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Dual roles of the inorganic aqueous phase on secondary organic aerosol growth from benzene and phenol

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Section S1. Time profile of sunlight intensity, temperature, relative humidity in the UF-APHOR chamber on October 19, 2022.

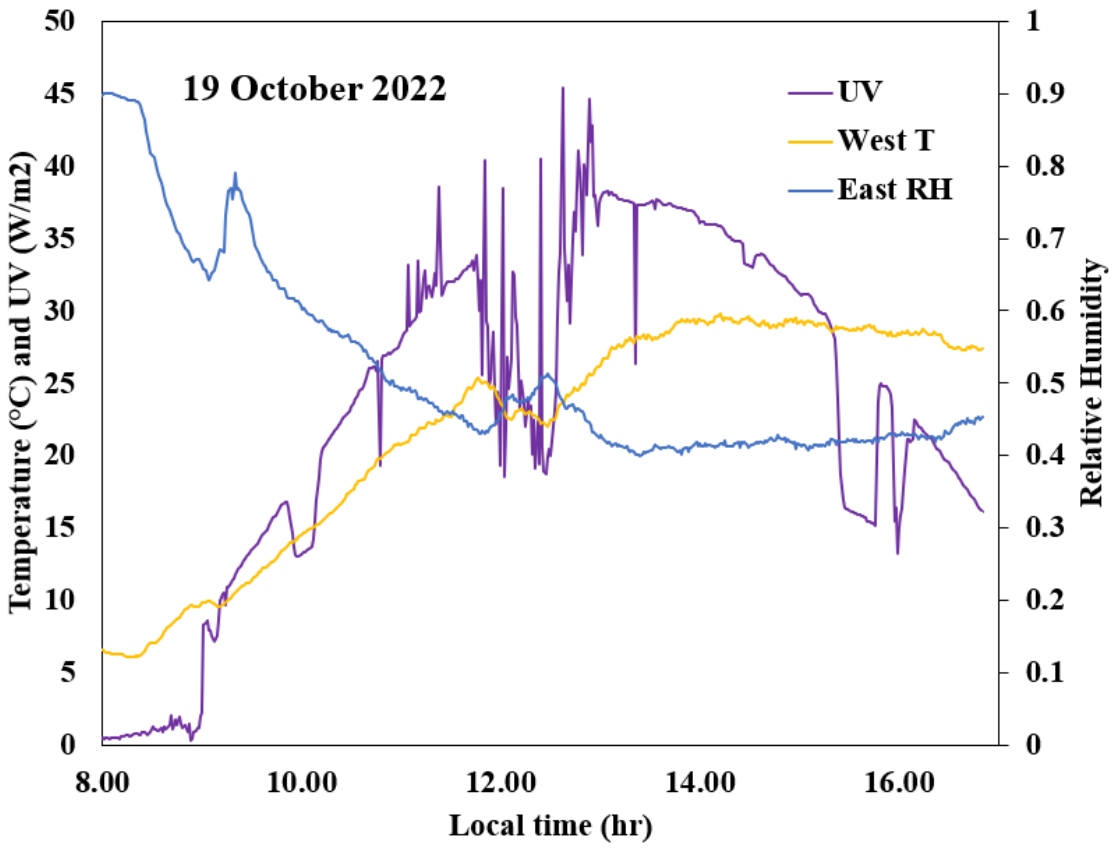


Figure S1. Time series data of sunlight intensity, temperature, and relative humidity in UF-APHOR chamber on October 19, 2022. This sunlight profiles has been used to simulate the sensitivity of the UNIPAR model to major variables such as temperature, humidity, and NO_x levels, and seed types.

Section S2. UNIPAR Model Structure

S2A. UNIPAR model description

(1) Gas Products Lumping Structure

The oxidation of phenol and benzene was simulated using the explicit gas mechanisms including MCM, v3.3.1 (Jenkin et al., 1997; Saunders et al., 2003; Jenkin et al., 2003), the mechanisms to form low-volatile HOM (Section 3.1.1), and the mechanisms to form PPR (Section 3.1.2) in the box model platform. The NO_x dependence of gas phase products was simulated with various HC/NO_x conditions (2-32 ppbC/ppb) under the same meteorological conditions (sunlight intensity, temperature, relative humidity) as on June 19, 2015. The resulting products were lumped into 50 lumping groups based on volatility and reactivity. This mass base 2D lumping array consists of 8 levels of volatility (10^{-8}, 10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, and 1 mmHg), 6 levels of aerosol phase reactivity (very fast (VF), fast (F), medium (M), slow (S), partitioning only (P), and multi-alcohol (MA)) and two additional reactive species (glyoxal (GLY), methylglyoxal (MGLY)) which are separately treated in UNIPAR model. The detailed products distribution was shown in SI tables S1-S2. The stoichiometric coefficient of resulting products are linked to the mathematical equation and applied to construct product array.

In addition, the mass based stoichiometric coefficient (α_i) of lumping group *i* in each NO_x levels is calculated with a fractional aging scale ($f'_A(t)$) ranging from 0 to 1, which is converted by the aging factor ($f_A(t)$).

$$f_A(t) = \frac{\log[HO_2]+[RO_2]}{[HC]_0} \quad \text{(Eq.1)}$$

$$f'_A(t) = \frac{f_A(aged)-f_A(t)}{f_A(aged)-f_A(fresh)} \quad \text{(Eq.2)}$$

$$\alpha_i = \left(1 - f'_A(t)\right)(fresh\ \alpha_i) + (f'_A(t))(aged\ \alpha_i) \quad \text{(Eq.3)}$$

In the equations above, $[HO_2]$ and $[RO_2]$ are the concentration of HO_2 and RO_2 radicals (in ppb) and [HC] represents the initial HC concentration (in ppbC). When the time (*t*) is small (fresh), (Eq.1) sets the lower boundary of $f_A(t)$. On the contrary, when *t* is big (aged), the upper boundary of $f_A(t)$ was decided. The fresh α_i and aged α_i be determined, respectively. As increasing aerosol acidity, the distribution of products is less aged due to the impact of PPR on gas oxidation (retarded production of $[HO_2]$ and $[RO_2]$).

