFD^2}}$$

PPFD : photosynthetic photon flux density (μmol m^{-2} s^{-1})

$$\alpha = 0.004 - 0.0005 \ln(P_{240})$$

$$C_p = 0.0468 \cdot \exp(0.0005 \cdot [P_{24} - P_s]) \cdot [P_{240}]^{0.6}$$

P_s : standard conditions for PPFD averaged over the past 24h (200 μmol m^{-2} s^{-1} for sun leaves and 50 μmol m^{-2} s^{-1} for shaded leaves)

P_{24} (P_{240}): average PPFD of the past 24h (240h)

(4) γ_T: gamma for emission response to temperature

$$\gamma_T = (1\text{-}LDF) \cdot \gamma_{T\_LIF} + LDF \cdot \gamma_{T\_LDF}$$

$$\gamma_{T\_LDF} = E_{opt} \frac{C_{T2} \cdot \exp(CT_1 \cdot x)}{C_{T2} - CT_1 \cdot (1 - \exp(C_{T2} \cdot x))}$$

$$x = \left(\frac{1}{T_{opt}} - \frac{1}{T}\right)/0.00831$$

$$E_{opt} = Ceo \cdot \exp(0.05 \cdot (T_{24} - T_s)) \cdot \exp(0.05 \cdot (T_{240} - T_s))$$

$$T_{opt} = 313 + (0.6 \cdot (T_{240} - Ts))$$

$$\gamma_{T\_LIF} = \exp(\beta \cdot (T - T_s))$$

LIF: light independent fraction

T_s : standard conditions for leaf temperature (297 K)

C_{T1}, C_{T2}, C_{eo}, β: Empiricially determined coefficients

- C_{T1} = 95, C_{T2} = 230, C_{eo} = 2, β=0.13 for isoprene

Biogenic emission estimate algorithm

- Based on MEGANv2.1 (Guenther et al., 2012)

$$\gamma = C_{CE} \cdot LAI \cdot \gamma_p \cdot \gamma_T \cdot \gamma_A \cdot \gamma_{SM} \cdot \gamma_C$$

(5) γ_A: gamma for emission response to leaf age

$$\gamma_A = F_{new} \cdot A_{new} + F_{gro} \cdot A_{gro} + F_{mat} \cdot A_{mat} + F_{sen} \cdot A_{sen}$$

A_{new}, A_{gro}, A_{mat}, A_{sen}: Empirical coefficients that describe the relative mission rates for new, growing, mature, and senescing leaves (=0.05, 0.6, 1.0, 0.9 for isoprene)

F_{new}, F_{gro}, F_{mat}, F_{sen}: leaf age fractions calculated by MEGAN

(6) γ_{SM}: gamma for emission response to soil moisture (only for isoprene)

$$\gamma_{SM} = 1 \qquad \theta > \theta_1$$
$$\gamma_{SM} = (\theta - \theta_w) / \Delta\theta_1 \qquad \theta_w < \theta < \theta_1$$
$$\gamma_{SM} = 0 \qquad \theta < \theta_w$$

θ: soil moisture (volumetric water content, $m^3\ m^{-3}$)

θ_w: wilting point (the soil moisture level below which plants cannot extract water from soil, $m^3\ m^{-3}$)

$\Delta\theta_1$: empirical parameter (0.04)

