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Review Article

Coupled VOC Oxidation Pathways and the Integrated Formation of Tropospheric Ozone and Secondary Organic Aerosols: A Systematic Review of Mechanistic Insights and Modelling Challenges

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ABSTRACT

Volatile organic compounds (VOCs) are key precursors of both tropospheric ozone and secondary organic aerosols (SOA), which are two major air pollutants in the troposphere. O_3 and SOA are often treated as two different species and are studied independently, while evidence of their formation coupling through shared VOC oxidation pathways is growing. Here, we performed a systematic review according to the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2020) guidelines to summarize current understanding of the mechanistic links between VOC oxidation, ozone formation and SOA production. A total of 3,425 articles retrieved from Web of Science, Scopus and Google Scholar were screened, and 36 peer-reviewed papers were selected based on defined criteria for qualitative synthesis. The review found that organic peroxy radical ($.RO_2$) is an important intermediate that dictates the competition between ozone producing pathways and aerosol forming pathways. It was shown that elevated NOx concentrations favours O_3 formation through the RO_2 + NOx reaction, whereas low-NOx conditions lead to autoxidation and $RO_2 + HO_2$ pathways that favour the formation of highly oxygenated organic molecules (HOMs) and SOA mass. The review also identified several persistent challenges with atmospheric models such as the incomplete treatment of intermediate-volatility organic compounds (IVOCs), uncertainties in RO_2 branching chemistry and shortcomings in multiphase process and autoxidation mechanism representations. The results demonstrate the necessity for integrated multi-pollutant control strategies and robust atmospheric models that represent the coupled O_3-SOA system. We link gas-phase oxidation chemistry and aerosol microphysics to provide an overall framework to advance air quality forecast and climate forcing estimate.

INTRODUCTION

The troposphere acts as a massive chemical reactor in which the oxidation of volatile organic compounds (VOCs) controls atmospheric chemistry. VOCs are released to the atmosphere from both biogenic and anthropogenic sources and follow complicated chemical transformation pathways, primarily initiated by hydroxyl radicals (OH), nitrate radicals (NO_3) and ozone (O_3) (Atkinson & Arey, 2003). These oxidation processes form the basis of simultaneous tropospheric ozone and secondary organic aerosol (SOA) formation, which are among two of the most significant issues in contemporary atmospheric chemistry (Hallquist et al., 2009). Ozone, in the troposphere, is both a greenhouse gas and an oxidant which negatively affects human health such as respiratory effects and agriculture such as impacts on crop yields (Monks et al., 2015). SOA forms a large component of fine particulate matter ($PM_{2.5}$) which influences radiative balance through scattering and absorption, and can cause cardio-vascular problems (Shrivastava et al., 2017). Due to the dual impact of tropospheric ozone and SOA, the chemical life cycle of VOCs needs to be understood in order to mitigate air pollution and climate change issues.

Although scientific research on the role of VOCs in atmospheric chemistry has been ongoing for decades, the formation of ozone and SOA have traditionally been isolated into distinct and non-interacting research fields. This has contributed to a piecemeal understanding of their coupled formation pathways and of their competition for key chemical intermediates. The ratio in which RO_2 key intermediate in VOC oxidation branches, for example, depends strongly on the nitrogen oxide (NOx) regime, but the non-linear interactions of the reaction mixtures in complex VOC sources have yet to be thoroughly characterized (McFiggans et al., 2019). Additionally, discrepancies exist between observations from laboratory experiments and predictions from atmospheric models. The most common chemical transport models use oversimplified surrogate mechanisms to represent critical reaction steps such as autoxidation, which produce highly oxygenated organic molecules (HOMs), and multiphase reactions taking place on particle surfaces (Ehn et al., 2014; Pye et al., 2010). The ability of the models to reproduce observations of SOA mass and oxidative potential, and the ability to accurately simulate sensitivity of ozone to changing precursor emissions in rapidly changing environments, remains poor.

There is an urgent need for an integrated mechanistic synthesis that bridges the gap between gas-phase kinetics and aerosol microphysics. Developing a unified perspective on the O_3 SOA nexus is scientifically imperative to resolve the missing SOA mass problem and to refine our understanding of atmospheric oxidative capacity. Such integration is of paramount importance for air quality policy, as emission control strategies must account for the co-benefits or potential trade-offs between reducing ozone and particulate matter (Zhu et al., 2025). This is particularly relevant for rapidly urbanizing regions, such as the Global South and East Asia, where complex "air pollution complexes" involve high concentrations of both NOx and diverse VOC species. Improved predictive capabilities are essential for designing robust climate forcing projections and effective public health interventions in these vulnerable regions.The objective of this review is to provide a comprehensive synthesis of the coupled pathways of VOC oxidation and their dual role in O_3 and SOA formation. This paper systematically evaluates the fundamental mechanistic links between gas phase radical chemistry and aerosol precursors, the influence of NO_x regimes and autoxidation on coupling efficiency and the prevailing limitations in current modelling frameworks. By identifying these critical constraints, the review aims to provide a roadmap for future experimental and computational research to improve the accuracy of atmospheric chemistry simulations.

MATERIALS AND METHODS

Literature Search Strategy

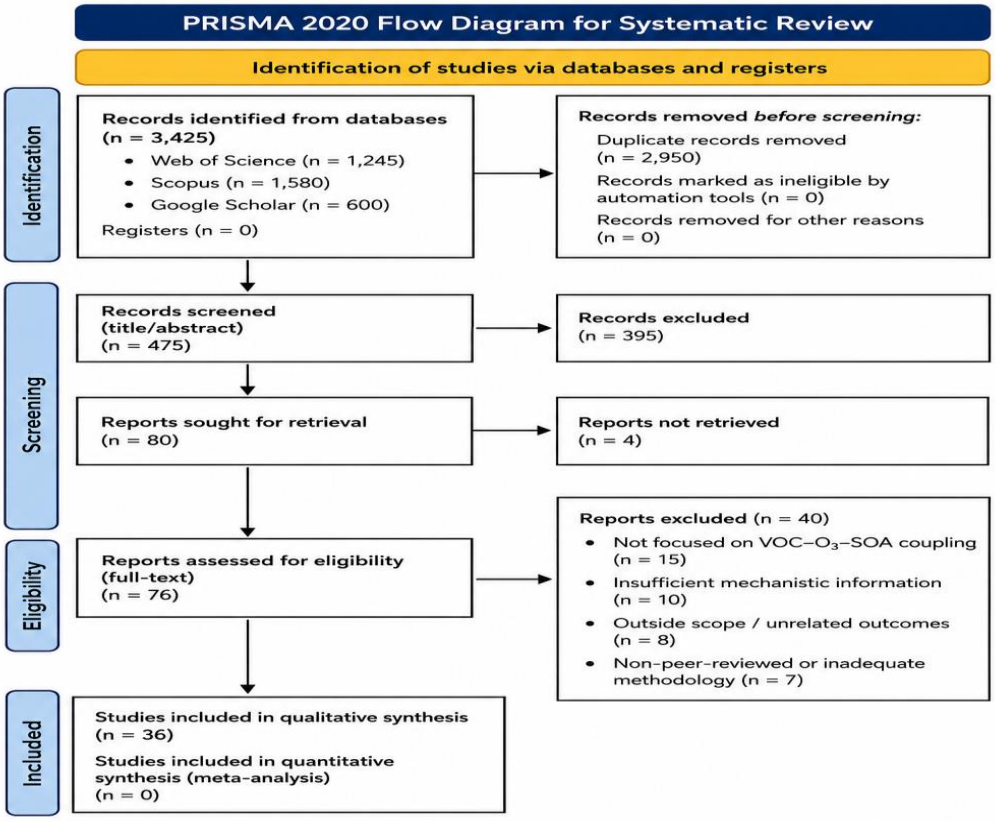
This review systematically identified, assessed, and integrated the existing literature pertaining to the coupled processes of VOC oxidation, ozone production, and SOA formation. Literature was identified through the use of electronic database searching of three major scientific journals: Web of Science, Scopus and Google Scholar. Searches were implemented through the use of Boolean operators (AND/OR) and the following terms: "VOC oxidation", "secondary organic aerosol (SOA) formation", "ozone photochemistry", "peroxy radical (RO) branching", "autoxidation", "atmospheric chemical transport models".

