Supporting information of

Comparing Secondary Organic Aerosols Schemes Implemented in Current Chemical Transport Models and the Policy Implications of Uncertainties

Ling Huang[1], Greg Yarwood[2,*], Katie Tuite[2], Pradeepa Vennam[2], Benjie Chen[1], Zi'ang Wu[1], Li Li[1]

[1]School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China
[2]Ramboll, Novato, California, 94945, USA
Correspondence to: Greg Yarwood (gyarwood@ramboll.com)

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List of Abbreviations

ALK4 Alkanes $5\times10^3 < k_{OH} < 1\times10^4$ (lumped class)

ALK5 Alkanes $1\times10^4 < k_{OH}$ (lumped class)

ARO1 Aromatics $k_{OH} < 2\times10^4$ (lumped class)

ARO2 Aromatics $k_{OH} > 2\times10^4$ (lumped class)

ASOA SOA formed from AVOC

AVOC Anthropogenic VOC

BENZ Benzene (explicit)

BSOA SOA formed from BVOC

BVOC Biogenic VOC

CG Condensable gases

CTM Chemical transport model

HUMULE Humulene (lumped sesquiterpene class)

ISOP Isoprene (explicit)

IVOC Intermediate volatility organic compounds

IV-SOA SOA formed from IVOC

LIMO Limonene (lumped class)

OA Organic aerosol

OLE1 Alkenes $k_{OH} < 7\times10^4$ (lumped class)

OLE2 Alkenes $k_{OH} > 7\times10^3$ (lumped class)

POA Primary organic aerosol

$PM_{2.5}$ Particulate matter with a diameter of 2.5 micrometers or less

SESQ Sesquiterpenes (lumped class)

SOA Secondary organic aerosol

SVOC Semivolatile organic compounds

SV-SOA SOA formed from SVOC

TERP Terpenes (lumped class)

TOL Toluene (lumped class)

VOC Volatile organic compounds

VBS Volatility basis set

XYL Xylenes (lumped class)

Table S1 Summary of SOA schemes implemented in CTMs reviewed in this study

Model (version)	SOA scheme	SOA precursors	Aging treatment	POA treatment	SOA photolysis	References
CAMx v7.20	SOAP2	BENZ/TOL/XYL ISOP/TERP/SESQ/IVOC	No aging effect	Non-volatile, no further reactions	$J_{SOA} = 0.1\% \times J_{NO2}$	Ramboll (2022) Koo et al. (2014)
	1.5D VBS		Gas-phase OH-oxidation aging for SOA formation from AVOC and IVOC	Semivolatile; gas-phase undergoes further oxidation		
CMAQ v5.4	AERO7	BENZ/TOL/XYL ISOP/TERP/SESQ/IVOC	Particle-phase of semivolatile products forms oligomers; products generated by TERP + NO_3 undergo hydrolysis to form low-volatile products.	Semivolatile; gas-phase undergoes further oxidation	NA	https://github.com/USEPA/CMAQ
	CRACMM	BENZ/TOL/XYM/XYE APIN/LIM/SESQ IEPOX/IVOC	OH oxidation aging resulting in functionalization and fragmentation based on modified 2-D VBS framework	Semivolatile; gas-phase undergoes further oxidation	NA	Pye et al. (2023)
GEOS-Chem v14.3.0	Simple	ISOP/TERP/SESQ Anthropogenic precursor scaled based on CO emissions	No aging effect	Non-volatile; 50% of POA is directly emitted; 50% is formed with a lifetime of 1.15 days, without dependence on local oxidation levels.	Described in literature but not found in source code	Pai et al. (2020), Pye et al. (2010) https://geos-chem.readthedocs.io/en/stable/
	Complex	BENZ/TOL/XYL/IVOC ISOP/MTPO/LIMO/SESQ		Semivolatile; gas-phase undergoes further oxidation with OH to form oxidized POA with lower volatility.		
CHIMERE v2023	VBS	ARO1/ARO2/ALK4/ALK5 /OLE1/OLE2/IVOC ISOP/TERP/HUMULE	OH oxidation aging with both functionalization and fragmentation; the aerosol phase undergoes oligomerization to form non-volatile products.	Semivolatile; gas-phase undergoes further oxidation.	Not available	Zhang et al. (2013); Shrivastava et al. (2015); Couvidat et al. (2018); CHIMERE (2023)