θ_1: $\theta_w + \Delta\theta_1$

Currently assumed to be 1 in CESM model

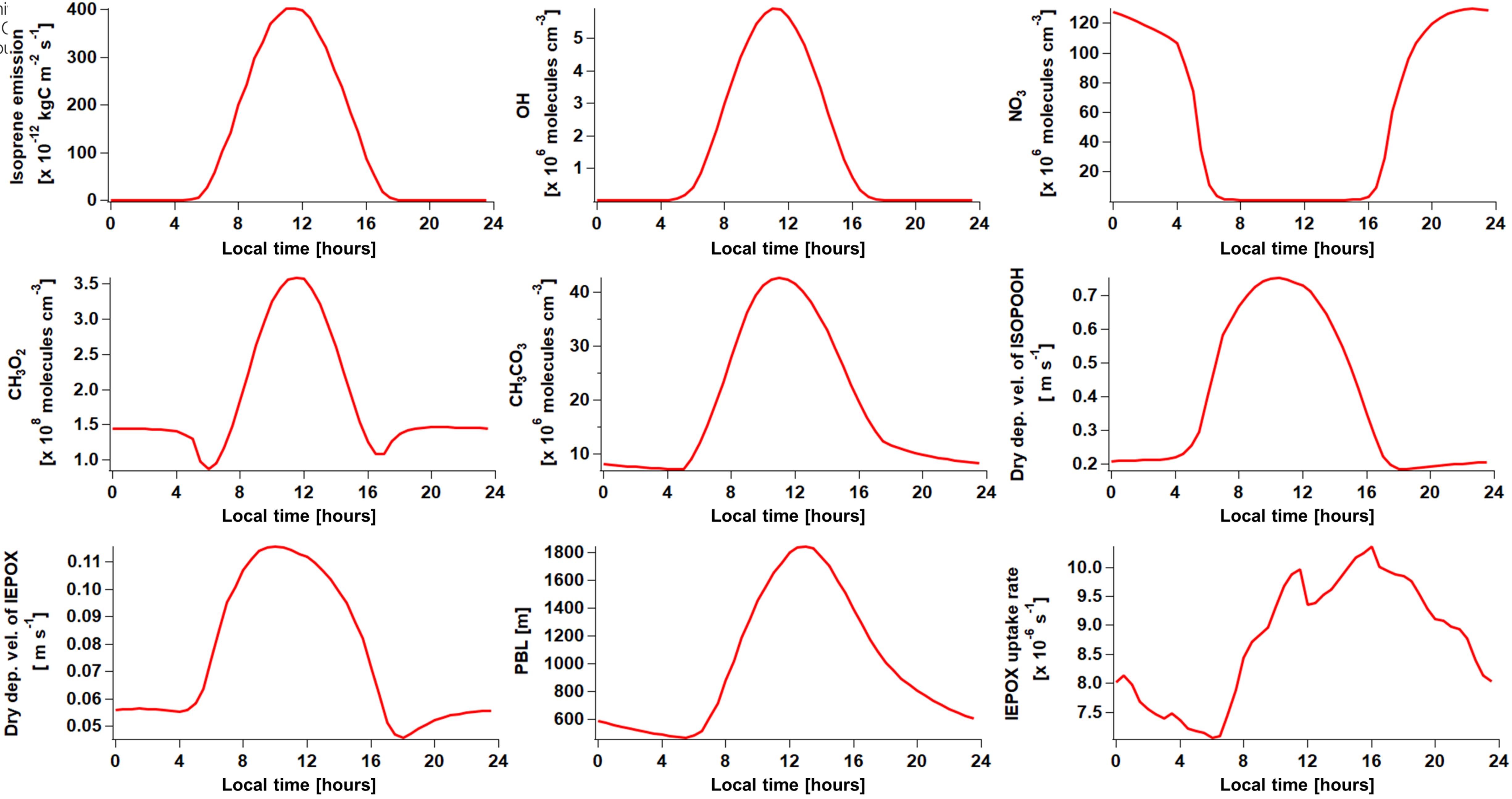
(6) γ_C: gamma for emission response to CO_2 inhibition (only for isoprene)

$$\gamma_C = I_{Smax} - \frac{I_{Smax} \cdot (C_i)^h}{(C*)^h + (C_i)^h}$$

Calculated for long-term (based on ambient CO_2) and short-term (based on intercellular CO_2) exposures

C_i: 0.7 x ambient CO_2 for long-term exposure
intracellular CO_2 for short-term exposure

C*, h, I_{Smax}: Empirically determined parameters (Heald et al., 2009)


