GEOS-Chem v11-02 Secondary Organic Aerosol (SOA) Mechanism Options

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There are 3 SOA scheme options available in v11-02:
1) Simple SOA
2) Complex SOA
3) Combined (1) and (2) (used in GEOS-Chem benchmarks to evaluate both schemes)

Below is a description of the simple and complex SOA schemes, how these are implemented in GEOS-Chem, guidance on where to make changes in the code or input files to switch from one mechanism to the next, and references for further information.

The irreversible isoprene SOA and organonitrate formation pathways in the complex scheme (detailed below) are used in all GEOS-Chem simulations, but in tropchem and standard chem the complex SOA scheme does not contribute to $PM_{2.5}$ or AOD. In complex SOA chem the simple SOA scheme does not contribute $PM_{2.5}$ or AOD. The decision for this is discussed on this wiki page.

All SOA compounds are transported and undergo wet and dry deposition in the model, unless stated otherwise.

See this GEOS-Chem wiki page for a descriptive list of chemical species in the model:
http://wiki.seas.harvard.edu/geos-chem/index.php/Species_in_GEOS-Chem.

Simple SOA Scheme

Quick Description: Irreversible formation of SOA using fixed yields.

Relevant Simulation(s): Used to estimate SOA in the Standard and Tropchem simulations. Replaced by the Complex SOA scheme in the SOA_SVPOA simulation.

Advantages:
- Rapid simulation (only 2 tracers and no detailed chemistry).
- Direct relationship between emissions and SOA yields.
- Easy to add or remove SOA sources in HEMCO.
- Compatible with TOMAS microphysics model.

Disadvantages:
- No dependence of yields on other factors (aqueous aerosol pH and water, pre-existing aerosol abundance, NO_x concentrations etc.).
- Not possible to track SOA from different sources (requires additional sensitivity simulations).
- Gas and aerosol phase chemistry aren't coupled (i.e. no loss of carbon from gas to aerosol phase).

Detailed Description:

Involves 2 tracers: **SOAP** (lumped SOA precursor) and **SOAS** (lumped simple SOA). SOAS is emitted directly and SOAS is formed in the atmosphere from SOAP with a default 1st-order lifetime of 1 day to form SOAS with 100% yield.

Mass yields of SOAP and SOAS are estimated by scaling monoterpene and isoprene emissions and CO emissions from biofuel (CO_{bf}), biomass burning (CO_{bb}), and fossil fuel use (CO_{ff}) and SOA formation from SOAP is assumed to take a day:

Isoprene:

$ISOP \rightarrow 1.5\%\ SOAS$

$ISOP \rightarrow 1.5\%\ SOAP \xrightarrow{\tau=1\ day} SOAS$

Total SOA mass yield from isoprene is 3% ([Kim et al., 2015](#))

Monoterpenes:

$MONX \rightarrow 5\ mass\ \%\ SOAS$

$MONX \rightarrow 5\ mass\ \%\ SOAP \xrightarrow{\tau=1\ day} SOAS$

Total SOA mass yield from monoterpene is 10% (as used historically in many SOA simulations, see [Chin et al. (2002)](#); note that this is double that from [Kim et al., (2015)](#)).

Biofuel, biomass burning, and fossil fuel:

$CO_{bf} \rightarrow 0.013\ g\ SOAP \xrightarrow{\tau=1\ day} SOAS$ ([Kim et al., 2015](#); [Cubison et al., 2011](#); [Shrivastava et al., 2017](#))

$CO_{bb} \rightarrow 0.013\ g\ SOAP \xrightarrow{\tau=1\ day} SOAS$ ([Kim et al., 2015](#); [Cubison et al., 2011](#); [Shrivastava et al., 2017](#))

$CO_{ff} \rightarrow 0.069\ g\ SOAP \xrightarrow{\tau=1\ day} SOAS$ ([Kim et al., 2015](#); [Hayes et al., 2015](#); [Hodzic and Jimenez, 2011](#))

Complex SOA Scheme

Quick Description: This scheme combines the volatility-based scheme (VBS) of [Pye et al. (2010)](#) for all SOA components with the aqueous-phase irreversible reactive uptake schemes of [Marais et al. (2016)](#) for isoprene SOA and [Fisher et al. (2016)](#) for organonitrate SOA.

Relevant Simulation(s): Used in the complex SOA and complex SOA_SVPOA simulations. Turned off in the standard and tropchem simulations.

Advantages:
- Track individual SOA components.
- Variable yields that depend on environmental factors (NO_x concentrations, pre-existing aerosol abundance, aqueous aerosol pH and water).
- Explicit mechanism that can be updated with new field and laboratory measurements.
- Gas and aerosol phase chemistry are coupled.