(2) Concentrations of Species in Multiphase

In the presence of wet-inorganic seed aerosol, the lumped products produced gas phase are separate into *g*, *or* and *in* phases by gas-aerosol absorptive partitioning model (Pankow, 1994). The *g-or* partitioning coefficient ($K_{or,i}$) (in $m^3\ \mu g^{-1}$) and *g-in* partitioning coefficient ($K_{in,i}$) are expressed as (Eq.4) and (Eq.5), respectively.

$$K_{or,i} = \frac{7.501RT}{10^9 MW_{or} \gamma_{or,i} p^\circ_{l,i}} \quad \text{(Eq.4)}$$

$$K_{in,i} = \frac{7.501RT}{10^9 \mathrm{MW_{in}} \gamma_{\mathrm{in},i} p^{\circ}_{\mathrm{l},i}} \quad \text{(Eq.5)}$$

R stands for the gas constant (8.314 J mol^{-1} K^{-1}). MW_{in} represents the average MW (g mol^{-1}) of inorganic aerosol. $p^{\circ}_{l,i}$ is the liquid vapor pressure (in mmHg) of the product *i* and is calculated using the group contribution method (Zhao et al., 1999). The activity coefficient ($\gamma_{or,i}$) of organic species *i* in *or* phase is treated as one (Im et al., 2014). The activity coefficient of *i* in *in* ($\gamma_{in,i}$) is predicted using a semi-empirically regression equation (Zhou et al., 2019). The theoretical $\gamma_{in,i}$ was estimated by using the thermodynamic Aerosol Inorganic-Organic Mixtures Functional Groups Activity Coefficients (AIOMFAC) (Zuend et al., 2011) for given set of conditions and aerosol parameters. $\gamma_{in,i}$ is a function of aerosol environment variables (RH ranging from 0 to 1 and fractional sulfate (FS = $[SO_4^{2-}]/[SO_4^{2-}]+[NH_4^+]$)) and the physicochemical parameters of species *i* such as the molecular weight (MW_i), the oxygen to carbon ratio ($O:C_i$), hydrogen bonding (HB_i) as follows,

$$\gamma_{in,i} = e^{0.035 \cdot MW_i - 2.704 \cdot \ln(O:C_i) - 1.121 \cdot HB_i - 0.330 \cdot FS - 0.022 \cdot (100 \cdot RH)} \quad \text{(Eq.6)}$$

$K_{or,i}$ and $K_{in,i}$ were applied to estimate the concentration (μg m^{-3}) of the lumping species in each phase (Fig. 1).

(3) Aerosol Phase Reaction

$OM_{AR,i}$ (in μg m^{-3}) forms via oligomerization in both *or* and *in* phases based on a second-order dimerization (Odian, 2004). The formed OM_{AR} is assumed to be nonvolatile and irreversible (Kleindienst and Bullock, 2006; Cao and Jang, 2010; Zhou et al., 2019). Oligomerization in the aqueous phase can be accelerated by acid-catalyzed reactions (Jang et al., 2002) and expressed as

$$\frac{dC_{\mathrm{or},i}}{dt} = -k_{or,i} C'^2_{\mathrm{or},i} \left(\frac{\mathrm{MW}_i \mathrm{OM}_T}{\rho_{\mathrm{or}} 10^3}\right) \quad \text{(Eq.7)}$$

$$\frac{dC_{\mathrm{in},i}}{dt} = -k_{in,i} C'^2_{\mathrm{in},i} \left(\frac{\mathrm{MW}_i \mathrm{M}_{in}}{\rho_{\mathrm{in}} 10^3}\right) \quad \text{(Eq.8)}$$

$k_{or,i}$ (L mol^{-1} s^{-1}) and $k_{in,i}$ are oligomerization rate constants in *or* and *in* phases, respectively. The average density of phenol and benzene aerosols (ρ_{or}) is 1.4 g cm^{-3} (Yee et al., 2013; Nakao et al., 2013; Nakao et al., 2011; Ng et al., 2007; Borrás and Tortajada-Genaro, 2012). The density of inorganic aerosol (ρ_{in} in g cm^{-3}) was calculated from a regression equation through the Extended Aerosol Inorganic Model (E-AIM) . The terms in brackets are conversion factors from aerosol-based concentrations ($C'_{or,i}$ and $C'_{in,I}$, mol L^{-1}) to air-based concentration (μg m^{-3}). $k_{or,i}$ (L mol^{-1} s^{-1}) and $k_{in,i}$ are semi-empirically estimated as a function of species reactivity (R_i), protonation equilibrium constant ($pK_{BH^+,i}$), excess acidity (X), water activity (a_w), and proton concentration ($[H^+]$) using the method developed by Jang et al. shown in (Eq.9) and (Eq.10) (Jang et al., 2005; Han and Jang, 2022; Beardsley et al., 2013; Zhou et al., 2019; Yu et al., 2021).

$$k_{o,i} = 10^{0.846 R_i + 0.22 pK_{BH^+ i} - 4.9} \quad \text{(Eq.9)}$$

$$k_{AC,i} = 10^{0.846 R_i + 0.22 pK_{BH^+ i} + 1.003 X + \log(a_w [H^+]) - 2.8} \quad \text{(Eq.10)}$$

$OM_{AR,i}$ in multiphase is calculated via a analytical solution of Eqs.11 and 12 (Im et al., 2014).

(4) Newtonian Method to Estimate Organic Mass via Partitioning

Schell et al. developed a partitioning model to predict SOA formation which Cao and Jang reconstructed to include OM formed via aerosol-phase reactions ($OM_{AR,i}$ in μg m^{-3}) from total species, i ($C_{T,i}$ in μg m^{-3}) (Schell et al., 2001; Cao and Jang, 2010). Mass balance equations as a function of the effective saturation concentration were employed to estimate the OM concentration formed from the total species during the partitioning process (OM_P in μg m^{-3}).

$$OM_P = \sum_{ij}[C_{T,i} - OM_{AR,i} - C^o_{g,i}\frac{\frac{C_{or,i}}{MW_i}}{\sum_{ij}\left(\frac{C'_{or,i}}{MW_i}+\frac{OM_{AR,i}}{MW_{oli,i}}\right)+\frac{OM_0}{MW_{oli,i}}}] \quad \text{(Eq.11)}$$

In (Eq.11), $MW_{oli,i}$ is the MW from oligomer (in g mol^{-1}) and OM_0 is the concentration of the preexisting OM (in mol m^{-3}). OM_p was solved for with the iteration method using the globally converging Newton-Raphson method (Press et al., 1996) at the end each step.

(5) Organosulfate Formation

In the presence of acidic aerosol, UNIPAR predicts the diorganosulfate (diOS) formation to calculate the change in aerosol hygroscopicity and acidity. For example, SA can be neutralized by ammonium or converted to diOS. Sulfate is applied into a semi-empirical equation as a function of free sulfate (Im et al., 2014; Beardsley and Jang, 2016). The PIL-IC experimental data provide ammonium ion concentrations and used for the calculation of aerosol acidity and diOS formation for SOA simulation as shown in (Eq.12).

$$\frac{[\mathrm{diOS}]_{\mathrm{model}}}{[SO_4^{2-}]_{\mathrm{free}}} = 1 - \frac{1}{1+f_{\mathrm{diOS}}\frac{N_{\mathrm{diOS}}}{[SO_4^{2-}]_{\mathrm{free}}}} \quad \text{(Eq.12)}$$

In (Eq.12), f_{diOS} is the diOS conversion factor (Im et al., 2014) and N_{diOS} denotes the numeric parameter for scaling lumping groups based on the effectiveness of diOS formation for each chemical species.

S2B. Model Parameters

(1) Physicochemical parameters

Table S1. Unified physicochemical parameters of lumping species from oxidation of phenol and benzene.