Isoprene emission [x 10^{-12} kgC m^{-2} s^{-1}]
0
100
200
300
400
OH [x 10^6 molecules cm^{-3}]
1
2
3
4
5
NO_3 [x 10^6 molecules cm^{-3}]
20
40
60
80
100
120
CH_3O_2 [x 10^8 molecules cm^{-3}]
1.0
1.5
2.0
2.5
3.0
3.5
CH_3CO_3 [x 10^6 molecules cm^{-3}]
10
20
30
40
Dry dep. vel. of ISOPOOH [m s^{-1}]
0.2
0.3
0.4
0.5
0.6
0.7
Dry dep. vel. of IEPOX [m s^{-1}]
0.05
0.06
0.07
0.08
0.09
0.10
0.11
PBL [m]
600
800
1000
1200
1400
1600
1800
IEPOX uptake rate [x 10^{-6} s^{-1}]
7.5
8.0
8.5
9.0
9.5
10.0
0
4
8
12
16
20
24
Local time [hours]

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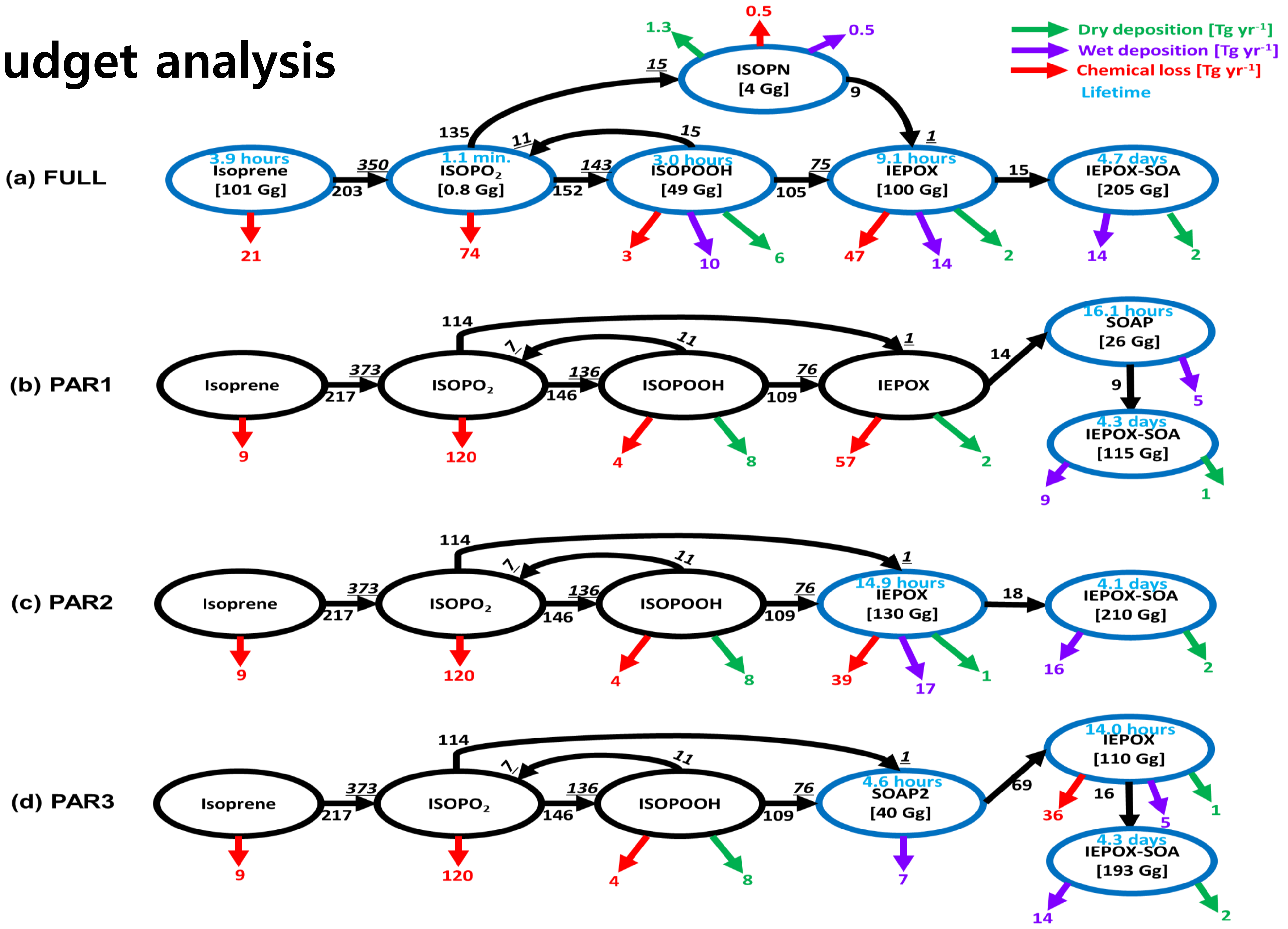
Budget analysis