Disadvantages:
- More expensive (run time and resources) than simple scheme.
- Relationship between emissions and SOA confounded by other factors.
- Some (currently unquantified) loss of carbon through organonitrate formation.
- Risk of double-counting (see notes below)

Detailed Description:

Involves many tracers listed below. Species used are named below. See this GEOS-Chem wiki page for a detailed description of these tracers.

This scheme is turned off by default in the standard and tropchem run directories and turned on by default in benchmark, complex SOA, and complex SOA_SVPOA run directories. The difference between these two is inclusion of SOA semivolatile POA in the complex SOA_SVPOA simulation.

The volatility-based approach depends on abundance of NO_x and volatility of pre-existing organic aerosol (C*). The aqueous phase reactive irreversible reactive uptake scheme for isoprene uses aerosol-phase reaction rates and solubilities (effective Henry's Law constant) to estimate uptake. Aqueous-phase isoprene SOA formation depends on sulfate aerosol as sulfate impacts aqueous aerosol acidity and water mass concentrations. Organonitrate formation in the model depends on pre-existing aerosol abundance.
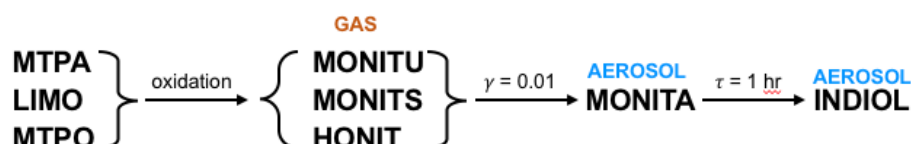
To activate the complex scheme in GEOS-Chem set the "Online COMPLEX SOA" option in the AEROSOL MENU in input.geos to "T" for true.

Monoterpenes:
Volatility-based scheme (Pye et al., 2010):
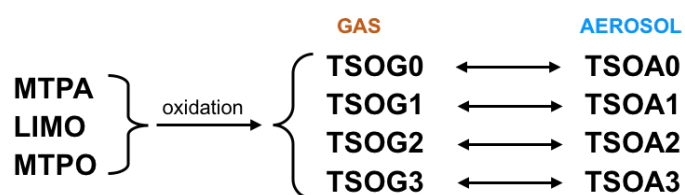
Irreversible uptake of monoterpene organonitrates to aerosols (Fisher et al., 2016):

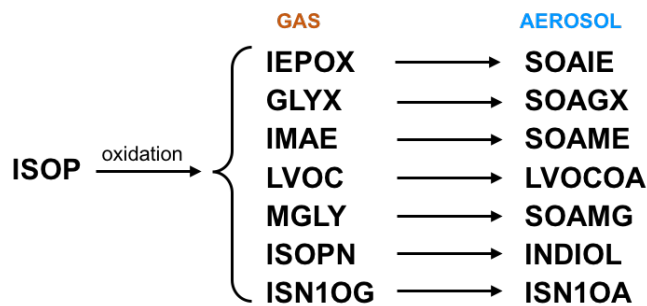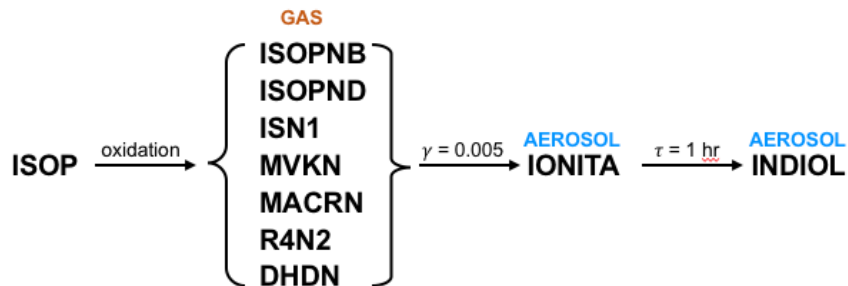**Isoprene:**
Volatility-based scheme (Pye et al., 2010):

Irreversible uptake to aqueous aerosols at RH > 35% (Marais et al., 2016):
Uptake coefficients are estimated to determine probability of SOA formation for each precursor. See Marais et al. (2016) for detailed description of calculation of uptake coefficients.