Lumped species	phenol			benzene		
	MW ($g\ mol^{-1}$)	O:C	H-bonding	MW ($g\ mol^{-1}$)	O:C	H-bonding
1VF	174.1082	1	2.6	174.1082	1	2.6
2VF	219.1058	1.333333	1	219.1058	1.333333	1
3VF	120.0609	1.666667	2.6	120.0609	1.666667	2.6
4VF	118.09	1	2	118.09	1	2
5VF	140.0936	0.666667	0	140.0936	0.666667	0
6VF	115.8671	1	0.898263	115.9067	1	0.917916
7VF	88.062	1	1	88.062	1	1
8VF	86.0462	1	0	86.0462	1	0
1F	0	0	0	0	0	0
2F	0	0	0	0	0	0
3F	0	0	0	0	0	0
4F	144.0823	1	1.6	204.9864	1.166277	1.001431
5F	118.5967	1.004738	1.990949	118.0894	1.000022	2
6F	0	0	0	198.9037	1.260374	0.000245
7F	116.07	1	0	116.07	1	4.97E-16
8F	84.65	0.5	0	84.08599	0.5	0
1M	159.5946	0.904116	3.747486	147.7398	1.018893	3.646408
2M	142.11	0.666667	2.6	142.11	0.666667	2.6
3M	125.0572	1.029092	3.037909	116.186	1.000004	2.607109
4M	145.0703	1.25	1.6	145.0703	1.25	1.6
5M	128.799	0.667997	1.568898	126.6408	0.525004	1.59185
6M	123.3449	1.036167	0.989723	123.4151	1.037009	0.987718
7M	74.03742	1.50006	1.6	74.03555	1.500002	1.6
8M	71.27919	1.065525	0.564863	65.0994	1.154774	0.687291
1S	0	0	0	0	0	0
2S	140.094	0.666667	2	140.094	0.666667	2
3S	157.4972	0.872951	1.886397	141.9989	0.996307	1.533303
4S	124.1794	0.503462	1	124.0853	0.50061	1
5S	161.07	1.5	0	161.07	1.5	0
6S	0	0	0	0	0	0
7S	108.0948	0.333333	0	108.0948	0.333333	0
8S	0	0	0	0	0	0
1P	155.1493	1.741777	4.562542	150.3565	2.134388	3.86065
2P	185.9148	1.081649	2.743808	169.5117	0.937519	2.990466
3P	184.1064	0.833333	1	184.1064	0.833333	1
4P	150.8352	0.732435	2.075105	128.9816	1.201975	2.481655
5P	139.1088	0.5	1	139.1088	0.5	1
6P	106.7159	0.69126	1.4343	133.8303	0.792327	1.28921

7P	110.1106	0.333333	1.6	142.1094	0.666667	1
8P	84.073	0.5	0	92.39821	0.223516	0.829453
1MA	169.2218	0.979188	5.098942	159.5576	0.848421	5.089731
2MA	142.11	0.666667	4	142.11	0.666667	4
3MA	0	0	0	0	0	0
4MA	0	0	0	92.11	0.5	3
5MA	0	0	0	0	0	0
6MA	0	0	0	0	0	0
7MA	0	0	0	0	0	0
8MA	0	0	0	0	0	0
MGLY	0	0	0	0	0	0
GLY	58.0361	1	0	58.0361	1	0

(2) Stoichiometric coefficients

The coefficients in the Tables (S2-S7) are integrated into the following mathematical equations to construct stoichiometric coefficient array of lumping species.

$$\alpha = A \times (\text{R\_V1N})\ \mathbf{3} + B \times (\text{R\_V1N})\ \mathbf{2} + C \times (\text{R\_V1N}) + D \quad \text{(Eq. 13)}$$

where R_V1N is the HC ppbC/NO_x ppb ratio .

Table S2. Stoichiometric coefficient array of lumping species generated from the oxidation of phenol under the sunlight without SA for the UNIPAR model.

Oxidation path: phenol + OH without SA								
Lumped species	Low NO_x (R_V1N ≥ 5)				High NO_x (R_V1N < 5)			
	A_1	B_1	C_1	D_1	A_1	B_1	C_1	D_1
1VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2VF	2.0766E-07	-1.3097E-05	2.1637E-04	1.3470E-03	-2.7092E-08	-1.7729E-05	4.5989E-04	-4.3263E-04
3VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6VF	7.9035E-08	-4.6010E-06	5.9991E-05	6.4261E-04	1.0674E-07	-5.8088E-06	7.9644E-05	5.2590E-04
7VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5F	3.2943E-07	-2.9298E-05	8.3827E-04	4.1888E-03	-3.6654E-06	1.5929E-04	-2.0059E-03	1.7901E-02
6F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7F	6.9208E-07	-3.7231E-05	3.6665E-04	6.2233E-03	4.5054E-06	-1.8427E-04	2.1984E-03	-1.0565E-03
8F	3.2481E-06	-2.2302E-04	4.5117E-03	4.4345E-03	1.8330E-05	-5.3990E-04	4.9067E-03	1.8265E-02
1M	-6.7149E-07	-1.1510E-05	2.3269E-03	7.5070E-02	1.0425E-04	-2.9654E-03	2.4701E-02	4.5574E-02
2M	-5.2114E-06	2.7051E-04	-1.9813E-03	6.0931E-02	7.9064E-05	-1.8536E-03	1.0206E-02	6.7842E-02
3M	1.4711E-07	-1.9121E-05	6.8469E-04	1.6073E-02	4.6980E-06	-1.2579E-04	1.0701E-03	1.8632E-02