Model (version)	SOA scheme	SOA precursors	Aging treatment	POA treatment	SOA photolysis	References
WRF-Chem v4.4	MOSAIC	ALK4/ALK5/ARO1/ARO2 OLE1/OLE2/IVOC ISOP/TERP/SESQ	No aging for AVOC and BVOC; gas-phase OH-oxidation of IVOC with 15% of mass added for each generation; no fragmentation.	Semivolatile; gas-phase undergoes further oxidation	Described in literature (Zawadowicz et al. 2020) but turned off in source code	Shrivastava et al. 2011

Table S2 Parameters for SOA formation in CAMx SOAP2 modified two-product scheme (adapted from Table 5-5 of Ramboll, 2022)

SOA mass-based yields (g/g) from anthropogenic precursors under low (top)/high (bottom) NOx conditions			
C* [μg/m^3] @ 300K	0	0.31	14
CG/SOA MW [g/mol]	220	150	160
ΔH_{vap} [kJ/mol]	-	147	116
Benzene	0	0.167	0.487
	0	0.391	0.248
Toluene	0.262	0.345	0.663
	0.044	0.293	0.304
Xylene	0.294	0.306	0.291
	0.025	0.049	0.084
IVOC	0.277	0.275	0
	0.129	0.225	0.012
SOA mass-based yields (g/g) from biogenic precursors under low (top)/high (bottom) NOx			
C* [μg/m^3] @ 300K	0	0.45	26
CG/SOA MW [g/mol]	220	180	180
ΔH_{vap} [kJ/mol]	-	123	118
Isoprene	0.011	0.029	0.156
	0	0.023	0.076
Monoterpene	0.070	0.090	0.150
	0.070	0.045	0.075
Sesquiterpene	0.270	0.400	0.136
	0.175	0.328	0.092

Table S3 Parameters for SOA formation in CAMx 1.5-D VBS (values adopted from CAMx source code)

C* [μg/m^3] @ 298K	0	1	10	100	1000
CG/SOA MW [g/mol]	172	167	163	158	153
ΔH_{vap} [kJ/mol]	35	35	35	35	35
SOA molar yield (ppm/ppm) under high (top)/low (bottom) NOx					
Benzene	0	0.001	0.079	0.148	0.222
	0	0.035	0.108	0.185	0.268
Toluene	0	0.006	0.145	0.281	0.432
	0	0.006	0.145	0.437	0.281
Xylene	0	0.001	0.127	0.201	0.301
	0	0.048	0.195	0.252	0.364
Isoprene	0	0	0.009	0.006	0
	0	0.004	0.013	0.006	0
Monoterpenes	0	0.01	0.101	0.173	0.451
	0	0.087	0.077	0.309	0.54
Sesquiterpenes	0	0.092	0.188	0.968	0.679
	0	0.092	0.188	0.968	0.679
SOA molar yield (ppm/ppm) for IVOC					
IVOG	0.022	0.098	0.373	0.699	0
IVOD	0.081	0.135	0.800	0.604	0
IVOA	0.081	0.135	0.800	0.604	0
IVOB	0.081	0.135	0.800	0.604	0
SOA molar yield (ppm/ppm) for NO_3 oxidation					
Monoterpenes	0.314	0.029	0	0.862	0

Table S4 Parameters for SOA formation from aromatics under high- (top row) and low- (bottom row) NO*x* conditions in CMAQ AERO7

C* [μg/m^3] @ 298K	0.01	1	10	100
ΔHvap [kJ/mol]	18	18	18	18
CG/SOA MW [g/mol]	198	179	169	158
Precursor	SOA molar yields			
Benzene	0	0.034	0	0.392
	0.146	0	0	0
Toluene	0	0.016	0.051	0.047
	0.14	0	0	0
Xylene	0	0.015	0.023	0.06
	0.193	0	0	0

Table S5 Parameters for SOA formation from monoterpenes and *α*-pinene in CMAQ AERO7

C* [μg/m^3] @ 298K	0.01	0.1	1	10	100	1000	10000
ΔHvap [kJ/mol]	102	91	80	69	58	47	36
CG/SOA MW [g/mol]	300	200	186	184	170	168	/
SOA molar yields	0.04	0.032	0.032	0.103	0.143	0.285	0.16

Table S6 Parameters for SOA formation from isoprene, sesquiterpenes, and IVOC in CMAQ AERO7

Precursor	Isoprene		Sesquiterpenes	IVOC
C* [μg/m^3] @ 298K	0.617	116.01	24.984	1E-05
ΔHvap [kJ/mol]	40	40	40	40
CG/SOA MW [g/mol]	132	133	273	170
SOA mass yields	0.0288	0.232	1.537	1.176