Inclusion and Exclusion Criteria

In order to reflect the current knowledge and scientific development of the field, the scope of the search was limited to peer-reviewed papers published between 2000 and 2025 to ensure that recent advancements in the field are included; such as the detection of HOMs and the determination of NOx dependent branching ratios. The criteria of selecting papers for this study included a central interest in gas or multiphase VOC oxidation mechanisms; direct reference to linkage between O_3 and SOA precursor chemistry; or analysis of the chemical mechanisms in numerical modelling schemes. Articles excluded were non-peer-reviewed literature (excluding key government reviews, such as IPCC), articles that exclusively analyse the indoor air chemistry without relation to the atmosphere, and articles without mechanistic description.

Screening and Selection Process

The selection procedure was conducted in line with Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) recommendations to maintain transparency and reproducibility (Page et al., 2021). Initial outputs were screened by title and abstract to exclude duplicates and ineligible studies, followed by full text eligibility review. Out of the total records identified and screened, 36 studies met the eligibility criteria and were retained for the final qualitative synthesis.



This PRISMA 2020 flow diagram shows the selection process of studies included in this systematic review on the mechanistic links between volatile organic compound (VOC) oxidation, tropospheric ozone (O_3), and secondary organic aerosol (SOA) formation.

Source: Page, M. J., McKenzie, J. E., Bossuyt, P. M., Boutron, I., Hoffmann, T. C., Mulrow, C. D., et al. (2021). The PRISMA 2020 statement: an updated guideline for reporting systematic reviews. *BMJ, 372*, n71. https://doi.org/10.1136/bmj.n71

Figure 1: PRISMA 2020 flow diagam for systematic review

Data Extraction and Synthesis Approach: Data were extracted and categorized using a thematic synthesis approach, focusing on three core dimensions of the VOC–O_3–SOA triad:

1. ***VOC Classification***: Differentiation between biogenic VOCs (isoprene, monoterpenes) and anthropogenic VOCs (aromatics, alkanes).
2. **Chemical Regimes:** Analysis of oxidation pathways under varying NOx concentrations (high-NOx vs. low-NOx/HO_2-dominated regimes).
3. ***Mechanistic Pathways***: Comparison of traditional multigenerational oxidation versus rapid autoxidation and the role of intermediate volatility organic compounds (IVOCs).

Modelling Assessment Framework

An important part of the methodology was an aggregation of modelling problems. This was performed by categorizing the models based on the complexity of their treatment of chemistry, varying from the fully explicit mechanisms such as Master Chemical Mechanism (MCM) down to the reduced/surrogate mechanisms, like the Volatility Basis Set (VBS) used in 3D CTMs. Through these categories, it was possible to isolate consistent biases in the current modeling of atmospheric oxidative capacity and aerosol mass loading.

RESULTS AND DISCUSSION

VOC Oxidation Mechanisms

Initiation of VOC Oxidation

Three main oxidants, the hydroxyl radical (OH), the nitrate radical (NO_3) and ozone (O_3), initiate the degradation of VOCs in the troposphere. OH radicals, otherwise known as the atmospheric detergent, drive most VOC oxidation during the daytime with rate constants with OH radicals (k OH) usually in the collision-limited regime ($1x10^{-10}$ cm^3 $molecule^{-1}$ s^{-1} for isoprene) (Atkinson & Arey, 2003). NO_3 radicals at night time become the main sink for unsaturated VOCs (specifically biogenic monoterpenes) and produce organic nitrates which can act as storage reservoirs for reactive nitrogen (Ng et al., 2017). Ozone reacts with only alkenes by cycloaddition into the C=C double bond to form primary ozonides which break down into Criegee intermediates (CIs), which can then form OH radicals or lead to particle formation (Ziemann & Atkinson, 2012).

Formation and Fate of Peroxy Radicals (RO_2)

Following the initial hydrogen abstraction or radical addition, the resulting alkyl radical (R·) reacts near instantaneously with molecular oxygen (O_2) to form organic peroxy radicals (RO_2). The RO_2 radical is the pivotal intermediate that links VOC degradation to both ozone and SOA production (Orlando & Tyndall, 2012). The chemical fate of RO_2 is determined by a competitive branching network influenced heavily by the local chemical environment, specifically the concentrations of NO, HO_2, and other RO_2 radicals.

NOx-Dependent Branching and Ozone Production

In NOx rich environments, typical of urban plumes, the dominant pathway is the reaction of RO_2 with nitric oxide (NO). This reaction primarily produces an alkoxy radical (RO) and nitrogen dioxide (NO_2):

$RO_2 + NO \rightarrow RO + NO_2$

The subsequent photolysis of NO_2 yields atomic oxygen, which reacts with O_2 to form tropospheric ozone. This sequence establishes the catalytic cycle of O_3 production. However, a minor branching channel in the RO2 + NO reaction produces organic nitrates ($RONO_2$), which effectively terminates the radical chain and sequesters NOx, thereby limiting ozone production potential (Wennberg et al., 2018). The branching ratio between these two channels is a critical parameter in modeling the non-linear sensitivity of O_3 to VOC and NOx emissions.

Autoxidation and the Formation of HOMs

In recent years, the discovery of rapid unimolecular autoxidation has shifted the paradigm of VOC oxidation, particularly for biogenic species like α-pinene and isoprene. Under conditions where bimolecular reactions (with NO or HO_2) are sufficiently slow, RO_2 radicals can undergo internal hydrogen shifts (H-shifts) followed by sequential oxygen addition (Crounse et al., 2013). This process, known as autoxidation, rapidly increases the oxygen-to-carbon (O=C) ratio of the molecule without carbon skeleton fragmentation.

$RO_2 \rightarrow .R'OOH \rightarrow .OO \rightarrow R'OOH$

This mechanism leads to the formation of Highly Oxygenated Organic Molecules (HOMs), which possess extremely low vapour pressures (ELVOCs) and are capable of driving new particle formation and rapid SOA growth (Ehn et al., 2014). Autoxidation rates are highly temperature dependent and vary significantly with the molecular structure of the precursor VOC, representing a major frontier in mechanistic atmospheric chemistry (Bianchi et al., 2019).