4M	5.7778E-07	-1.0384E-05	-9.5318E-04	2.5974E-02	-2.2103E-06	-1.4838E-04	3.9223E-03	-5.9922E-03
5M	-2.7520E-06	1.6694E-04	-2.4506E-03	2.7819E-02	6.4887E-06	-9.1579E-05	-2.6698E-04	2.1763E-02
6M	-2.3238E-06	7.4349E-05	1.5573E-03	1.3654E-01	-5.0510E-06	-3.2821E-04	1.3656E-02	5.5938E-02
7M	2.0321E-06	-1.2938E-04	2.2491E-03	1.1644E-02	1.0723E-06	-1.3205E-04	2.8774E-03	6.3892E-03
8M	-2.2289E-07	1.3125E-05	-1.9692E-04	2.1221E-03	7.3661E-07	-2.6192E-05	3.2878E-04	-2.1454E-04
1S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2S	8.0515E-08	-5.1791E-06	8.8631E-05	2.3209E-03	8.9440E-07	-2.1284E-05	7.7544E-05	3.3077E-03
3S	-6.1820E-08	3.5322E-06	-4.5906E-05	2.2749E-04	-4.1715E-08	2.0124E-06	-1.4974E-05	3.0443E-05
4S	1.4362E-07	-9.4814E-06	1.7118E-04	5.8243E-03	2.0350E-06	-4.6534E-05	1.3903E-04	8.1248E-03
5S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7S	3.0179E-07	-2.3242E-05	5.5786E-04	3.2594E-02	-2.1753E-06	8.5178E-05	-9.7760E-04	3.9622E-02
8S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1P	-6.4645E-07	1.8106E-05	5.2763E-04	-4.5717E-03	-3.2836E-06	1.2555E-04	-9.1700E-04	1.5044E-03
2P	-3.4764E-06	2.2287E-04	-3.7977E-03	2.1333E-02	-4.9438E-07	3.7573E-05	-3.0767E-04	6.0435E-04
3P	4.5544E-08	-2.0191E-06	-3.8996E-06	1.1829E-03	-5.4651E-08	-5.8139E-06	1.4551E-04	1.5017E-04
4P	2.0902E-05	-1.1662E-03	1.2873E-02	2.5087E-01	2.9294E-05	-3.5584E-03	6.8138E-02	-6.1945E-02
5P	1.5743E-06	-7.3109E-05	4.8235E-05	5.6623E-02	-6.9809E-06	-2.2322E-04	7.9286E-03	2.5637E-03
6P	-2.1914E-05	1.3168E-03	-1.8586E-02	2.3671E-01	-1.0403E-04	4.2824E-03	-5.0154E-02	3.2231E-01
7P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8P	-4.6166E-07	2.7186E-05	-3.9515E-04	2.0953E-02	1.8031E-05	-5.6681E-04	5.3563E-03	5.2854E-03
1MA	-6.4868E-06	4.0243E-04	-6.4528E-03	6.1163E-02	7.1431E-06	-1.1327E-04	1.4221E-04	3.1532E-02
2MA	-2.1163E-06	1.1144E-04	-9.0582E-04	1.9559E-02	-1.4892E-05	6.1160E-04	-7.0862E-03	4.3110E-02
3MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
MGLY	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
GLY	1.1516E-05	-7.5023E-04	1.3399E-02	8.5479E-02	5.1907E-05	-2.0514E-03	2.5959E-02	5.2439E-02

Table S3. Stoichiometric coefficient array of oxygenated products from the oxidation of phenol under the sunlight with SA for the UNIPAR model.

Oxidation path: phenol + OH with SA								
Lumped species	Low NO_x				High NO_x			
	A_1	B_1	C_1	D_1	A_1	B_1	C_1	D_1
1VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2VF	-3.4594E-08	2.6512E-06	-6.4020E-05	6.5047E-04	-7.3419E-07	1.5381E-05	-6.7714E-05	1.0401E-04
3VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

1F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8F	-2.2516E-07	1.7834E-05	-4.5778E-04	5.7682E-03	-3.4846E-06	5.5382E-05	7.0124E-05	-1.2963E-04
1M	-2.7275E-08	1.9277E-06	-3.8238E-05	4.3398E-04	-4.9267E-07	9.6955E-06	-2.9508E-05	4.4596E-05
2M	-3.3041E-08	2.2244E-06	-3.4950E-05	4.9960E-04	-5.7853E-07	1.1127E-05	-2.0524E-05	2.3881E-05
3M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4M	-1.6596E-06	1.3048E-04	-3.2511E-03	3.4909E-02	-1.1615E-05	9.8518E-05	1.4417E-03	1.3576E-03
5M	-2.5888E-06	1.7007E-04	-2.0434E-03	7.1508E-02	-2.0588E-05	-2.7932E-05	9.9658E-03	-1.0573E-02
6M	2.1932E-06	-1.9177E-04	5.4713E-03	1.0110E-01	-5.1505E-06	1.8081E-04	3.4396E-04	1.2155E-01
7M	-9.1750E-08	6.9709E-06	-1.6718E-04	4.2991E-03	-1.4529E-06	2.3131E-05	2.8672E-05	2.0524E-03
8M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7S	7.6882E-08	-7.5916E-06	2.1924E-04	7.2760E-02	1.9889E-05	-6.2890E-04	6.4125E-03	5.3094E-02
8S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2P	-8.8834E-09	5.9116E-07	-6.2845E-06	1.7227E-04	-1.1236E-07	1.5326E-06	1.3413E-05	-1.1921E-05
3P	-1.9651E-07	1.6005E-05	-4.1933E-04	4.7707E-03	2.9630E-07	-2.9381E-05	4.0412E-04	6.0635E-04
4P	-3.0474E-09	-1.1645E-05	4.0863E-04	7.2726E-01	1.9990E-04	-6.3673E-03	6.4773E-02	5.1913E-01
5P	2.8654E-06	-1.9611E-04	4.0691E-03	2.8444E-01	-2.7302E-04	9.2718E-03	-1.0048E-01	6.5872E-01
6P	-1.9629E-06	1.5638E-04	-3.9168E-03	4.8265E-02	-1.0652E-05	1.9085E-06	3.1936E-03	1.3545E-03
7P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8P	-7.9313E-07	5.9987E-05	-1.3717E-03	1.3907E-02	-1.1363E-05	2.0356E-04	-3.9335E-04	5.0072E-04
1MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2MA	-6.3920E-10	-5.9913E-08	5.7115E-06	9.0706E-05	5.3856E-08	-2.2021E-06	3.0962E-05	2.7302E-06
3MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
MGLY	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
GLY	2.9570E-06	-2.3189E-04	5.4447E-03	9.8720E-03	-1.3145E-05	5.4935E-04	-4.9025E-03	4.9154E-02

Table S4. Stoichiometric coefficient array of fresh, oxygenated products from the oxidation of benzene under the sunlight without SA for the UNIPAR model.

