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


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
IEPOX-SOA: main source of isoprene-derived aerosol

de Sa et al. (2017)
IEPOX-SOA fractions of OA: up to 36%
Schematic diagram of IEPOX-SOA chemistry

For SOAS condition
Blue: IEPOX-SOA making pathway
Red: other pathways

Isoprene → ISOPO$_2$ → ISOPN → IEPOX

Dry deposition: 2.3% NO, 9.7% NO$_3$, 0.7% ISOPN, 4.5% OH

Self-reaction: 2.6% CH$_3$O$_2$, 3.3% CH$_3$CO$_3$

Isomerization: 8.6% OH, 6.0% ISOPN

Dry deposition: 1.6% OH, 8.4% ISOPN

For SOAS condition
Blue: IEPOX-SOA making pathway
Red: other pathways

IEPOX → Aerosol

pH, Surface area, Organic coating
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.
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)

Parameterization

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

Chemical Reactions

Parameterization development

Box model (KinSim)

Chemical transport model (full reactions)

Chemical transport model (parameterization)

Numerical fitting

Comparison

Parameterization
Objective: Develop a parameterization of IEPOX-SOA without an additional heavy computational cost.
<table>
<thead>
<tr>
<th>#</th>
<th>Reactions</th>
<th>Reaction rate</th>
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<tr>
<td>1</td>
<td>ISOP Reactions: Geoscientific Model Development</td>
<td>1.00E+10 exp(350/T)</td>
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<td>5</td>
<td>ISOP Reactions: © Author(s) 2019. This work is distributed under the Creative Commons Attribution 4.0 License.</td>
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<td>12</td>
<td>ISOP Reactions: 4Laboratoire d’Aérologie, Université de Toulouse, CNRS, UPS, Toulouse, France</td>
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<td>13</td>
<td>ISOP Reactions: 5Department of Physics and Astronomy, University of Leicester, Leicester, UK</td>
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<td>14</td>
<td>ISOP Reactions: Received: 12 Jan 2019 – Accepted for review: 04 Feb 2019 – Discussion started: 05 Feb 2019</td>
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<td>15</td>
<td>ISOP Reactions: 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</td>
<td>8.0E+18</td>
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<tr>
<td>16</td>
<td>ISOP Reactions: IEPOX dry deposition</td>
<td>2.5 cm s^-1 / [PBL depth]</td>
</tr>
<tr>
<td>17</td>
<td>ISOP Reactions: IEPOX dry deposition</td>
<td>2.5 cm s^-1 / [PBL depth]</td>
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<tr>
<td>18</td>
<td>ISOP Reactions: IEPOX dry deposition</td>
<td>2.5 cm s^-1 / [PBL depth]</td>
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### Reactions

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<th>Reaction rate</th>
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<tbody>
<tr>
<td>1</td>
<td>ISOP + OH -&gt; 1.0 ISOPO₂</td>
<td>3.1E-11 ( \exp(350/T) )</td>
</tr>
<tr>
<td>2</td>
<td>ISOP + O₃ -&gt; other products</td>
<td>1.00E-14 ( \exp(-1970/T) )</td>
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<tr>
<td>3</td>
<td>ISOP + NO₃ -&gt; other products</td>
<td>3.3E-12 ( \exp(-450/T) )</td>
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<td>4</td>
<td>ISOPO₂ + HO₂ -&gt; 0.937 ISOPOOH</td>
<td>2.12E-13 ( \exp(1300/T) )</td>
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<td>ISOPO₂ + NO -&gt; 0.023 ISOPND + 0.047ISOPNB</td>
<td>2.7E-12 ( \exp(350/T) )</td>
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<td>6</td>
<td>ISOPO₂ + CH₃O₂ -&gt; other products</td>
<td>2.00E-12</td>
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<td>7</td>
<td>ISOPO₂ + ISOPO₂ -&gt; other products</td>
<td>2.30E-12</td>
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<tr>
<td>8</td>
<td>ISOPO₂ + CH₃CO₃ -&gt; other products</td>
<td>1.40E-11</td>
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<td>9</td>
<td>ISOPO₂ -&gt; other products</td>
<td>4.07E+08 ( \exp(-7694/T) )</td>
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<tr>
<td>10</td>
<td>ISOPOOH + OH -&gt; 0.387 ISOPO₂</td>
<td>4.75E-12 ( \exp(200/T) )</td>
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<tr>
<td>11</td>
<td>ISOPOOH + OH -&gt; 0.850 IEPOX</td>
<td>1.9E-11 ( \exp(390/T) )</td>
</tr>
</tbody>
</table>

\[
f_{\text{Isoprene} \rightarrow \text{ISOPO}_2} = \frac{k_1 \times [\text{OH}]}{k_1 \times [\text{OH}] + k_2 \times [\text{O}_3] + k_3 \times [\text{NO}_3]}
\]