Low-NOx Pathways and SOA Precursors

In pristine or low-NOx environments, RO_2 radicals predominantly react with hydroperoxy radicals (HO_2) to form organic hydroperoxides (ROOH):

$RO_2 + HO_2 \rightarrow ROOH + O_2$

ROOH species are significant contributors to SOA mass, as they are often less volatile than their precursors and can undergo further condensed phase reactions (Hallquist et al., 2009). Additionally, RO_2–RO_2 cross reactions can lead to the formation of alcohols, carbonyls, or even covalently bonded dimers (R−OO−R). These dimers are particularly important for SOA as they represent high-molecular-weight species that partition effectively into the aerosol phase (Shrivastava et al., 2017).

Table 1: Atmospheric Reaction Rate Constants (At 298 K) and Dominant Products for Key VOC Classes

VOC Class	Reactant	Rate Constant (k) (cm3 molecule-1 s-1)	Dominant Product(s)	Reference
Isoprene (C_5H_8)	OH	1.0×10^{-10}	MVK, MACR, Formaldehyde	Atkinson & Arey (2003)
	O_3	1.2×10^{-17}	Criegee Intermediates, OH	Atkinson & Arey (2003)
	NO_3	6.0×10^{-13}	Isoprene Nitrooxy Hydroperoxides	Ng et al. (2017)
Monoterpenes (alpha-Pinene)	OH	5.3×10^{-11}	Pinonaldehyde, HOMs	Atkinson & Arey (2003)
	O_3	8.6×10^{-16}	Highly Oxygenated Molecules (HOMs)	Ehn et al. (2014)
	NO_3	6.1×10^{-12}	Organic Nitrates, SOA Precursors	Ng et al. (2017)
Aromatics (Toluene)	OH	5.6×10^{-12}	Benzaldehyde, Cresols, Epoxides	Atkinson & Arey (2003)
	O_3	$< 1.0 \times 10^{-20}$	Negligible in Troposphere	Atkinson & Arey (2003)
	NO_3	7.0×10^{-17}	Nitrotoluene	Atkinson & Arey (2003)
Alkanes (n-Butane)	OH	2.4×10^{-12}	Alkyl Radicals, Carbonyls	Atkinson & Arey (2003)
	O_3	$< 1.0 \times 10^{-20}$	Negligible in Troposphere	Atkinson & Arey (2003)
	NO_3	4.6×10^{-17}	Alkyl Nitrates	Atkinson & Arey (2003)

Tropospheric Ozone Formation

The Fundamental NO–NO_2–O_3 Cycle

Tropospheric ozone is produced through the photolysis of NO_2. In a simple system containing only nitrogen oxides, ozone is at the photo stationary state known as the Leighton cycle, in which NO_2 photolysis generates atomic oxygen, which in turn reacts with O_2 to produce ozone. In turn, ozone reacts with nitric oxide (NO) to re-form NO_2, leaving no net increase in ozone (Monks et al., 2015). There is net production of ozone only when oxidation of VOCs short-circuits this cycle by re-oxidizing NO to NO_2 with no consumption of an ozone molecule (Seinfeld & Pandis, 2016) by means of the production of peroxy radicals (RO_2 or HO_2).

Radical Propagation and Termination

The HOx radical cycle (OH + HO_2 + RO_2) governs the propagation and termination of tropospheric ozone formation. The cycle is initiated primarily by OH reactions with VOCs, producing peroxy radicals (RO_2), which are subsequently converted to HO_2 and recycled back to OH through reaction with NO, sustaining ozone production. Radical termination occurs when reactive species are removed from the cycle. Under high NOx conditions, a major termination pathway involves the reaction between hydroxyl radicals and nitrogen dioxide, forming nitric acid (HNO_3):

$OH + NO_2 \rightarrow HNO_3$

This reaction effectively removes both OH and NOx from the active photochemical cycle, thereby limiting further ozone production (Thornton et al., 2002).

Under low-NOx conditions, termination is more likely to occur through radical-radical reactions, particularly the recombination of HO_2 and RO_2 species, forming peroxides and organic accretion products that reduce radical availability.

VOC–NOx Sensitivity Regimes

The relationship between O_3, NOx, and VOCs is non-linear and is characterized by two distinct chemical regimes. In the NOx-limited regime (common in rural areas), O_3 production increases with increasing NOx and is relatively insensitive to VOCs. In the VOC limited (or radical-limited) regime (typical of urban centers), high NOx concentrations suppress O_3 formation by scavenging OH radicals. In this regime, reducing NOx can lead to an increase in O3, whereas reducing VOCs is the most effective control strategy (Sillman, 1999).

Ozone Production Efficiency (OPE)

A critical metric for assessing the coupling between NOx and O_3 is the Ozone Production Efficiency (OPE), defined as the number of O_3 molecules produced per molecule of NOx oxidized to terminal sinks. OPE is higher in rural areas (ranging from 10 to 20) where NOx is low and VOCs are abundant, and lower in polluted urban plumes (ranging from 2 to 7) due to the rapid removal of radicals by NO_2 (Kleinman et al., 2002; Monks et al., 2015). Understanding OPE variability is essential for evaluating how VOC oxidation drives the regional ozone budget.

Table 2: Ozone Formation Efficiencies and Yields for Representative VOCs

VOC	NOx Regime	O_3 Yield (molecules O_3 / molecule VOC)	Temperature / Humidity Conditions	Reference
Methane (CH_4)	Low NOx (Remote)	~0.5 – 1.0	Global average; Variable RH	Monks et al. (2015)
	High NOx (Polluted)	~3.5 – 4.0	Global average; Variable RH	Seinfeld & Pandis (2016)
Ethane (C_2H_6)	High NOx	~2.0	298 K; Dry (<10% RH)	Carter (2010)
n-Butane (C_4H_{10})	High NOx	~2.5 – 3.0	300 K; Moderate RH	Jenkin et al. (2015)
Isoprene (C_5H_8)	Low NOx	~0.8 – 1.5	303 K; High RH (Tropical)	Wennberg et al. (2018)
	High NOx	~3.0 – 5.0	298 K; 40–60% RH	Monks et al. (2015)
alpha-Pinene ($C_{10}H_{16}$)	High NOx	~3.0 – 4.5	295 K; 50% RH	Carter (2010)
Toluene (C_7H_8)	High NOx	~2.8 – 4.0	298 K; Dry to Moderate RH	Carter (2010)
Formaldehyde (HCHO)	High NOx	~1.5 – 2.0	Photolysis-driven; Variable	Seinfeld & Pandis (2016)

Secondary Organic Aerosol (SOA) Formation

Gas-Particle Partitioning Theory

Partitioning of SVOCs between gas and particle phase is a key process controlling SOA formation. The tendency for an oxidation product to partition into the particle phase is a thermodynamic property and is controlled by the partition coefficient (Kp) which is inversely related to the compound's saturation vapor pressure (Pankow, 1994; Kroll & Seinfeld, 2008). As a VOC is oxidized it develops more polar functional groups such as -OH, -COOH and -OOH which systematically decrease the vapor pressure of the carbon backbone. SOA formation then occurs as these products nucleate from vapor or dissolve into existing organic aerosol organic mass, when their concentrations exceed saturation (Hallquist et al., 2009).