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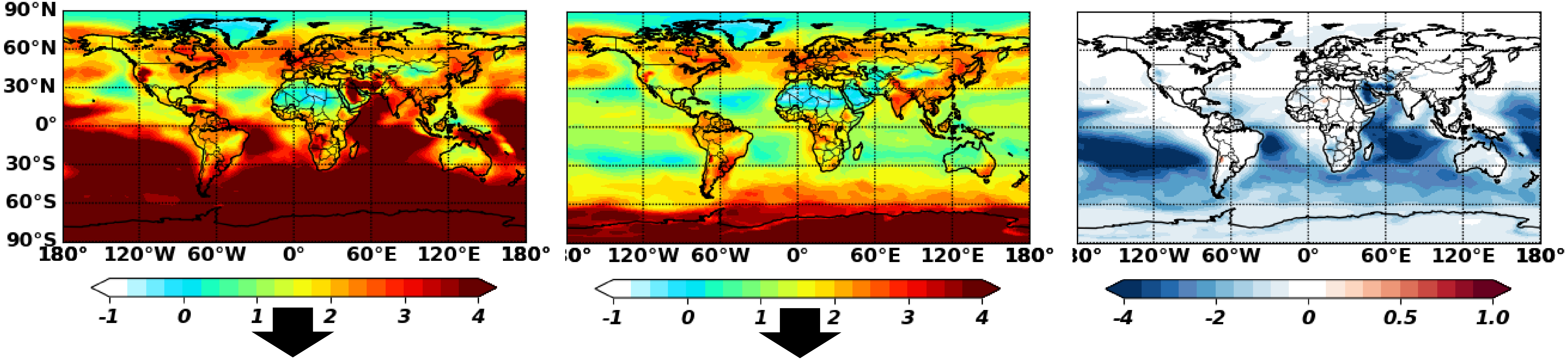
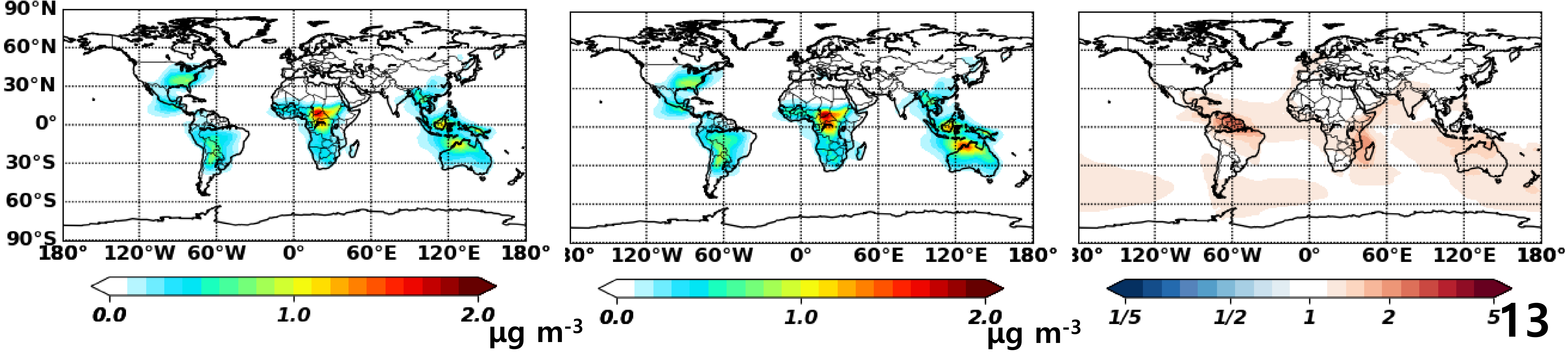
Surface 2-D map of pHs in GEOS-Chem


(a) Base case pH

(b) pH w/o sea salt

(b) – (a)