16 | ISOPND + O₃ -> other products                                             | 3E-10                         |
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]      |
$\text{IEPOX-SOA}_{\text{PAR}} = Y_{\text{IEPOX-SOA}} \times E_{\text{Isoprene}}$

$Y_{\text{IEPOX-SOA}} = f(\text{OH, O}_3, \text{NO}_3, \text{HO}_2, \text{NO}, \text{CH}_3\text{O}_2, \text{CH}_3\text{CO}_3, \text{pH}, \text{Aerosol surface area, organic coating})$

<table>
<thead>
<tr>
<th>#</th>
<th>Species</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO [ppt]</td>
<td>1, 5, 10, 50, 100, 500, 1000, 5000, 10^4, 5×10^4, 10^5, 5×10^5, 10^6</td>
</tr>
<tr>
<td>2</td>
<td>OH [molecules cm^-3]</td>
<td>10^4, 5×10^4, 10^5, 5×10^5, 10^6, 2×10^6, 3×10^6, 4×10^6, 5×10^6</td>
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<tr>
<td>3</td>
<td>HO_2 [ppt]</td>
<td>1, 2, 5, 10, 20, 50, 100</td>
</tr>
<tr>
<td>4</td>
<td>pH [unitless]</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Aerosol</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>O_3 [ppt]</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>NO_3 [ppt]</td>
<td></td>
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<tr>
<td>8</td>
<td>CH_3 [ppt]</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>CH_3CO_3 [ppt]</td>
<td>0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10</td>
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<tr>
<td>10</td>
<td>Aerosol radius [nm]</td>
<td>50, 100, 150, 200, 250, 300, 500, 1000</td>
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<tr>
<td>11</td>
<td>Organic coating fraction [unitless]</td>
<td>0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0</td>
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<tr>
<td>12</td>
<td>Temperature [K]</td>
<td>288, 293, 298, 303, 308, 313, 318</td>
</tr>
<tr>
<td>13</td>
<td>Planetary boundary layer height [m]</td>
<td>100, 200, 500, 1000, 1500, 2000, 2500, 3000, 3500, 4000</td>
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<tr>
<td>14</td>
<td>Photolysis rate of ISOPOOH [s^-1]</td>
<td>10^-7, 5×10^-7, 10^-6, 5×10^-6, 10^-5, 2×10^-5</td>
</tr>
</tbody>
</table>
Schematic diagram of IEPOX-SOA chemistry

For SOAS condition
Blue: IEPOX-SOA making pathway
Red: other pathways

Isoprene → ISOPN → IEPOX

O₃  NO₃  OH

Isoprene → ISOPO₂ → ISOPOOH → IEPOX

Isomerization  8.6%  6.0%

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\( Y_{\text{IEPOX-SOA}} = f(\text{OH}, O_3, NO_3, HO_2, NO, CH_3 O_2, CH_3 CO_3, pH, \text{Aerosol surface area, organic coating}) \)

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</tr>
<tr>
<td>2</td>
<td>OH [molecules cm(^{-3})]</td>
<td>10^4, 5x10^4, 10^5, 5x10^5, 10^6, 2x10^5, 3x10^5, 4x10^5, 5x10^6</td>
</tr>
<tr>
<td>3</td>
<td>HO(_2) [ppt]</td>
<td>1, 2, 5, 10, 20, 50, 100</td>
</tr>
<tr>
<td>4</td>
<td>p(_H)</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Aerosol radius</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>CH(_3)O(_2)</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>CH(_3)CO(_3)</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Aerosol radius</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Organic coating</td>
<td></td>
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<td>Temperature [K]</td>
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<td>12</td>
<td>Photolysis rate of ISOPOOH [s(^{-1})]</td>
<td>10^{-7}, 5x10^{-7}, 10^{-6}, 5x10^{-6}, 10^{-5}, 2x10^{-5}</td>
</tr>
</tbody>
</table>
ISOP emission → IEPOX-SOA

Δt = IEPOX-SOA(t) + \{1 - \exp\left(-\frac{\Delta t}{\tau}\right)\} \times SOAP(t)

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

Chemical loss by OH
Dry deposition

upTake (\gamma)