Oxidation path: benzene + OH without SA								
Lumped species	Low NO_x				High NO_x			
	A_1	B_1	C_1	D_1	A_1	B_1	C_1	D_1
1VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2VF	-2.8096E-09	6.6597E-07	-1.5082E-05	9.5787E-05	4.7594E-09	-1.7838E-08	-4.3120E-08	1.9081E-07
3VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6VF	-1.2139E-08	5.4537E-07	-1.9853E-06	1.0665E-05	-1.9499E-08	7.1166E-07	-2.3902E-06	3.6705E-06
7VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5F	-1.6013E-07	8.7023E-06	-7.2527E-05	5.3907E-04	-2.8216E-07	9.6309E-06	-2.5341E-05	4.0104E-05
6F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7F	-1.3113E-06	4.2492E-05	1.1592E-03	1.3422E-02	-4.3202E-06	6.4009E-05	2.3475E-03	1.0696E-03
8F	1.1554E-06	-2.9470E-05	-1.2617E-03	1.3025E-01	4.1068E-06	-7.6406E-05	-1.6878E-03	1.3717E-01
1M	-8.4936E-07	7.7954E-05	-1.5696E-03	9.6022E-03	1.6862E-07	2.1075E-06	-1.1523E-05	2.0462E-05
2M	-2.1143E-06	1.6675E-04	-3.2573E-03	1.9299E-02	5.3170E-07	-3.1896E-06	1.5719E-06	1.0219E-05
3M	-1.9577E-07	1.1194E-05	-9.7347E-05	7.3196E-04	-3.8472E-07	1.3161E-05	-3.8670E-05	5.7347E-05
4M	2.2279E-08	-9.7797E-07	1.7037E-05	-9.2185E-05	-8.3304E-10	1.3879E-07	-8.2404E-07	1.2760E-06
5M	-2.0702E-06	1.3922E-04	-2.4872E-03	1.4161E-02	1.7159E-07	5.8843E-06	-4.0697E-05	6.8317E-05
6M	-3.6132E-07	1.3815E-04	-2.4108E-03	2.0995E-02	-1.1162E-06	5.9252E-05	3.1704E-04	7.2838E-04
7M	-2.8228E-07	1.8048E-05	-2.3053E-04	1.3777E-03	-2.6858E-07	1.1115E-05	-4.1080E-05	6.2786E-05
8M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2S	-2.5806E-08	1.5115E-06	-1.7692E-05	1.0052E-04	-2.7581E-08	1.0925E-06	-4.6827E-06	6.4690E-06
3S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4S	-6.2736E-08	3.6301E-06	-3.9872E-05	2.5372E-04	-7.7030E-08	2.8269E-06	-8.4150E-06	1.3217E-05
5S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7S	-2.7735E-07	1.3047E-05	1.1917E-05	1.9504E-03	-5.8745E-07	1.2560E-05	2.1127E-04	1.3704E-04
8S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3P	-7.1788E-09	4.7806E-07	-5.4632E-06	3.3436E-05	-8.5592E-09	3.5877E-07	-1.2492E-06	1.9546E-06
4P	1.4971E-06	-6.4197E-05	1.2686E-03	-6.2614E-03	-8.5536E-07	3.4432E-05	-1.1469E-04	1.7754E-04
5P	-1.1611E-09	-7.5198E-07	4.6876E-04	1.5472E-03	-1.1952E-06	2.6275E-05	4.1765E-04	2.8203E-04
6P	-2.2796E-06	1.7180E-05	3.0425E-03	8.7528E-02	-6.2805E-06	4.0057E-05	4.7605E-03	7.0277E-02
7P	2.4253E-07	-2.3513E-05	8.5025E-04	2.2063E-03	-6.7094E-07	-8.0488E-06	9.5508E-04	2.6400E-04
8P	7.9088E-06	-3.7110E-04	-1.1205E-03	8.2553E-01	1.8685E-05	-4.0207E-04	-6.6894E-03	8.7905E-01
1MA	-1.5845E-07	1.0536E-05	-1.4557E-04	7.3669E-04	-4.3833E-08	3.8043E-06	-2.3598E-05	3.6245E-05
2MA	-4.8471E-07	2.5091E-05	-1.6646E-04	1.1966E-03	-1.0761E-06	3.6733E-05	-1.3929E-04	1.8282E-04
3MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4MA	-5.4104E-08	1.2230E-06	6.4131E-05	3.6928E-04	-3.2711E-07	6.5832E-06	7.4429E-05	-5.8772E-05

5MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
MGLY	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
GLY	-1.1020E-06	5.6963E-05	-2.8675E-04	2.1932E-01	-1.9315E-06	4.4927E-05	5.5594E-04	2.1228E-01

Table S5. Stoichiometric coefficient array of aged, oxygenated products from the oxidation of benzene under the sunlight without SA for the UNIPAR model.

Oxidation path: benzene + OH without SA								
Lumped species	Low NO_x				High NO_x			
	A_1	B_1	C_1	D_1	A_1	B_1	C_1	D_1
1VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2VF	-8.2681E-08	6.6507E-06	-1.7858E-04	2.6107E-03	-6.2419E-07	4.3219E-06	1.7603E-04	-3.0008E-04
3VF	4.4691E-09	-6.1259E-07	2.4201E-05	-1.9251E-04	3.0753E-08	-3.0515E-07	5.4434E-07	3.2952E-07
4VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6VF	-2.2453E-07	1.6948E-05	-4.2435E-04	3.8445E-03	-4.6322E-07	7.8899E-06	-1.3024E-05	5.5402E-04
7VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5F	-3.9335E-08	3.4059E-06	-9.1369E-05	1.4440E-03	6.3257E-08	2.5292E-05	-7.2212E-04	5.5743E-03
6F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7F	-3.5953E-06	2.6582E-04	-6.4664E-03	5.4697E-02	-1.1635E-06	-1.5919E-05	-2.3152E-04	1.6631E-02
8F	-2.1166E-06	1.5599E-04	-3.7667E-03	3.2324E-02	1.4166E-05	-3.9980E-04	2.3995E-03	9.5229E-03
1M	-5.0775E-07	2.5884E-05	1.3326E-04	4.0026E-03	1.0089E-04	-2.8411E-03	2.1735E-02	-2.0619E-02
2M	-5.2920E-07	3.4065E-05	-5.7965E-04	6.0043E-03	5.7832E-05	-1.5832E-03	1.1353E-02	-8.1318E-03
3M	-3.4356E-07	2.1060E-05	-2.3424E-04	5.2158E-03	2.2029E-05	-6.4502E-04	5.2118E-03	-2.8069E-03
4M	2.1999E-06	-5.9710E-05	-3.0652E-03	1.4111E-01	-1.9072E-04	4.8442E-03	-2.5911E-02	3.9562E-02
5M	-1.7929E-07	1.4575E-05	-3.4260E-04	7.9012E-03	8.6639E-06	-2.8194E-04	2.7930E-03	-2.4513E-03
6M	-1.4396E-06	1.1152E-04	-2.5606E-03	6.1435E-02	2.3732E-05	-9.6441E-04	1.1874E-02	2.0267E-03
7M	-4.0252E-06	2.9585E-04	-7.1648E-03	5.9180E-02	-1.4482E-05	2.9679E-04	-1.2173E-03	5.9069E-03
8M	6.4447E-07	-5.2669E-05	1.5286E-03	-7.9964E-03	3.1840E-06	-8.7697E-05	1.0432E-03	-1.5693E-03
1S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2S	-1.1686E-08	8.9287E-07	-1.9654E-05	1.4033E-03	2.2549E-06	-6.1829E-05	4.2365E-04	1.1374E-03
3S	4.0136E-07	-3.4460E-05	9.9247E-04	-7.0812E-03	8.1178E-07	-6.7712E-06	3.3655E-06	3.1874E-05
4S	5.7598E-08	-5.3180E-06	1.7817E-04	1.7947E-03	5.6441E-06	-1.5090E-04	1.0272E-03	2.7462E-03
5S	-3.2807E-08	3.1826E-06	-1.1329E-04	2.0461E-03	-2.2709E-06	5.4865E-05	-2.6336E-04	3.2554E-04
6S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7S	-4.9990E-07	3.4844E-05	-7.3255E-04	1.9065E-02	8.0962E-06	-2.2853E-04	1.5191E-03	1.5281E-02
8S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1P	1.0162E-05	-7.8149E-04	2.0027E-02	-1.3253E-01	6.3750E-06	9.5480E-05	-1.4008E-03	2.9418E-03