Formation of Low-Volatility Products (LVOCs and ELVOCs)

The partitioning framework has been recently extended to a larger range of volatilities. With the VBS (Volatility Basis Set) scheme, organic vapors are grouped into 'bins' according to their effective saturation concentrations (Donahue et al., 2006). It is now known that a large amount of SOA mass may originate from Extremely Low Volatility Organic Compounds (ELVOCs) and Low Volatility Organic Compounds (LVOCs). Such molecules are often generated through the autoxidation mechanism mentioned in section

3.1.4, and may transfer onto the particle phase permanently regardless of the background aerosol mass (Ehn et al., 2014). The formation of Highly Oxygenated Organic Molecules (HOMs) is extremely rapid and this allows relatively small precursors VOCs to contribute to SOA mass early in the oxidation chain rather than much later, as traditionally thought using multi-generational aging mechanisms (Bianchi et al., 2019).

Aqueous-Phase and Heterogeneous Reactions

Apart from physical partitioning, SOA mass is dramatically increased through chemical reactions either in the condensed phase or gas-particle interface. High yields of small water-soluble carbonyls, such as glyoxal and methylglyoxal, are produced through the oxidation of isoprene and aromatics, and can dissolve in cloud droplets or aqueous deliquesced particles. After entering the aqueous phase, these products undergo oligomerization, oxidation and acid-catalyzed reactions, resulting in non-volatile species after water evaporation (Ervens et al., 2011). Moreover, heterogeneous reactions, such as uptake of Criegee intermediates, or acid-catalyzed reactive uptake of isoprene-derived epoxydiols (IEPOX) lead to huge SOA yields bypassing gas-phase partitioning constraints (Surratt et al., 2010).

Role of Organic Nitrates and Peroxides

The chemical composition and mass yields of SOA are sensitive to the oxidant used, and critically to the NOx regime. Under low NOx conditions, the RO_2 + HO_2 pathway results in organic hydroperoxides (ROOH), which can be dominant products of biogenic SOA because they are less volatile and can react further in the condensed phase (Kroll & Seinfeld, 2008). In contrast, under high-NOx conditions the RO_2 + NO pathway produces organic nitrates ($RONO_2$). While smaller organic nitrates are likely to be sufficiently volatile to exist in the gas phase, higher order organic nitrates formed from long-chain alkanes and monoterpenes are sufficiently non-volatile to be partitioned into the aerosol phase (Ng et al., 2017). These nitrates contribute to the overall mass yield of SOA, and provide a temporary or permanent sink for reactive nitrogen, which will be important in the regional nitrogen cycle, and subsequent ozone production (Ziemann, & Atkinson, 2012).

Table 3: Secondary Organic Aerosol (SOA) Mass Yields from Representative VOC Precursors

VOC	Oxidant	Yield (%)	Conditions (T, RH, NOx)	Reference
Isoprene (C_5H_8)	OH	1% – 4%	298 K, Low NOx, Acidic Seeds	Surratt et al. (2010)
	OH	< 1%	298 K, High NOx, Dry	Kroll & Seinfeld (2008)
alpha-Pinene ($C_{10}H_{16}$)	O_3	15% – 40%	295 K, Low NOx, Dark	Hallquist et al. (2009)
	OH	10% – 25%	298 K, High NOx, Moderate RH	Ng et al. (2007)
	NO_3	10% – 15%	298 K, Night-time proxy	Ng et al. (2017)
Limonene ($C_{10}H_{16}$)	O_3	30% – 60%	298 K, Low NOx, Dry	Zhu et al. (2025)
beta-Caryophyllene ($C_{15}H_{24}$)	O_3	60% – 100%	298 K, Low NOx, Various RH	Lee et al. (2006)
Toluene (C_7H_8)	OH	5% – 15%	298 K, High NOx, Dry	Ng et al. (2007)
	OH	15% – 30%	298 K, Low NOx, Moderate RH	Shrivastava et al. (2017)
m-Xylene (C_8H_{10})	OH	10% – 25%	298 K, Low NOx, Dry	Ng et al. (2007)
n-Dodecane ($C_{12}H_{26}$)	OH	10% – 30%	298 K, Low NOx, High MW Alkane	Loza et al. (2014)

Coupled O3–SOA Formation

Shared Precursors and Radical Intermediates

The processes of tropospheric ozone and SOA formation are linked as they share a pool of precursors and intermediates. Both processes are triggered off by the same atmospheric oxidants (OH, NO_3, O_3) acting upon the same parents VOC molecules. The central linking mechanism is the peroxy radical (RO2) intermediate. In the gas phase this radical provides a pathway for ozone formation (via reaction with NO) but the chemistry which this specific RO_2 radical undertakes (either bimolecular reactions or unimolecular autoxidation) determines the volatility and degree of functionalization of the organic molecules which will form SOA (Orlando & Tyndall 2012). Recent work has shown that in mixtures the species will compete for these radical species and a non-linear cocktail effect will occur whereby the presence of one VOC will lead to either increase or decrease in either SOA yield or ozone production potential of another VOC (McFiggans et al 2019).

Competition between Reaction Pathways

The coupling is characterized by a direct competition between reaction pathways that favor either O_3 or SOA. This competition is primarily modulated by the NOx concentration. In high-NOx urban environments, the reaction of RO_2 with NO is prioritized, maximizing O_3 production. However, this same pathway can lead to the fragmentation of the organic carbon skeleton, creating smaller, more volatile products that are less likely to form SOA. Conversely, in low-NOx or NO depleted conditions, RO_2 radicals react preferentially with HO_2 or undergo autoxidation, pathways that preserve or increase the carbon chain length and oxygen content, thereby maximizing SOA mass (Kroll & Seinfeld, 2008). This mechanistic see-saw implies that air quality strategies aimed at reducing NOx to control ozone may inadvertently increase the formation of SOA by shifting RO2 radicals toward aerosol-productive pathways (Shrivastava et al., 2017).

Influence of Environmental Variables

Environmental variables including temperature, relative humidity (RH) and solar radiation act as double-edged swords in O_3-SOA coupling. Particularly for temperature, it increases VOC emissions rate (particularly biogenic isoprene and terpene) and H-shift reaction rate in autoxidation (resulting in more rapid cycling of O_3 and fast formation of HOMs for SOA (Ehn et al., 2014)). However, elevated temperatures promote the re-partitioning of semi volatile compounds into gas phase, which might decrease SOA mass yet ensure the availability of precursors for other O3-producing oxidation. In terms of RH, it contributes to O_3-SOA linkage in terms of providing aqueous phase for multiphase chemistry where water-soluble O_3 oxidation products (Glyoxal) would be turned into SOA mass, leading to reduced atmospheric oxidative capacity (Ervens et al., 2011).

Feedback Mechanisms and Radiative Effects

An important though often overlooked aspect of the coupling is the feedback between the gas and particle phase. Once SOA has been formed, it affects ozone photochemistry in a number of ways. Firstly, SOA scatters and absorbs sunlight and so affects the photolysis rate (J - value) of NO_2 and O_3 which has a direct effect on the production rate of O_3 (Zhu et al., 2025). Secondly, there are potential sink sites at the surface of organic aerosols for HO_2, NO_3 and N_2O_5. Removal of radicals from the gas phase via heterogeneous uptake onto SOA can remove radicals that would otherwise contribute to the O3 production cycle (Pye et al., 2010). Thus the aerosol-chemistry feedback implies that O3 and SOA are not simply co-pollutants but are inter-linked and can effectively control one another through these processes.