Table S7 Aging effect for different SOA precursors in CMAQ AERO7

SOA precursors	Aging effect treatment
Aromatics	Under high-NO*x* conditions, oxidation products form non-volatile oligomers (AOLGA) at a rate of 9.49×10^{-6} s^{-1}; under low-NO*x* conditions, oxidation products do not form oligomers, i.e., no aging effect.
Isoprene/Sesquiterpene	Aging is NO*x*-independent; oxidation products form non-volatile oligomers (AOLGB) at a rate of 9.49×10^{-6} s^{-1}
Monoterpenes	There is no aging effect for OH and O_3 oxidation products; NO_3 oxidation products undergo hydrolysis to form a non-volatile product (AMTHYD) at a rate of 9.26×10^{-5} s^{-1}
IVOC	No aging effect

Table S8 SOA yield[1] parameterization of GOES-Chem Complex scheme (adopted from Pye et al. 2010)

C* [μg/m3] @ 298K	Mass yields (g/g) under high (top)/low (bottom) NO*x* conditions					ΔH_{vap} [kJ/mol]
	Non-volatile	0.1	1	10	100	
ISOP	0	0	0.0306	0.0000	0.0945	42
MTPA[2]	0	0.04	0.0095	0.0900	0.0150	42
	0	0.08	0.0190	0.1800	0.0300	
LIMO	0	0	0.4743	0.1174	1.4190	42
	0	0	0.3661	0.3214	0.8168	
SESQ	0	0	0.0005	1.1463	2.9807	42
	0	0	0.0000	0.5738	1.4893	
BENZ	0	0	0.0778	0.0000	0.7932	42
	0.37	0	0.0000	0.0000	0.0000	
TOL	0	0	0.0315	0.0944	0.0800	42
	0.30	0	0	0.0000	0.0000	
XYL	0	0	0.0250	0.0360	0.0899	42
	0.36	0	0	0.0000	0.0000	
IVOC[3]	0	0	0.0390	0.2960	0.2350	42
	0.73	0	0	0.0000	0.0000	

[1]SOA yield for OH and O_3 oxidation. SOA yields from NO_3 oxidation with isoprene and terpenes are not presented in this table.
[2] α-pinene and similar monoterpenes
[3] Use naphthalene as a proxy

Table S9 SOA yield parameterization in CHEMIERE VBS (Zhang et al., 2013; CHIMERE, 2023)

C* [μg/m^3] @ 300K	Mass yields under high (top)/low (bottom) NO*x* conditions (molar-based)[2]				ΔH_{vap} [kJ/mol]	CG/SOA MW [g/mol]
	1	10	100	1000		
ISOP	0.0003	0.0225	0.015	0	30	180
	0.009	0.03	0.015	0		
TERP[1]	0.012	0.1215	0.201	0.507	30	180
	0.1073	0.0918	0.3587	0.6075		
HUMULE	0.075	0.15	0.75	0.9	30	180
	0.075	0.15	0.75	0.9		
ARO1	0.003	0.165	0.3	0.435	30	150
	0.075	0.225	0.375	0.525		
ARO2	0.0015	0.195	0.3	0.435	30	150
	0.075	0.3	0.375	0.525		
ALK4	0	0.0375	0	0	30	120
	0	0.075	0	0		
ALK5	0	0.15	0	0	30	150
	0	0.3	0	0		
OLE1	0.0008	0.0045	0.0375	0.15	30	120
	0.0045	0.009	0.06	0.225		
OLE2	0.003	0.0225	0.0825	0.27	30	120
	0.0225	0.0435	0.129	0.375		

[1] Same mass yields are used for APINEN, BPINEN, OCIMEN, and LIMONE. Use TERP to represent all monoterpene species.
[2] Yields for OH and O_3 oxidation are the same for biogenic VOCs.

Table S10 SOA yield (g/g) parameterization of WRF-Chem MOSAIC (adopted from Shrivastava et al. 2011).