2P	1.6488E-06	-1.3359E-04	3.6497E-03	-2.4840E-02	1.5276E-06	1.3982E-05	-2.4949E-04	5.4524E-04
3P	2.7406E-07	-2.3346E-06	-6.7471E-04	2.0778E-02	-1.6767E-05	4.1388E-04	-1.9715E-03	4.8614E-03
4P	-1.2442E-05	9.4897E-04	-2.4707E-02	3.5372E-01	-1.5964E-04	2.7386E-03	5.4771E-03	5.1843E-03
5P	-3.6689E-06	3.3364E-04	-1.1065E-02	2.0295E-01	-1.3200E-04	3.0603E-03	-1.2826E-02	5.5431E-02
6P	1.0112E-05	-8.5927E-04	2.5195E-02	-4.9321E-02	9.6870E-05	-2.0938E-03	1.0440E-02	1.5124E-01
7P	5.7397E-06	-4.7054E-04	1.3355E-02	-9.2718E-02	8.7848E-06	-7.5843E-06	-1.0509E-03	7.6372E-03
8P	-9.1182E-06	6.2982E-04	-1.2933E-02	1.7278E-01	-5.5269E-05	2.5501E-03	-4.2546E-02	3.4038E-01
1MA	-8.3685E-08	-1.9244E-05	2.0738E-03	-8.8182E-03	2.3911E-05	-5.6619E-04	3.5178E-03	1.0425E-02
2MA	-1.7522E-07	1.1237E-05	-1.9015E-04	1.9361E-03	-3.3980E-07	7.2889E-05	-1.7225E-03	1.1467E-02
3MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4MA	-3.6381E-08	2.3528E-06	-4.1904E-05	3.8505E-04	-2.5151E-07	1.9157E-05	-3.6699E-04	2.1866E-03
5MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
MGLY	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
GLY	-8.2527E-06	7.0429E-04	-2.0076E-02	2.5097E-01	3.6943E-05	-1.2900E-03	1.0129E-02	9.4244E-02

Table S6. Stoichiometric coefficient array of fresh, oxygenated products from the oxidation of benzene under the sunlight with SA for the UNIPAR model.

Oxidation path: benzene + OH with SA								
Lumped species	Low NO_x				High NO_x			
	A_1	B_1	C_1	D_1	A_1	B_1	C_1	D_1
1VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2VF	1.1816E-09	-2.6779E-07	1.9346E-05	-1.7937E-04	-9.8873E-09	6.2405E-07	-3.4202E-06	5.4908E-06
3VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6VF	1.3952E-09	-2.7796E-07	1.5749E-05	1.5378E-04	-2.2177E-08	3.8472E-07	2.1917E-05	-3.5720E-05
7VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7F	2.8491E-08	-5.4607E-06	2.9059E-04	5.4734E-02	7.6815E-06	-4.4097E-04	8.4424E-03	3.8436E-03
8F	-7.2634E-08	1.5142E-05	-9.3898E-04	6.9353E-02	-3.6685E-06	2.4011E-04	-5.6937E-03	1.0336E-01
1M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4M	4.8949E-08	-1.0259E-05	6.4294E-04	6.9815E-04	-6.6826E-07	1.9113E-05	4.2214E-04	-6.9633E-04
5M	3.4856E-08	-7.3058E-06	4.7665E-04	-2.2592E-03	-5.3763E-07	2.3721E-05	-2.4305E-05	-1.8356E-05
6M	1.2720E-07	-2.9827E-05	2.3257E-03	-3.6166E-03	4.4524E-07	-3.0596E-05	1.9433E-03	1.5474E-03

7M	1.7643E-08	-3.6720E-06	2.2773E-04	6.9377E-04	-2.3420E-07	5.5725E-06	1.9782E-04	-3.0684E-04
8M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7S	1.5658E-08	-3.2277E-06	1.9714E-04	6.4149E-03	6.7168E-07	-4.4251E-05	1.0672E-03	1.4778E-04
8S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3P	1.0536E-08	-2.1850E-06	1.3416E-04	3.0840E-04	-1.2166E-07	2.9220E-06	1.0874E-04	-1.2885E-04
4P	4.5796E-07	-9.4357E-05	5.7573E-03	1.7944E-01	1.8463E-05	-1.2271E-03	2.9957E-02	3.8028E-03
5P	2.3355E-07	-4.8406E-05	2.9691E-03	1.1556E-01	8.7698E-06	-5.8591E-04	1.4471E-02	3.1913E-02
6P	-5.2807E-11	1.5550E-06	-3.1334E-04	8.5335E-02	-1.1475E-06	4.0749E-05	-3.6878E-04	8.0398E-02
7P	-1.0911E-08	2.2615E-06	-1.3752E-04	1.4509E-02	2.8183E-06	-1.4266E-04	2.1638E-03	3.2806E-03
8P	-7.1069E-07	1.4658E-04	-8.9451E-03	6.1229E-01	-2.6543E-05	1.7829E-03	-4.4202E-02	8.7044E-01
1MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
MGLY	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
GLY	1.0489E-08	-2.2826E-06	1.5811E-04	2.2089E-01	1.9514E-06	-1.1357E-04	2.2518E-03	2.0782E-01

Table S7. Stoichiometric coefficient array of aged, oxygenated products from the oxidation of benzene under the sunlight with SA for UNIPAR model.

Oxidation path: benzene + OH with SA								
Lumped species	Low NO_x				High NO_x			
	A_1	B_1	C_1	D_1	A_1	B_1	C_1	D_1
1VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2VF	8.2907E-11	1.9299E-09	-3.1343E-06	6.5202E-04	6.1044E-08	-4.4570E-06	1.0224E-04	-1.4608E-04
3VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6VF	-6.5453E-10	1.4359E-07	-1.0404E-05	4.0958E-04	1.1750E-07	-4.8013E-06	4.0715E-05	3.7377E-04
7VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8VF	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