Table 4: Comparative Analysis of Atmospheric Conditions Favouring Ozone (O_3) Versus Secondary Organic Aerosol (SOA) Formation

Condition (T, RH, NOx, VOC type)	Favoured Product	Mechanistic Explanation	Reference
High NOx (Urban/Industrial)	O_3	RO_2 + NO reaction dominates, producing NO2 which photolyzes to O_3; high NOx promotes carbon fragmentation, reducing SOA yields.	Monks et al. (2015); Kroll & Seinfeld (2008)
Low NOx (Rural/Remote)	SOA	RO_2 + HO_2 or RO_2 + RO_2 reactions dominate, forming peroxides and alcohols with lower volatility than products of NO-pathways.	Shrivastava et al. (2017); Hallquist et al. (2009)
High Temperature (>30°C)	O_3	Increased biogenic emissions (isoprene) and faster radical initiation; thermal instability of PANs releases NOx to participate in O_3 cycling.	Akimoto (2016); Monks et al. (2015)
High Relative Humidity (>70%)	SOA (aqSOA)	Facilitates aqueous-phase processing of water-soluble carbonyls (e.g., glyoxal) and reactive uptake of IEPOX into deliquesced particles.	Ervens et al. (2011); Surratt et al. (2010)
Low NOx + Low T	SOA	Favors rapid autoxidation and formation of HOMs; lower temperatures significantly decrease the vapor pressure of semi-volatile compounds.	Ehn et al. (2014); Bianchi et al. (2019)
High VOC:NOx Ratio	SOA	Radical-radical termination becomes competitive with NO reactions; promotes functionalization over fragmentation.	McFiggans et al. (2019); Seinfeld & Pandis (2016)
Low VOC:NOx Ratio	O_3	Radical-limited regime where O_3 production is sensitive to VOC levels; high NO_2 scavenges OH, suppressing both O_3 and SOA.	Sillman (1999); Zhu et al. (2025)
Large/Cyclic VOCs (terpenes, aromatics)	SOA	High carbon number and structure allow for multiple functionalization steps and lower saturation vapor pressures.	Atkinson & Arey (2003); Hallquist et al. (2009)
Small Alkanes (ethane, propane)	O_3	Oxidation products (e.g., formaldehyde) are too volatile to condense but highly efficient at driving the catalytic NOx cycle.	Atkinson & Arey (2003); Jenkin et al. (2015)

Modelling Approaches and Challenges

Representative Chemical Mechanisms: From Explicit to Reduce

To evaluate the performance of chemical mechanisms within atmospheric models for VOC-O_3-SOA system, mechanisms varying in complexity are commonly used. The MCM provides near-explicit representation of atmospheric oxidation of hundreds of primary VOCs, with thousands of elementary reactions involved (Jenkin et al., 2003; Jenkin et al., 2015). This highly detailed mechanism is most suitable for box model simulation and inter-comparison, but too intensive for direct application to 3D CTMs. In the CTM application, a simplified mechanism (SAPRC mechanism or CB6 mechanism) is commonly adopted instead. This type of mechanism reduces the complexity through lumping of VOCs into groups with common carbon bond type or reactivities (Carter & Heo, 2013). Such aggregation often causes oversimplification that fails to retain the required structural information for producing low volatility SOA precursors correctly and hence resulting in the discrepancy between simulated and observed aerosol mass (Ziemann, & Atkinson, 2012).

VOC Representation and Missing Reactivity

An important limitation in modelling efforts is the lack of representation of the VOC precursor pool. Conventional modelling has primarily considered light NMVOCs (non-methane volatile organic compounds), yet often lacks adequate representation of IVOCs and SVOCs. These groups, frequently produced by the emission from diesel exhaust or from consumer goods, have significantly higher SOAs yields than the lighter alkanes (Robinson et al., 2007). This problem is then exacerbated by the missing OH reactivity problem, identified in many field studies in which measured total OH reactivity has been larger than the sum of measured VOC reactivity; the implication of this problem is that organic precursors are unaccounted for, directly affecting the simulations of both O_3 and SOAs, as the radical budget cannot be well constrained (Mao et al., 2012).

SOA Parameterization and Volatility Basis Set (VBS) Limitations

The initial representation of SOA relied on a two-product model which was derived from yields measured in chamber experiments. The development of the Volatility Basis Set (VBS), which segregates organic compounds into bins of equivalent saturation concentrations (Donahue et al. 2006), has largely supplanted this. Though a significant improvement in capturing the evolution and dilution of SOA, the VBS method has limitations in representing fast autoxidation and formation of Extremely Low Volatility Organic Compounds (ELVOCs). Most common CTM representations of the VBS method do not explicitly consider the formation of Highly Oxygenated Organic Molecules (HOMs) from biogenic compounds, resulting in a persistent underprediction of SOA at remote locations (Shrivastava et al. 2017). Furthermore, parameterizations are being developed which can handle multiphase reactions (e.g., the acid-catalyzed reaction of isoprene products) but the implementation is still computationally intensive and inherently uncertain (Pye et al. 2010).

Uncertainties in Radical Chemistry and NOx Sensitivity

The accuracy of O_3–SOA coupling in models is highly sensitive to the representation of peroxy radical (RO_2) chemistry. Many reduced mechanisms use simplified branching ratios for the RO_2 + NO vs. RO_2 + HO_2 pathways, which may not hold true under the complex, fluctuating NOx regimes of transitional urban-to-rural areas (McFiggans et al., 2019). Furthermore, recent discoveries regarding HOx recycling in the oxidation of isoprene have forced a re-evaluation of radical budgets in low-NOx, high-isoprene environments. Models that fail to account for these recycling mechanisms tend to underestimate OH concentrations, subsequently under predicting the rate of both O_3 production and SOA precursor formation (Wennberg et al., 2018).

Box Models vs. Chemical Transport Models (CTMs)

The choice of modelling scale involves a trade-off between chemical complexity and physical realism. Zero-dimensional box models (e.g., MCM-based simulations, Jenkin et al., 2015) can explicitly represent detailed gas-phase chemistry, making them suitable for chamber studies and mechanistic interpretation at a single location. However, they cannot represent spatial gradients or transport processes. In contrast, chemical transport models (CTMs), such as GEOS-Chem, CMAQ, and WRF-Chem, are three-dimensional (3D) Eulerian models with an explicit time dimension, used to simulate the spatiotemporal evolution of atmospheric composition. These models are therefore often described as 3D CTMs (with temporal integration) rather than “4D CTMs,” a term that may cause confusion in atmospheric chemistry literature. Although CTMs provide the necessary framework for regional and global air quality and climate applications, they rely on simplified chemical mechanisms due to computational constraints (Seinfeld & Pandis, 2016). This introduces limitations in representing fast-forming intermediates such as ELVOCs and multiphase autoxidation chemistry. Emerging hybrid approaches, including machine-learning emulators and nested chemical schemes, offer promising pathways to improve chemical realism while retaining computational efficiency.