\gamma_{IEPOX-SOA}

SOAP → IEPOX-SOA

\tau

IEPOX → IEPOX-SOA

Formation time scale by parameterization [x 10^3 s]

\[ y = 0.98826x + 612.21 \]

\[ R^2 = 0.98888 \]
\( \tau : \text{E-folding time in the first order kinetic equation} \)

\[
\text{IEPOX-SOA}(t+\Delta t) = \text{IEPOX-SOA}(t) + \{1 - \exp\left(-\frac{\Delta t}{\tau}\right)\} \times \text{SOAP}(t)
\]

\[
\tau = f(L_{\text{ISOP}}, L_{\text{ISOPOOH}}, L_{\text{IEPOX}}, L_{\text{ISOPN}}, \text{NO}, \text{HO}_2)
\]

- Chemical loss by OH
- Dry deposition
Objective: Develop a parameterization of IEPOX-SOA without an additional heavy computational cost.
Annual mean IEPOX-SOA surface maps and scatterplots for troposphere

(a) FULL

(b) PAR1/FULL

PAR1 vs. FULL

\[ Y = 0.7X - 0.01 \]
\[ R^2 = 0.9 \]

(c) VBS/FULL

VBS vs. FULL

\[ Y = 0.3X - 0.0 \]
\[ R^2 = 0.51 \]

(d) PAR2/FULL

PAR2 vs. FULL

\[ Y = 0.34X + 0.0 \]
\[ R^2 = 0.71 \]

(e) FIXED/FULL

FIXED vs. FULL

\[ Y = 1.33X - 0.01 \]
\[ R^2 = 0.88 \]

(f) PAR3/FULL

PAR3 vs. FULL

\[ Y = 1.13X - 0.01 \]
\[ R^2 = 0.94 \]

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
- 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

**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

<table>
<thead>
<tr>
<th>Unit: [s]</th>
<th>Chemistry</th>
<th>Transport</th>
<th>Dry deposition</th>
<th>Wet deposition</th>
<th>Total</th>
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<tr>
<td>FULL</td>
<td>559</td>
<td>172</td>
<td>30</td>
<td>380</td>
<td>1141</td>
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<tr>
<td>VBS</td>
<td>7</td>
<td>120</td>
<td>20</td>
<td>253</td>
<td>400</td>
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<td>PAR1</td>
<td>47</td>
<td>34</td>
<td>7</td>
<td>84</td>
<td>172</td>
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<tr>
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<td>13</td>
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<td>7</td>
<td>84</td>
<td>138</td>
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<td>PAR3</td>
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<td>52</td>
<td>7</td>
<td>127</td>
<td>234</td>
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<tr>
<td>FIXED</td>
<td>1</td>
<td>34</td>
<td>3</td>
<td>42</td>
<td>80</td>
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Moving from GEOS-Chem to CAM-chem for future simulations of SOA

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<tr>
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<th>GEOS-Chem</th>
<th>CAM-chem</th>
</tr>
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<tbody>
<tr>
<td>Aerosol scheme</td>
<td>Bulk aerosol scheme</td>
<td>Modal aerosol scheme (MAM4: 4 modes)</td>
</tr>
<tr>
<td>Species</td>
<td>BC, POA, SOA, Sulfate, Nitrate, Ammonium, Sea salt, Dust</td>
<td>BC, POA, SOA, Sulfate, Sea salt, Dust, Number + Nitrate, Ammonium (MOSAIC)</td>
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<tr>
<td>Thermodynamics</td>
<td>ISORROPIA II</td>
<td>MOSAIC</td>
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<tr>
<td>Mixing state</td>
<td>External</td>
<td>External(between modes) + Internal (within modes)</td>
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<tr>
<td>Condensation and coagulation</td>
<td>No</td>
<td>Yes</td>
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<td>Aging of BC and POA</td>
<td>Fixed e-folding time scale (1.15 days)</td>
<td>Directly calculated</td>
</tr>
<tr>
<td>Time required for 1 year simulation</td>
<td>~ 5 days</td>
<td>~12 hours</td>
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Aerosol pH fields from CESM2.1 (MOSAIC)

Aitken mode

Accumulation mode

Coarse mode

Liu et al. (2016) + Ca$^{2+}$, Cl$^-$, NH$_4^+$, NO$_3^-$, CO$_3^{2-}$ (MOSAIC)
Evaluating SOA under Future Climate

Historical simulation (BCHIST) 2010 CMIP6-SSP5-8.5 Scenario Interactive atmosphere, land, ocean, and ice 2050

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

18
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.
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.