GAS | AEROSOL

ISOP —oxidation→ {
IEPOX ——→ SOAIE
GLYX ——→ SOAGX
IMAE ——→ SOAME
LVOC ——→ LVOCOA
MGLY ——→ SOAMG
ISOPN ——→ INDIOL
ISN1OG ——→ ISN1OA
}

Irreversible uptake of isoprene organonitrates to all aerosol types (Fisher et al., 2016):

GAS

ISOP —oxidation→ {
ISOPNB
ISOPND
ISN1
MVKN
MACRN
R4N2
DHDN
} —$\gamma = 0.005$→ **AEROSOL** IONITA —$\tau = 1\ hr$→ **AEROSOL** INDIOL
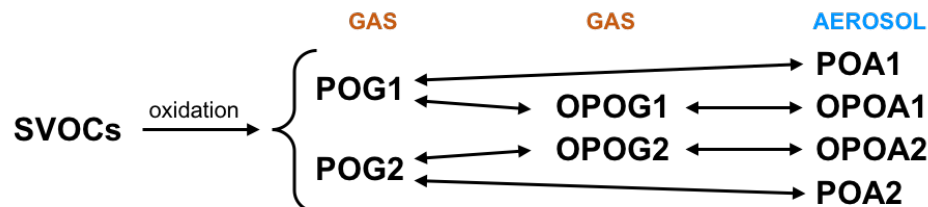
Anthropogenic, biofuel, and biomass burning:
Includes aromatics and semivolatile POA (SVPOA) formed by reversible partitioning (Pye et al., 2010). The SVPOA can be (de)activated using a switch in input.geos (see notes below for details).

Aromatics:
Volatility-based scheme (Pye et al., 2010):

GAS | AEROSOL

BENZ
TOLU
XYLE
IVOC
} —oxidation→ {
ASOGN ——→ ASOA0
ASOG1 ←——→ ASOA1
ASOG2 ←——→ ASOA2
ASOG3 ←——→ ASOA3
}

SVPOA:

GAS | GAS | AEROSOL

SVOCs —oxidation→ {
POG1
POG2
}
POA1
OPOG1 ←→ OPOA1
OPOG2 ←→ OPOA2
POA2

NOTES:
- **INDIOL** is not transported and does not contribute to aerosol mass (including PM$_{2.5}$) or AOD calculations in the model, as the hydrolysis of organonitrates in the aerosol phase is uncertain (Fisher et al., 2016). **IONITA** and **MONITA** do not include any stable forms and are assumed to fully hydrolyse with a lifetime of 1 hour. More research is needed to constrain this pathway for the dominant organonitrate compounds.

- There is the risk of double-counting using this approach, as there is likely overlap between the volatility-based and irreversible schemes (see Marais et al., 2016 for evaluation of the irreversible scheme against observations).

  To **turn off the isoprene volatility-based scheme** in the model go into carbon_mod.F in the ./GeosCore/ directory and set ALPHA values for isoprene SOA to zero:

  This portion of the code in carbon_mod.F will change from this:

```
!----------------------------
! ISOP
!----------------------------
NOX = 1 ! low NOx/all OH rxn
ALPHA(NOX,1,PARENTISOP) = 0.0306e+0_fp
ALPHA(NOX,2,PARENTISOP) = 0.0000e+0_fp
ALPHA(NOX,3,PARENTISOP) = 0.0945e+0_fp
NOX = 2 ! NO3 rxn
ALPHA(NOX,1,PARENTISOP) = 0.0000e+0_fp
ALPHA(NOX,2,PARENTISOP) = 0.2171e+0_fp
ALPHA(NOX,3,PARENTISOP) = 0.0919e+0_fp
```

  To this:

```
!----------------------------
! ISOP
!----------------------------
NOX = 1 ! low NOx/all OH rxn
ALPHA(NOX,1,PARENTISOP) = 0.0+0_fp
ALPHA(NOX,2,PARENTISOP) = 0.0+0_fp
ALPHA(NOX,3,PARENTISOP) = 0.0+0_fp
NOX = 2 ! NO3 rxn
ALPHA(NOX,1,PARENTISOP) = 0.0e+0_fp
ALPHA(NOX,2,PARENTISOP) = 0.0e+0_fp
ALPHA(NOX,3,PARENTISOP) = 0.0e+0_fp
```

- To **turn off the SVPOA pathway only** in the model set the "=> Semivolatile POA?" option in the AEROSOL MENU in input.geos to "F" for false.

- The only way to only use the VBS SOA scheme or switch between Fisher et al. (2016) and Marais et al. (2016) representation of organonitrates is to edit the KPP *.eqn files and rebuild the mechanism.

- There is inconsistency between Marais et al. (2016) and Fisher et al. (2016) in the treatment of isoprene nitrates. Currently, the code follows Fisher et al. (2016).