(c) IEPOX-SOA

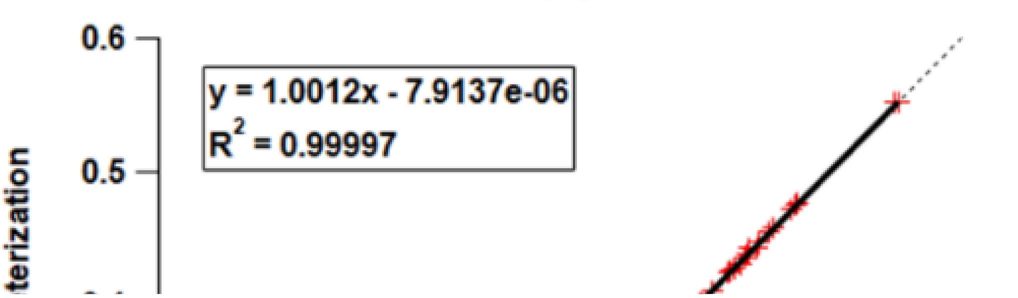
(d) IEPOX-SOA

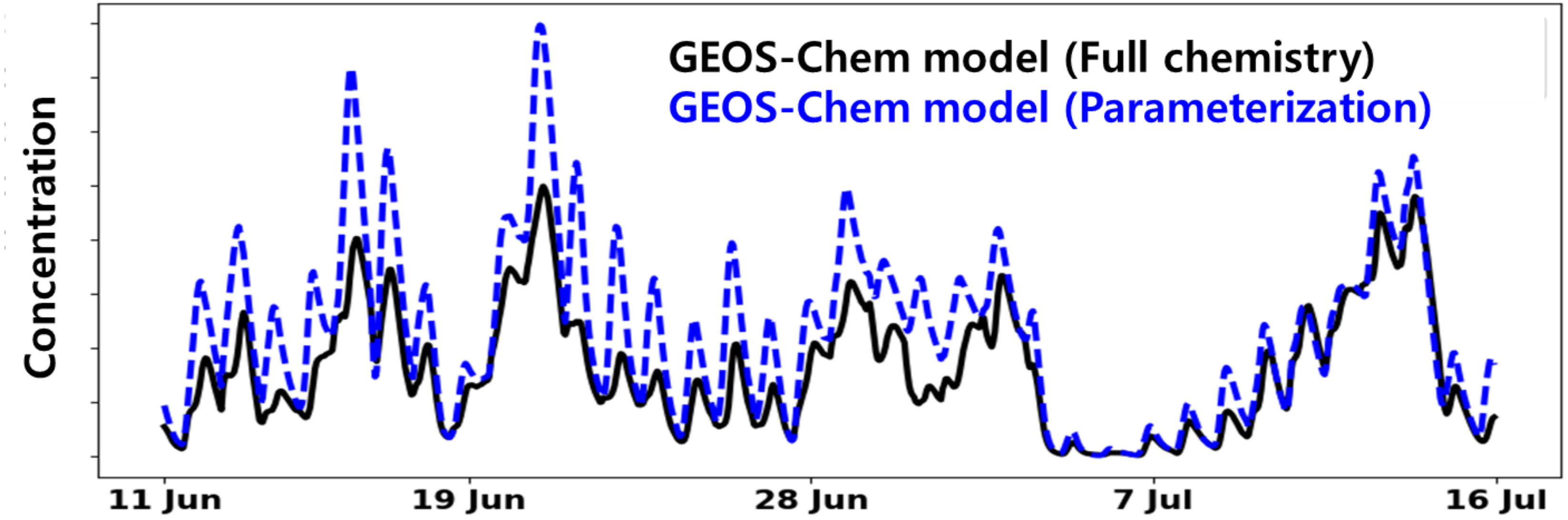
(d) / (c)

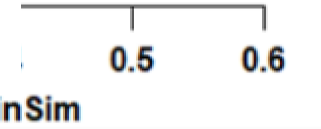
$\text{IEPOX-SOA}_{\text{PAR}} = Y_{\text{IEPOX-SOA}} \times E_{\text{Isoprene}}$

$$Y_{\text{IEPOX-SOA}} = f(OH, O_3, NO_3, HO_2, NO, CH_3O_2, CH_3CO_3, pH, \text{Aerosol surface area}, \text{organic coating})$$