4F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6F	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7F	-1.0974E-08	2.3910E-06	-1.7017E-04	1.0812E-02	-1.6978E-06	9.4237E-05	-1.7903E-03	2.0215E-02
8F	-5.9004E-09	1.2770E-06	-8.9543E-05	5.3936E-03	-3.7528E-07	2.4790E-05	-5.9008E-04	8.9520E-03
1M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4M	1.2452E-07	-2.3067E-05	9.9847E-04	9.7610E-02	1.4018E-05	-7.4110E-04	1.3136E-02	2.7219E-02
5M	9.7667E-11	-5.3174E-08	1.0555E-05	4.3323E-03	1.0951E-06	-5.7424E-05	9.5387E-04	-5.1360E-04
6M	3.4323E-08	-7.3472E-06	5.0156E-04	2.1507E-02	-5.2049E-07	-1.5204E-05	1.5909E-03	8.0462E-03
7M	6.7384E-10	7.1083E-08	-3.6990E-05	6.7307E-03	6.6587E-07	-3.2675E-05	4.8808E-04	3.7472E-03
8M	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5S	3.3413E-09	-7.1046E-07	4.7057E-05	-1.4064E-04	-1.1240E-07	4.8267E-06	-2.5249E-05	3.5646E-05
6S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7S	-5.4305E-10	1.1587E-07	-8.4854E-06	1.3458E-02	5.9006E-07	-3.0343E-05	4.8304E-04	1.0974E-02
8S	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2P	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3P	-1.6183E-08	4.0034E-06	-3.6179E-04	2.7778E-02	5.5086E-06	-2.4852E-04	2.9230E-03	1.7147E-02
4P	-2.2330E-07	4.6115E-05	-2.9003E-03	4.0179E-01	3.2744E-05	-1.5518E-03	1.9812E-02	3.1579E-01
5P	3.3461E-08	-6.0784E-06	1.8361E-04	2.9654E-01	-3.2890E-05	1.6771E-03	-2.6570E-02	4.2813E-01
6P	-2.1939E-08	5.2238E-06	-4.2887E-04	1.1456E-01	7.8744E-06	-3.7418E-04	4.9973E-03	9.2595E-02
7P	2.8532E-09	-7.3132E-07	7.1020E-05	2.8915E-03	-1.2644E-06	5.9949E-05	-7.9522E-04	6.4258E-03
8P	5.2831E-08	-1.5608E-05	1.8314E-03	1.1461E-01	-3.2091E-05	1.5034E-03	-1.9406E-02	1.9821E-01
1MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8MA	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
MGLY	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
GLY	-3.4545E-08	7.5117E-06	-5.3108E-04	6.9518E-02	-4.9695E-06	2.8060E-04	-5.4594E-03	9.8983E-02

(3) Major oxygenated products in lumping groups

Reactivity scales of the oxidation products are determined according to the number of reactive functional groups in their chemical structure. The reactivity bins used in UNIPAR are very fast (VF, α-hydroxybicarbonyls and tricarbonyls), fast (F, 2 epoxides or aldehydes,), medium (M, 1 epoxide or aldehyde), slow (S, ketones), partitioning only (P) and multi-alcohol (MA, 3 or more alcohols). The explicit chemical structures of oxidation products from phenol and benzene are summarized in Table S9-S10 as examples.

Table S8. Major oxygenated products distribution in gas phase for phenol oxidation under aged and low NO_x (HC/NO_x=16) condition.

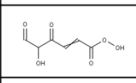
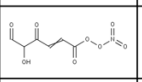
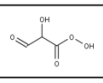
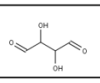
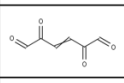
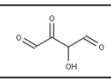
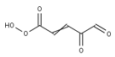
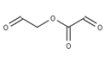
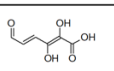
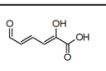
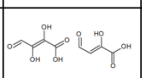
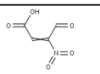
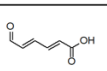
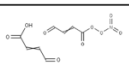
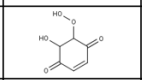
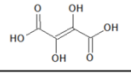
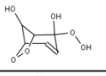
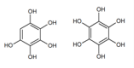
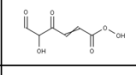
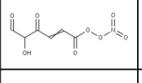
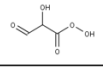
$\alpha_{m,n}$		Phenol: Vapor Pressure (mmHg) [n]							
		n = 1 (10^{-8})	n = 2 (10^{-6})	n = 3 (10^{-5})	n = 4 (10^{-4})	n = 5 (10^{-3})	n = 6 (10^{-2})	n = 7 (10^{-1})	n = 8 (10^{0})
Reactivity [m]	VF								
	F								
	M								
	S								
	P								
	MA								
	R								GLY 

Table S9. Major oxygenated products distribution in gas phase for benzene oxidation under aged and low NO_x (HC/NO_x=14) condition.

$\alpha_{m,n}$		Benzene: Vapor Pressure (mmHg) [n]							
		n = 1 (10^{-8})	n = 2 (10^{-6})	n = 3 (10^{-5})	n = 4 (10^{-4})	n = 5 (10^{-3})	n = 6 (10^{-2})	n = 7 (10^{-1})	n = 8 (10^{0})
Reactivity [m]	VF								
	F								
	M								
	S								
	P								
	MA								
	R								GLY

Section S3. Gas oxidation mechanism

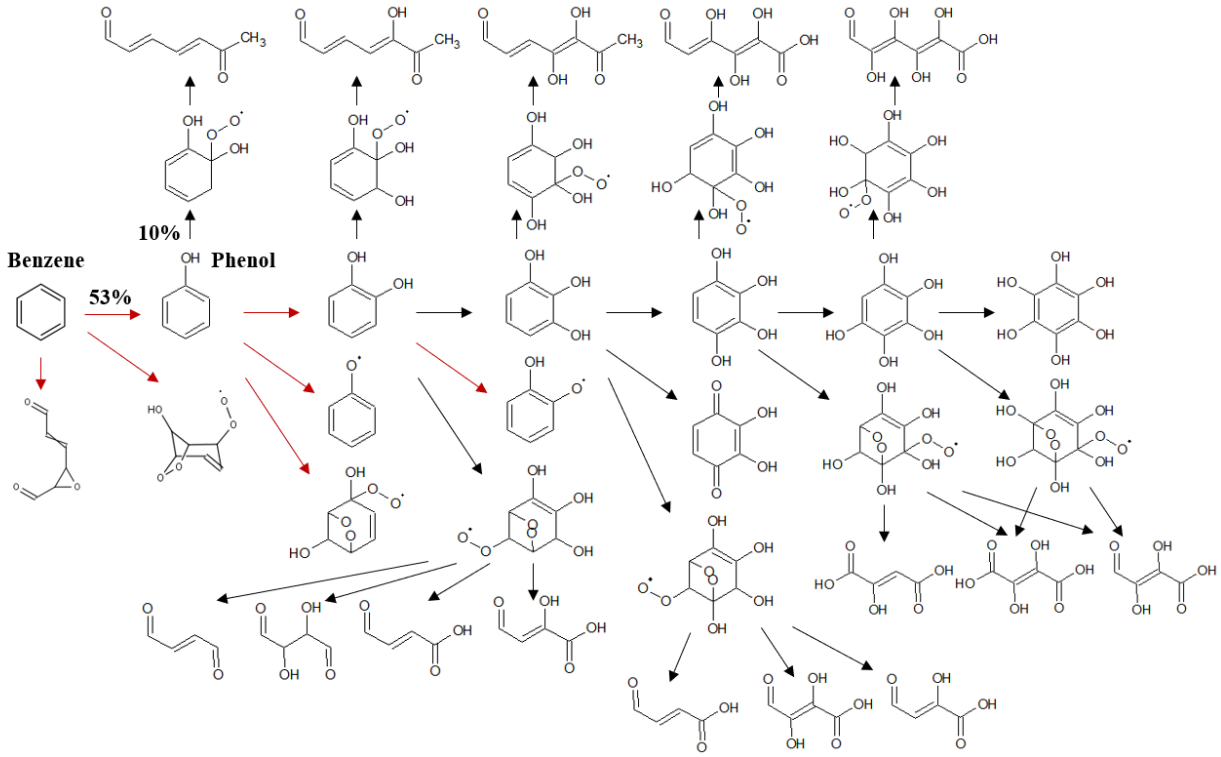


Figure S2. The benzene and phenol oxidation mechanisms to form low volatility products originating from multi-hydroxybenzenes.