Table 5: Comparison of major atmospheric chemical mechanisms used in O_3 and SOA modelling

Mechanism	VOC Coverage	O_3 Representation	SOA Formation Treatment	Limitations	Reference
MCM (Master Chemical Mechanism)	Very High: Near-explicit; >140 primary VOCs and >17,000 reactions.	Highly detailed radical propagation; explicit branching ratios for O3 cycling.	Provides explicit precursor concentrations; usually coupled with external VBS or partitioning modules.	Computationally prohibitive for 3D Chemical Transport Models (CTMs); mostly used for box models.	Jenkin et al. (2015)
SAPRC (Statewide Air Pollution Research Center)	Moderate: Lumped by chemical reactivity and structural characteristics.	Optimized for VOC–NOx sensitivity; excellent for regulatory O3 simulations.	Integrated via VBS (Volatility Basis Set) or fixed-yield parameterizations.	Lumping may obscure specific low-volatility intermediates (e.g., HOMs) critical for SOA.	Carter & Heo (2013)
CB6 (Carbon Bond Mechanism)	Moderate: Lumped by carbon bond types (e.g., paraffinic, olefinic).	Highly efficient; designed for long-range 3D CTMs (e.g., CMAQ, CAMx).	Linked to aerosol modules (e.g., AERO6) using volatility-based surrogates.	Over-simplification of organic radical chemistry; poor representation of autoxidation pathways.	Yarwood et al. (2010)
VBS (Volatility Basis Set - *Framework*)	N/A: Often integrated into SAPRC or CB6.	Indirectly impacts O3 via radical removal during organic aging.	High: Categorizes species by saturation concentration (C*) and chemical aging.	Often lacks explicit oxidant-specific chemistry; relies on empirical chamber yields.	Donahue et al. (2006)
GECKO-A (Generator of Explicit Chem. & Kinet. of Organics)	Extreme: Fully explicit; millions of reactions generated by computer code.	Mechanistically comprehensive; covers all known radical pathways.	High: Explicitly calculates vapor pressures for all products to model partitioning.	Extreme computational demand; limited by availability of kinetic data for all species.	Aumont et al. (2005)

Discussion

Synthesis of the VOC–O_3–SOA Nexus

This consolidation of existing research has proven that tropospheric O_3 and SOA are not separate pollutants, but twin products resulting from one central VOC oxidation sequence. RO_2 serves as the linchpin between the two products, and the choice made by a particular RO_2 molecule whether to react with NO (producing O_3 and potential fragmentation) or whether to undergo self-reaction with RO_2 followed by autoxidation and reaction with HO_2 (producing aerosol mass) determines the level of oxidant capacity and aerosol loading of a particular area (Orlando & Tyndall, 2012). The separate study of these two fields has concealed the non-linear seesaw effect: in many environments, decreasing NOx concentrations to decrease ozone production will, conversely, result in an increased production of SOA as the RO_2 molecule branches toward aerosol-producing unimolecular and HO 2 reaction (McFiggans et al., 2019; Shrivastava et al., 2017).

Contrasting Urban and Biogenic Systems

A key insight from this synthesis is that O_3–SOA coupling differs fundamentally between urban and biogenic chemical regimes. Urban environments are dominated by anthropogenic VOC emissions from combustion sources and are typically characterized by high NO_x concentrations. Under these conditions, ozone formation is efficient due to rapid RO_2 + NO reactions, while SOA formation is often limited by radical fragmentation pathways and reduced autoxidation efficiency.

In contrast, biogenic environments are dominated by emissions of isoprene and monoterpenes from vegetation. Under low-NO_x conditions, these systems favor autoxidation processes and the formation of highly oxygenated organic molecules (HOMs), leading to enhanced SOA production (Ehn et al., 2014; Glasius & Goldstein, 2016; Carlton et al., 2009). At the interface between urban and biogenic systems, a mixed regime emerges where anthropogenic NO_x interacts with biogenic VOCs. In this study, this is referred to as the Anthropogenic–Biogenic Interaction (ABI) regime, defined as atmospheric conditions in which co-located anthropogenic NO_x emissions and biogenic VOC emissions interact to produce non-linear enhancements in both ozone and secondary organic aerosol formation. This ABI regime is particularly important because it produces synergistic effects, where SOA yields exceed those predicted from isolated precursor systems due to radical recycling and enhanced oxidant production.

Regional Relevance and Challenges in Developing Regions

The mechanistic coupling between O_3 and SOA is extremely relevant for fast urbanizing regions in the Global South like the Indo-Gangetic Plain and the Pearl River Delta, where high temperatures and solar insolation speed up oxidation of VOCs while a multi-pollutant cocktail comprising high NOx, SO_2 and a wide variety of VOCs establish unusual chemical regimes (Lu et al., 2018). High concentrations of ammonia and acidic aerosols found in many mega cities in China cause increased uptake of SOA oxidation products, resulting in concurrent spikes of O_3 and PM 2.5 secondary haze (Guo et al., 2014). The existing models derived from the North America or European parameterizations do not account for the severe conditions at these regions, and that represents a great lack of understanding in global modeling of chemical species.

Policy and Regulatory Implications

From a regulatory point of view the multi-pollutant control required by the integrated O_3-SOA framework implies that efforts previously aimed solely at NOx and VOC reduction in order to regulate O_3 will also have effects on $PM_{2.5}$. Since different VOC's can vary widely in their OCP and SOA yield for example, the control of a high-OCP VOC could potentially fail to significantly decrease SOA mass (Zhu et al., 2025). It is therefore essential that policy addresses and controls highly effective precursors such as aromatics and intermediate-volatility organic compounds (IVOCs) which have the largest impact on both O_3 and aerosols (Robinson et al., 2007).

Model Limitations vs. Atmospheric Complexity

On the other hand, a brief analysis of current modelling approaches shows that this complexity gap is still present. Even though near-explicit models, such as the MCM, have high mechanistic completeness, their computational costs are far too high for being used within 3D chemical transport models (CTMs), commonly used for policy-making. CTMS lack, however, enough structural detail to reproduce fast ELVOCs formation by autoxidation or multistep organic nitrates multiphase chemistry (Pye et al., 2010). The lack of observed OH reactivity, further suggests that a sizable portion of the VOC-O_3-SOA cycle is missing from current simulation schemes (Mao et al., 2012). Filling this gap likely involves developing new hybrid modelling approaches that could use machine learning for emulating computationally expensive gas-phase chemistry.

Future Research Directions

To resolve remaining uncertainties in the coupled O_3–SOA system, several key research frontiers are emerging in recent atmospheric chemistry literature. First, improved representation of multiphase chemistry and aqueous processing remains a priority particularly given growing evidence that cloud and aerosol phase reactions significantly alter organic aerosol mass and radical budgets (Ervens et al., 2011; Shrivastava et al., 2017). Second, the role of complex VOC mixtures (chemical cocktails) is increasingly recognized as non-additive, with recent chamber and field studies demonstrating strong interaction effects between anthropogenic and biogenic emissions that cannot be captured using single-precursor approaches (McFiggans et al., 2019; Glasius & Goldstein, 2016). Third, temperature dependent autoxidation pathways and their sensitivity to climate warming are an active area of investigation, with recent studies showing that increasing temperature can significantly alter RO_2 fate and HOM formation rates, thereby modifying SOA yields under future climate scenarios (Bianchi et al., 2019; Wennberg et al., 2018). Finally, emerging work on intermediate-volatility organic compounds (IVOCs) and volatile chemical products (VCPs) highlights their importance as previously underrepresented precursors in urban atmospheres, particularly in rapidly developing regions (Robinson et al., 2007; Pye et al., 2010). Collectively, these research directions indicate that the O_3–SOA system remains an active frontier in atmospheric chemistry rather than a resolved mechanistic framework.