#	Species	Values
1	NO [ppt]	1, 5, 10, 50, 100, 500, 1000, 5000, 10^4, $5x10^4$, 10^5, $5x10^5$, 10^6
2	OH [molecules cm^{-3}]	10^4, $5x10^4$, 10^5, $5x10^5$, 10^6, $2x10^6$, $3x10^6$, $4x10^6$, $5x10^6$
3	HO_2 [ppt]	1, 2, 5, 10, 20, 50, 100
4	pH [unitless]	
5	Aeros	
6	O_3 [p	
7	NO_3 [	
8	CH_3C	
9	CH_3C	
10	Aeros	
11	Orga	
12	Temp	
13	Planetary boundary layer height [m]	100, 200, 500, 1000, 1500, 2000, 2500, 3000, 3500, 4000
14	Photolysis rate of ISOPOOH [s^{-1}]	10^{-7}, $5x10^{-7}$, 10^{-6}, $5x10^{-6}$, 10^{-5}, $2x10^{-5}$





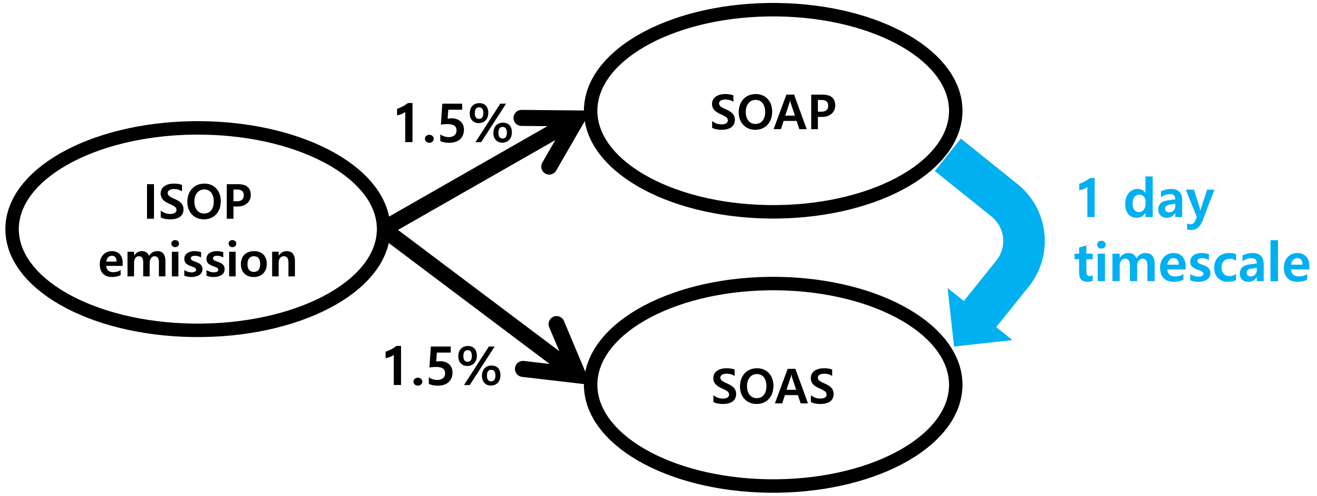


Global models tend to simplify secondary organic aerosol formation mechanism in order to reduce computational cost

- For example,

The default SOA scheme in the next GEOS-Chem (v11-02) is simplified SOA scheme.
→ For isoprene SOA, constant 3% yield is applied. (1.5% mass yield SOAP, 1.5% mass yield SOAS)