C* ($\mu g/m^3$) @ 298K	Mass yields (g/g) of each bin under high (top)/low (bottom) NO*x* conditions				MW [g/mol]
	1	10	100	1000	
ISOP	0.001	0.023	0.015	0	250
	0.009	0.03	0.15	0	
TERP	0.012	0.122	0.201	0.5	250
	0.107	0.092	0.359	0.6	
SESQ	0.075	0.15	0.75	0.9	250
	0.075	0.15	0.75	0.9	
ARO1	0.01	0.24	0.45	0.7	250
	0.01	0.24	0.7	0.7	
ARO2	0.01	0.24	0.45	0.7	250
	0.01	0.24	0.7	0.7	
ALK4	0	0.38	0	0	250
	0	0.075	0	0	
ALK5	0	0.15	0	0	250
	0	0.3	0	0	
OLE1	0.001	0.005	0.038	0.15	250
	0.005	0.009	0.06	0.225	
OLE2	0.003	0.026	0.083	0.27	250
	0.023	0.044	0.129	0.375	

Table S11 Ranking (from lowest to highest) initial SOA yield from different precursors by each scheme under high and low NO*x* conditions (ref. Table 1 for specific numbers)

Ranking	CAMx SOAP2	CAMx VBS	CMAQ AERO7	CMAQ CRAMM	GOES-Chem Simple	GEOS-Chem Complex	CHIMERE VBS	WRF-Chem MOSAIC
				High NOx conditions				
1	ISOP	ISOP	ISOP	XYL	ISOP	ISOP	IVOC	IVOC
2	XYL	TERP	XYL	TOL	TERP	XYL	ISOP	ISOP
3	TERP	BEZN	TOL	SESQ	SESQ	TOL	TERP	TERP
4	IVOC	XYL	BENZ	BENZ	BENZ / TOL / XYL	TERP	XYL	BENZ
5	TOL	TOL	TERP	TERP		BENZ	BENZ	TOL
6	BENZ	SESQ	SESQ			IVOC	TOL	XYL
7	SESQ	IVOC	IVOC			SESQ	SESQ	SESQ
				Low NOx conditions				
1	ISOP	ISOP	ISOP	TERP	ISOP	ISOP	IVOC	IVOC
2	TERP	TERP	TERP	TOL	TERP	TERP	ISOP	ISOP
3	BENZ	TOL	TOL	BENZ	SESQ	TOL	SESQ	TERP
4	IVOC	SESQ	XYL	XYL	BENZ / TOL / XYL	XYL	TERP	BENZ
5	SESQ	BENZ	BENZ	SESQ		BENZ	XYL	TOL
6	XYL	XYL	SESQ			SESQ	BENZ	XYL
7	TOL	IVOC	IVOC			IVOC	TOL	SESQ

Table S12 Initial and aged SOA yields (g/g) for CMAQ CRACMM IVOC types at 298 K and C_{OA} of 10 µg/m^3. The aging effect is for 24-hour exposure to OH concentration of 3×10^6 molecules/cm^3.

SOA yield	NO*x* condition	Alkane IVOC[1]	Emitted oxygenated IVOC	Aromatic IVOC[1]	Average[1]
Initial	High	0.296	0.121	0.019	0.209
	Low	0.245	0.121	0.035	0.183
Aged	High	0.077	0.121	0.015	0.099
	Low	0.039	0.121	0.190	0.080

[1] Weighted average of ~C12 (ROCP6ALK), ~C14 (ROCP5ALK), ~C18 (ROCP4ALK), and ~C21 (ROCP3ALK) IVOC yields. Weighting factors for each IVOC category are adopted from Table S1 of Zhang et al., (2013).

[2] Arithmetic average of less volatile (ROCP5ARO) and more volatile aromatic (ROCP6ARO) IVOC yields.

[3]Aromatic IVOC are excluded from averaging due to disagreement with Pye et al. (2023) values.

Table S13 Ratio of high/low NO*x* SOA yields for different precursors in each scheme. Numbers in red indicate higher yields under low NO*x* conditions (ref. Table 1 for specific numbers).

Precursor	CAMx		CMAQ		GEOS-Chem		CHIMERE	WRF-Chem
	SOAP2	VBS	AERO7	CRACMM	Simple	Complex	VBS	MOSAIC
BENZ	1.25	0.53	0.39	0.35	/	0.39	0.54	0.89
TOL	0.52	0.90	0.27	0.19	/	0.28	0.54	0.89
XYL	0.16	0.51	0.14	0.10	/	0.14	0.51	0.89
IVOC	0.65	1.00	1.00	1.14	/	0.28	1.00	1.00
ISOP	0.52	0.47	1.00	/	1.00	1.00	0.53	0.56
TERP	0.67	0.52	1.00	8.02	1.00	0.50	0.53	0.52
SESQ	0.74	1.00	1.00	0.12	1.00	2.00	1.00	1.00

Table S14 Ratio of aged SOA yields (**Error! Reference source not found.**2) to initial SOA yields (**Error! Reference source not found.**1) from different precursors simulated by different schemes. Shaded values indicate no aging processes implemented. Values in red indicate cases when aging decreases SOA yields.