Section S4. The mechanisms to produce a phenoxy radical in aqueous aerosol

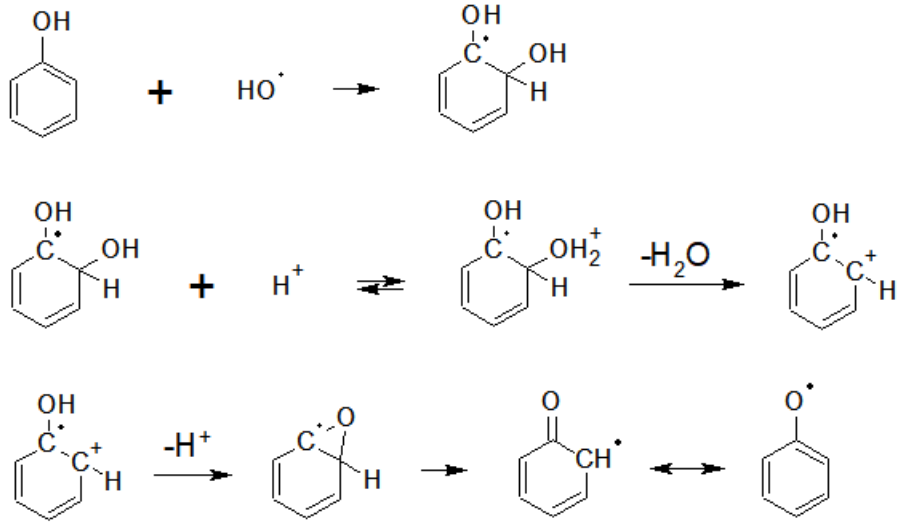


Figure S3. The scheme of phenol oxidation path to form phenoxy radicals in aqueous phase.

OH radical formation in aqueous aerosol

The radical species produced in gas phase and ozone can be partitioned to aqueous phase. K_p denotes the gas-particle partitioning constant and K_a, the acid dissociation constant. Additionally, radicals can be produced via the photolysis of H_2O_2 and HONO, or aqueous phase reaction (Liang and Jacobson, 1999). k_{aq} denotes the reaction rate constant of a radical in aqueous phase and k_{ph}, the photolysis rate constant of chemical species. Term V = NA×V(aq), where Na (6.022×1023molecule mol-1) is the Avogadro constant and V(aq) (L cm-3) is the volume concentration of inorganic salt seeded aqueous phase in the air.

$OH\ (g) \leftrightarrow OH\ (aq)$ $K_{p,OH} = 4.58\times10^{-20}\exp(5250/T) \times T/(V(aq)\rho in)$ (SR1)

(Hanson et al., 1992; Jacob, 1986)

$HO_2(g) \leftrightarrow HO_2(aq)$ $K_{p,HO_2} = 3.95\times10^{-20}\exp(6600/T) \times T/(V(aq)\rho in)$ (SR2)

(Hanson et al., 1992; Jacob, 1986)

$O_3\ (g) \leftrightarrow O_3\ (aq)$ $K_{p,O_3} = 3.07\times10\text{-}19\exp(2380/T) \times T/(V(aq)\rho in)$ (SR3)

(Chameides, 1984; Jacob, 1986)

$HO_2(aq) \leftrightarrow O_2^- + H^+$ $K_{a,HO_2} = 1.17\times10^{-3}\exp(-1046.4/T)$ (SR4)

(Bielski et al., 1985)

$HO_2(aq) + HO_2(aq) \rightarrow H_2O_2(aq) + O_2(aq)$ $k_{aq,S5}$ = 7.14×10^{9}exp(-2700/T)/V (SR5)

(Bielski et al., 1985)

$O_2^- + O_3(aq) \rightarrow OH(aq) + OH^- + 2O_2(aq)$ $k_{aq,S6}$ = 2.30×10^{11}exp(-1500/T)/V (SR6)

(Sehested et al., 1983; Bielski et al., 1985)

$H_2O_2(aq) + h\nu \rightarrow 2OH(aq)$ k_{ph,H_2O_2} = j[H_2O_2_to_OH] (SR7)

(Lin et al., 1978; Molina and Molina, 1981; Nicovich and Wine, 1988)

$HONO(aq) + h\nu \rightarrow OH(aq) + NO(aq)$ $k_{ph,HONO}$ = j[HONO_to_OH] (SR8)

(Bongartz et al., 1991; Atkinson et al., 1997)

Phenoxy radical formation via the reaction with an OH radical in aqueous aerosol

$C_6H_5OH\ (g) \rightarrow C_6H_5OH\ (aq)$ $K_p = 2.89 \times 10^{-5}$ (SR9)

(Dohnal and Fenclova, 1995; Abd-El-Bary et al., 1986)

$OH\ (aq) + C_6H_5OH\ (aq) \rightarrow HO\text{-}C_6H_5^{\bullet}OH\ (aq)$ $k_{aq,S10} = 6.6 \times 10^9\ M^{-1}\ s^{-1}$ (SR10)

(Ross et al., 1998)

$HO\text{-}C_6H_5^{\bullet}OH\ (aq) \rightarrow C_6H_5O^{\bullet}\ (aq) + H_2O$

$k_{aq,S11} = 2.0 \times 10^6\ s^{-1}$ (for *p*-adduct $k = 1.8 \times 10^3 s^{-1}$) (SR11)

(Mvula et al., 2001; Das, 2005)

$HO\text{-}C_6H_5^{\bullet}OH\ (aq) \xrightarrow{H^+} C_6H_5O^{\bullet}\ (aq) + H_2O$

$k_{aq,S12} = 2.0 \times 10^7\ M^{-1}\ s^{-1}$ (for *o- & p- adduct* $k = 6.7 \times 10^8\ M^{-1}\ s^{-1}$) (SR12)

(Mvula et al., 2001; Das, 2005)

Phenoxy radical formation via irradiation under UV light

$ArOH \xrightarrow{h\nu} Ar^{\bullet+}OH - e^-$ (SR13)

(Siano et al., 2020)

$Ar^{\bullet+}OH \xrightarrow{k_H} ArO^{\bullet} + H^+$ (SR14)

(Dixon and Murphy, 1976; Siano et al., 2020)

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