CONCLUSION

This systematic review has demonstrated that tropospheric ozone (O_3) and secondary organic aerosol (SOA) are tightly coupled products of a shared volatile organic compound (VOC) oxidation system, mediated primarily through peroxy radical (RO_2) chemistry. The evidence consistently shows that RO_2 branching determines whether atmospheric oxidation favours ozone formation under high-NO_x conditions or aerosol production under low-NO_x, autoxidation-dominated regimes. A key outcome of this synthesis is the recognition of autoxidation as a central paradigm shift in atmospheric chemistry, enabling rapid formation of highly oxygenated organic molecules (HOMs) and extremely low-volatility compounds that substantially contribute to SOA mass. This coupled chemistry creates a non-linear "see-saw" relationship between ozone and aerosol formation, with important implications for air quality management, human health, and climate forcing. Current chemical transport models (CTMs) remain limited in their ability to fully represent this complexity due to simplified chemical mechanisms, incomplete treatment of intermediate-volatility organic compounds (IVOCs), and insufficient representation of multiphase and autoxidation processes. These limitations lead to systematic uncertainties in predicting both oxidant levels and aerosol burdens.

Accordingly, this review highlights the need for enhanced atmospheric modelling frameworks that integrate explicit or semi-explicit chemical mechanisms within 3D CTMs, rather than relying on overly simplified reaction schemes. Bridging this gap is essential for improving predictive accuracy and for supporting more effective multi-pollutant air quality and climate mitigation strategies. Finally, the findings emphasise that future progress will depend on integrating laboratory kinetics, field observations, and advanced modelling approaches to better resolve the coupled O_3–SOA system across diverse atmospheric environments.

RECOMMENDATIONS

Based on the results of this systematic review, the following recommendations can be made for the advancement of scientific knowledge, accuracy of atmospheric modelling, and air quality management strategies for the coupled formation of tropospheric ozone (O_3) and secondary organic aerosols (SOA).

1. Future atmospheric chemistry studies should use a coupled approach to study ozone and SOA formation as a combined atmospheric process, rather than as separate components of atmospheric chemistry, because both ozone and SOA formation are closely linked via common VOC oxidation pathways and peroxy radical (RO) chemistry.
2. The oxidation mechanisms responsible for the formation of highly oxygenated organic molecules (HOMs), especially under low NOx conditions, should receive further scientific attention and should be better characterized through chamber and field studies quantifying temperature, humidity, and VOC molecular structure effects on RO branching ratios and SOA yields.
3. The persistent under prediction of SOA mass and oxidative capacity in CTMs can be reduced by representing intermediate volatility organic compound (IVOC) and semi volatile organic compound (SVOC) emissions and multiphase chemistry more explicitly, and by representing rapid autoxidation chemistry in the models more accurately.
4. More chamber and field studies with mixed, real-world VOC mixtures should be performed to further characterize the non-linear 'cocktail' effects and the competition between ozone-forming and aerosol-forming processes at the rural-urban interface where anthropogenic NOx coexists with biogenic VOC emissions.
5. More atmospheric chemistry studies should be performed in rapid growing urban areas of the Global South such as the cities of Africa, where a combination of high temperatures, intense solar radiative, biomass burning and coexisting biogenic and anthropogenic VOC emissions produce a unique atmospheric chemical regime that is not well represented by global models.

REFERENCES

Akimoto, H. (2016). *Atmospheric Reaction Chemistry*. Springer Japan. https://link.springer.com/book/10.1007/978-4-431-55870-5

Atkinson, R., & Arey, J. (2003). Gas-phase tropospheric chemistry of biogenic volatile organic compounds: a review. *Atmospheric environment*, *37*, 197-219. https://www.sciencedirect.com/science/article/abs/pii/S1352231003003911

Aumont, B., Szopa, S., & Madronich, S. (2005). Modelling the evolution of organic carbon during its atmospheric processing. *Atmospheric Chemistry and Physics*, 5(9), 2497–2517. https://acp.copernicus.org/articles/5/2497/2005/

Bianchi, F., Kurtén, T., Riva, M., Mohr, C., Rissanen, M. P., Roldin, P., & Ehn, M. (2019). Highly oxygenated organic molecules (HOM) from gas-phase autoxidation involving peroxy radicals: A key contributor to atmospheric aerosol. *Chemical reviews*, *119*(6), 3472-3509. https://pubs.acs.org/doi/full/10.1021/acs.chemrev.8b00395

Carlton, A. G., Wiedinmyer, C., & Kroll, J. H. (2009). A review of Secondary Organic Aerosol (SOA) formation from isoprene. *Atmospheric Chemistry and Physics*, *9*(14), 4987-5005. https://acp.copernicus.org/articles/9/4987/2009/

Carter, W. P., & Heo, G. (2013). Development of revised SAPRC aromatics mechanisms. Atmospheric Environment, 77, 404–414. https://www.sciencedirect.com/science/article/abs/pii/S1352231013003646

Crounse, J. D., Nielsen, L. B., Jørgensen, S., Kjaergaard, H. G., & Wennberg, P. O. (2013). Autoxidation of organic compounds in the atmosphere. *The Journal of Physical Chemistry Letters*, *4*(20), 3513-3520. https://pubs.acs.org/doi/abs/10.1021/jz4019207

Donahue, N. M., Robinson, A. L., Stanier, C. O., & Pandis, S. N. (2006). Coupled partitioning, dilution, and chemical aging of semivolatile organics. *Environmental science & technology*, *40*(8), 2635-2643. https://pubs.acs.org/doi/abs/10.1021/Es052297c

Ehn, M., Thornton, J. A., Kleist, E., Sipilä, M., Junninen, H., Pullinen, I., & Mentel, T. F. (2014). A large source of low-volatility secondary organic aerosol. *Nature*, *506*(7489), 476-479. https://www.nature.com/articles/nature13032

Ervens, B. T. B. W. R., Turpin, B. J., & Weber, R. J. (2011). Secondary organic aerosol formation in cloud droplets and aqueous particles (aqSOA): a review of laboratory, field and model studies. *Atmospheric Chemistry and Physics*, *11*(21), 11069-11102. https://acp.copernicus.org/articles/11/11069/2011/

Glasius, M., & Goldstein, A. H. (2016). Recent discoveries and future challenges in atmospheric organic chemistry, 50(6), 2754–2764. https://pubs.acs.org/doi/full/10.1021/acs.est.5b05105

Guo, S., Hu, M., Zamora, M. L., Peng, J., Shang, D., Zheng, J., & Zhang, R. (2014). Elucidating severe urban haze formation in China. *Proceedings of the National Academy of Sciences*, *111*(49), 17373-17378. https://www.pnas.org/doi/abs/10.1073/pnas.1419604111

Hallquist, M., Wenger, J. C., Baltensperger, U., Rudich, Y., Simpson, D., Claeys, M., & Wildt, J. (2009). The formation, properties and impact of secondary organic aerosol: current and emerging issues. *Atmospheric chemistry and physics*, *9*(14), 5155-5236. https://acp.copernicus.org/articles/9/5155/2009/

Jenkin, M. E., Saunders, S. M., Wagner, V., & Pilling, M. J. (2003). Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part B): tropospheric degradation of aromatic volatile organic compounds. *Atmospheric Chemistry and Physics*, *3*(1), 181-193. https://acp.copernicus.org/articles/3/181/2003/