Precursor	NO*x* condition	CAMx		CMAQ		GEOS-Chem		CHIMERE	WRF-Chem	Multi-model averages[2]
		SOAP2	VBS	AERO7	CRACMM[1]	Simple	Complex	VBS	MOSAIC	
BENZ	high	1.0	6.9	1.6	/	1.0	1.0	4.1	1.0	2.4
	low	1.0	4.9	1.0	/	1.0	1.0	3.1	1.0	1.9
TOL	high	1.0	6.9	1.5	/	1.0	1.0	4.1	1.0	2.4
	low	1.0	6.3	1.0	/	1.0	1.0	3.1	1.0	2.1
XYL	high	1.0	6.3	1.5	/	1.0	1.0	3.9	1.0	2.2
	low	1.0	4.4	1.0	/	1.0	1.0	2.9	1.0	1.8
IVOC	high	1.0	2.2	1.0	/	/	1.0	60	4448	645
	low	1.0	2.2	1.0	/	/	1.0	60	4448	645
ISOP	high	1.0	1.0	1.3	/	1.0	1.0	2.3	1.0	1.2
	low	1.0	1.0	1.3	/	1.0	1.0	1.8	1.0	1.2
TERP	high	1.0	1.0	1.0	/	1.0	1.0	4.1	1.0	1.4
	low	1.0	1.0	1.0	/	1.0	1.0	3.2	1.0	1.3
SESQ	high	1.0	1.0	1.8	/	1.0	1.0	4.2	1.0	1.6
	low	1.0	1.0	1.8	/	1.0	1.0	4.2	1.0	1.6

[1] Ratio for CRACMM is not applicable as the initial SOA yields are zero.

[2] Excluding CRACMM.

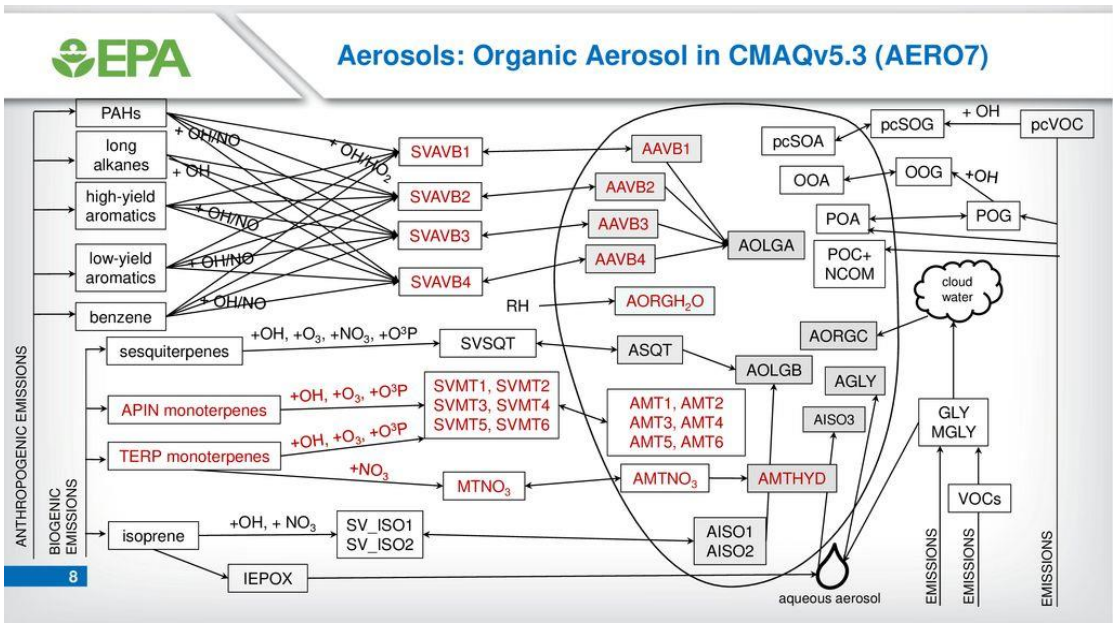

Figure S1 Schematic of AERO7 scheme (Murphy et al. 2018)

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