Thank you!
Back-up slides
Factors affecting isoprene emissions

- light, temperature, leaf age, leaf area index, and CO₂
Gamma values change (2050/2010) for biogenic emissions

\[ \gamma = C_{CE} \cdot \text{LAI} \cdot \gamma_p \cdot \gamma_T \cdot \gamma_A \cdot \gamma_SM \cdot \gamma_C \]
Future changes of IEPOX-SOA precursors and oxidants

Isoprene change

ISOPOOH change

IEPOX change

OH change

HO₂ change

NO change

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

(a) IsoPPOOH + OH
(k(T)x[OH])

(b) ISOPO2 + NO
(k(T)x[NO])

IEPOX change

Future changes of chemical pathways affecting IEPOX-SOA (2050/2010)
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 $\gamma = 1$ 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. $\gamma_p$: gamma for emission response to light (applied separately for the sunlit and shaded leaves)

   \[ \gamma_p = (1 - LDF) + LDF \cdot \gamma_{p \_LDF} \]

   $LDF$: light dependent fraction (1 for isoprene)

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

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

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

   $P_s$: 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. $\gamma_T$: gamma for emission response to temperature

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

   \[ \gamma_{T \_LDF} = \frac{E_{opt} \cdot \exp(0.05 \cdot (T_{24} - T_s))}{C_{eo} \cdot \exp(0.05 \cdot (T_{240} - T_s))} \cdot \frac{1 - \exp(C_{T_2} \cdot x)}{C_{T_2} \cdot \exp(CT_1 \cdot x)} \]

   \[ E_{opt} = C_{eo} \cdot \exp(0.05 \cdot (T_{24} - T_s)) \cdot \exp(0.05 \cdot (T_{240} - T_s)) \]

   \[ T_{opt} = 313 + (0.6 \cdot (T_{240} - T_s)) \]

   $LIF$: light independent fraction

   $T_s$: standard conditions for leaf temperature (297 K)

   $C_{T_1}$, $C_{T_2}$, $C_{eo}$, $\beta$: Empirically determined coefficients

   - $C_{T_1} = 95$, $C_{T_2} = 230$, $C_{eo} = 2$, $\beta = 0.13$ 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) \( \gamma_A \): 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) \( \gamma_{SM} \): gamma for emission response to soil moisture (only for isoprene)

\[ \gamma_{SM} = \begin{cases} 1 & \theta > \theta_1 \\ (\theta - \theta_w) / \Delta \theta_1 & \theta_w < \theta < \theta_1 \\ 0 & \theta < \theta_w \end{cases} \]

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

\( \theta_w \): 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)

\( \theta_1, \theta_w + \Delta \theta_1 \)

Currently assumed to be 1 in CESM model

(6) \( \gamma_C \): gamma for emission response to CO\(_2\) inhibition (only for isoprene)

\[ \gamma_C = I_{S_{max}} \cdot \frac{(C_i)^h}{(C^*)^h + (C_i)^h} \]

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

\( C^*, h, I_{S_{max}} \): Empirically determined parameters (Heald et al., 2009)
Budget analysis
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)

\[ \text{Surface 2-D map of pHs in GEOS-Chem} \]

\[ \text{(a) Base case pH} \]

\[ \text{(b) pH w/o sea salt} \]

\[ \text{(b) – (a)} \]

\[ \text{(c) IEPOX-SOA} \]

\[ \text{(d) IEPOX-SOA} \]

\[ \text{(d) / (c)} \]
\[ \text{IEPOX-SOA}_{\text{PAR}} = Y_{\text{IEPOX-SOA}} \times E_{\text{Isoprene}} \]

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

<table>
<thead>
<tr>
<th>#</th>
<th>Species</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NO [ppt]</td>
<td>1, 5, 10, 50, 100, 500, 1000, 5000, 10^4, 5x10^4, 10^5, 5x10^5, 10^6</td>
</tr>
<tr>
<td>2</td>
<td>OH [molecules cm(^{-3})]</td>
<td>10^4, 5x10^4, 10^5, 5x10^5, 10^6, 2x10^5, 3x10^5, 4x10^5, 5x10^6</td>
</tr>
<tr>
<td>3</td>
<td>HO_2 [ppt]</td>
<td>1, 2, 5, 10, 20, 50, 100</td>
</tr>
</tbody>
</table>

Aerosol:

6 O_3 [p]  
7 NO_3 [ ]
8 CH_3C
9 CH_3C
10 Aeros
11 Organ
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
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.