Kroll, J. H., & Seinfeld, J. H. (2008). Chemistry of secondary organic aerosol: Formation and evolution of low-volatility organics in the atmosphere. *Atmospheric Environment*, *42*(16), 3593-3624. https://www.sciencedirect.com/science/article/abs/pii/S1352231008000253

Lee, A., Goldstein, A. H., Keywood, M. D., Gao, S., Varutbangkul, V., Bahreini, R., & Seinfeld, J. H. (2006). Gas-phase products and secondary aerosol yields from the ozonolysis of ten different terpenes. *Journal of Geophysical Research: Atmospheres*, *111*(D7). https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2005JD006437

Loza, C. L., Craven, J. S., Yee, L. D., Coggon, M. M., Schwantes, R. H., Shiraiwa, M., ... & Seinfeld, J. H. (2014). Secondary organic aerosol yields of 12-carbon alkanes. *Atmospheric Chemistry and Physics*, *14*(3), 1423-1439. https://acp.copernicus.org/articles/14/1423/2014/

Mao, J., Ren, X., Zhang, L., Van Duin, D. M., Cohen, R. C., Park, J. H., & Brune, W. H. (2012). Insights into hydroxyl measurements and atmospheric oxidation in a California forest. *Atmospheric Chemistry and Physics*, *12*(17), 8009-8020. https://acp.copernicus.org/articles/12/8009/2012/

McFiggans, G., Mentel, T. F., Wildt, J., Pullinen, I., Kang, S., Kleist, E., & Kiendler-Scharr, A. (2019). Secondary organic aerosol reduced by mixture of atmospheric vapours. *Nature*, *565*(7741), 587-593. https://www.nature.com/articles/s41586-018-0871-y

Monks, P. S., Archibald, A. T., Colette, A., Cooper, O., Coyle, M., Derwent, R., & Williams, M. L. (2015). Tropospheric ozone and its precursors from the urban to the global scale from air quality to short-lived climate forcer. *Atmospheric chemistry and physics*, *15*(15), 8889-8973. https://acp.copernicus.org/articles/15/8889/2015/

Ng, N. L., Kroll, J. H., Chan, A. W. H., Chhabra, P. S., Flagan, R. C., & Seinfeld, J. H. (2007). Secondary organic aerosol formation from m-xylene, toluene, and benzene. *Atmospheric Chemistry and Physics*, *7*(14), 3909-3922. https://acp.copernicus.org/articles/7/3909/2007/

Orlando, J. J., & Tyndall, G. S. (2012). Laboratory studies of organic peroxy radical chemistry: an overview with emphasis on recent issues of atmospheric significance. *Chemical Society Reviews*, *41*(19), 6294-6317. https://pubs.rsc.org/en/content/articlelanding/2008/qd/c2cs35166h/unauth

Page, M. J., McKenzie, J. E., Bossuyt, P. M., Boutron, I., Hoffmann, T. C., Mulrow, C. D., & Moher, D. (2021). The PRISMA 2020 statement: an updated guideline for reporting systematic reviews. *bmj*, *372*. https://www.bmj.com/content/372/bmj.n71.short

Pankow, J. F. (1994). An absorption model of gas/particle partitioning of organic compounds in the atmosphere. *Atmospheric Environment*, *28*(2), 185-188. https://www.sciencedirect.com/science/article/abs/pii/1352231094900930

Pye, H. O. T., Chan, A. W. H., Barkley, M. P., & Seinfeld, J. H. (2010). Global modeling of organic aerosol: the importance of reactive nitrogen (NO x and NO 3). *Atmospheric Chemistry and Physics*, *10*(22), 11261-11276. https://acp.copernicus.org/articles/10/11261/2010/

Robinson, A. L., Donahue, N. M., Shrivastava, M. K., Weitkamp, E. A., Sage, A. M., Grieshop, A. P., ... & Pandis, S. N. (2007). Rethinking organic aerosols: Semivolatile emissions and photochemical aging. *Science*, *315*(5816), 1259-1262. https://www.science.org/doi/abs/10.1126/science.1133061

Seinfeld, J. H., & Pandis, S. N. (2016). *Atmospheric chemistry and physics: from air pollution to climate change*. John Wiley & Sons. https://books.google.com.ng/books?hl=en&lr=&id=n_RmCgAAQBAJ&oi=fnd&pg=PR5&dq=Seinfeld,+J.+H.,+%26+Pandis,+S.+N.+(2016).+Atmospheric+Chemistry+and+Physics:+From+Air+Pollution+to+Climate+Change.+John+Wiley+%26+Sons.&ots=gTMeIOsigl&sig=xl7mn14Km-wpQm0af8Zj3mztQVE&redir_esc=y#v=onepage&q&f=false

Shrivastava, M., Cappa, C. D., Fan, J., Goldstein, A. H., Guenther, A. B., Jimenez, J. L., & Zhang, Q. (2017). Recent advances in understanding secondary organic aerosol: Implications for global climate forcing. *Reviews of Geophysics*, *55*(2), 509-559. https://agupubs.onlinelibrary.wiley.com/doi/full/10.1002/2016RG000540

Sillman, S. (1999). The relation between ozone, NOx and hydrocarbons in urban and polluted rural environments. *Atmospheric environment*, *33*(12), 1821-1845. https://www.sciencedirect.com/science/article/abs/pii/S1352231098003458

Snyder, H. (2019). Literature review as a research methodology: An overview and guidelines. *Journal of business research*, *104*, 333-339. https://www.sciencedirect.com/science/article/pii/S0148296319304564

Surratt, J. D., Chan, A. W., Eddingsaas, N. C., Chan, M., Loza, C. L., Kwan, A. J., & Seinfeld, J. H. (2010). Reactive intermediates revealed in secondary organic aerosol formation from isoprene. *Proceedings of the National Academy of Sciences*, *107*(15), 6640-6645. https://www.pnas.org/doi/abs/10.1073/pnas.0911114107

Wennberg, P. O., Bates, K. H., Crounse, J. D., Dodson, L. G., McVay, R. C., Mertens, L. A., & Seinfeld, J. H. (2018). Gas-phase reactions of isoprene and its major oxidation products. *Chemical reviews*, *118*(7), 3337-3390. https://pubs.acs.org/doi/abs/10.1021/acs.chemrev.7b00439

Xiao, Y., & Watson, M. (2019). Guidance on conducting a systematic literature review. *Journal of planning education and research*, *39*(1), 93-112. https://journals.sagepub.com/doi/abs/10.1177/0739456X17723971

Yarwood, G., Jung, J., Whitten, G. Z., Heo, G., Mellberg, J., & Estes, M. (2010, October). Updates to the Carbon Bond mechanism for version 6 (CB6). In *9th Annual CMAS Conference, Chapel Hill, NC* (pp. 11-13). https://cmascenter.org/conference/2010/abstracts/emery_updates_carbon_2010.pdf

Zhu, X., Wang, H., Han, Y., Zhang, D., Liu, S., Zhang, Z., & Liu, Y. (2025). Reconstructing the VOC–Ozone Research Framework Through a Systematic Review of Observation and Modeling. *Sustainability*, *17*(16), 7512.

Ziemann, P. J., & Atkinson, R. (2012). Kinetics, products, and mechanisms of secondary organic aerosol formation. *Chemical Society Reviews*, *41*(19), 6582-6605. https://pubs.rsc.org/en/content/articlelanding/2012/cs/c2cs35122f/unauth