✓ SOAP : gas-phase precursor of SOA
✓ SOAS : SOA in particle phase


ISOP emission
1.5%
SOAP
1.5%
SOAS
1 day timescale

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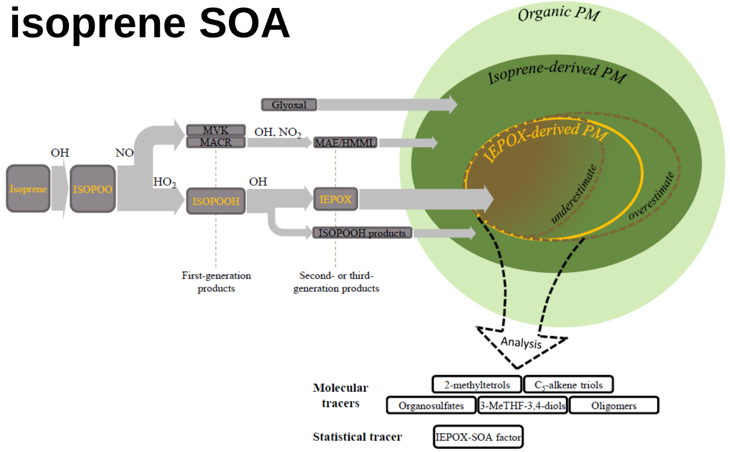
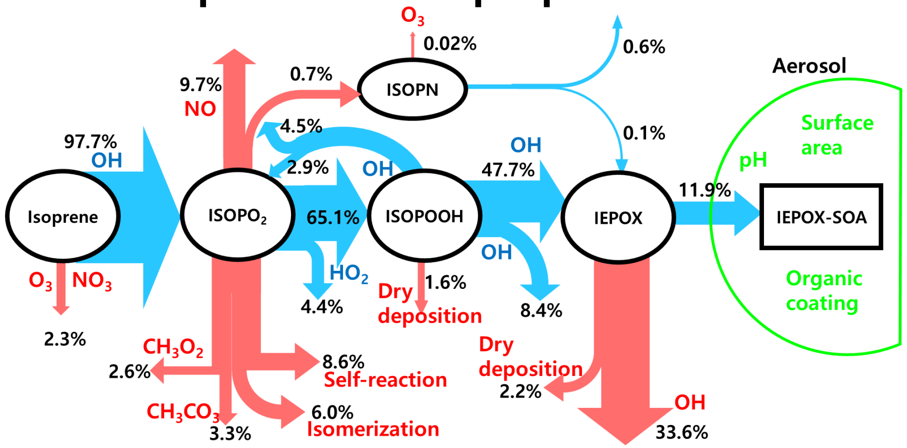
Summary

IEPOX-SOA is thought to contribute the dominant fraction of total isoprene SOA

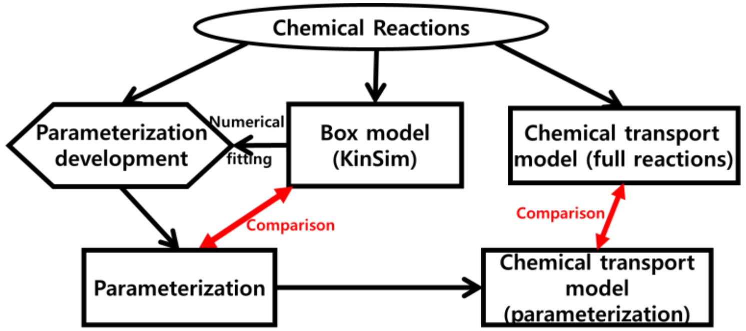


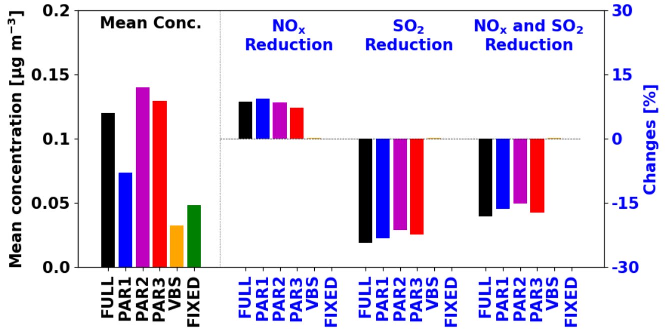
IEPOX-SOA formation depends on oxidants, aerosol pH and other properties



But current SOA parameterizations (e.g. VBS) used in chemistry models consider only simple chemistry such as VOC + OH

New IEPOX-SOA parameterizations retaining key physico-chemical dependencies were developed, and they captured the response to changes on emissions





With a new MAM-MOSAIC framework and updated isoprene and monoterpene chemistry, CESM2.1 can be a best tool for investigating future SOA changes