Reviewer #1

Huang et al. presents a comparison of 8 different air quality models/mechanisms in how these models produce secondary organic aerosol (SOA). They run these models offline, e.g., using a box model, so that same initial conditions are used and initial results can be compared. They find that each model/mechanism lead to very different yields of the similarly tracked species (aromatics, biogenics). Though this could be a good reference paper for modeling community and insight into how to compare and/or improve models, the paper currently as presented is not ready to be published in ACP, for the following reasons:

Response: We appreciate the reviewer's positive comment. We provide point-by-point responses below.

1) The first 16 pages of the manuscript currently reads more as a review of SOA modeling schemes than a research article. Though this compilation of models is useful for an easily digestable reference, I recommend that the authors and/or editor determine if this paper should be a review, a research article, or a measurement report, as I will discuss next.

Response: We appreciate the reviewer's constructive feedback regarding the manuscript's structure. We agree that the research focus should be more prominent. Following this suggestion, we have maintained the manuscript as a research article but implemented two major structural and content revisions to transition it away from a review-style format.

First, we moved the detailed Section 3 ("Parameterization of SOA scheme in different CTMs") to the Supporting Information to avoid a purely descriptive compilation in the main text. Instead, the revised main text now provides a high-level overview of the schemes (Section 2.1), focusing on conceptual similarities and differences in their underlying physics and chemistry (e.g., partitioning, aging mechanisms). We moved Table S1, which summarizes scheme details, from Supporting Information to the main text (now Table 1), to provide a concise reference for the subsequent quantitative analysis.

The revised text of Section 2.1 follows in italics:

"A comparative overview of the SOA schemes is presented in Table 1 while comprehensive details regarding their specific parameterizations can be found in Section S1 of the Supporting Information.
The review of these SOA schemes reveals diverse parameterizations ranging from simplified, non-volatile assumptions to complex, multi-dimensional volatility basis sets. CAMx offers two distinct approaches: the SOAP2 scheme (based on Strader et al., 1999) and the 1.5-D VBS (Koo et al., 2014). SOAP2 has non-volatile POA and a two product

SOA scheme (Figure 1) with yields fitted to the aged VBS scheme of Hodzic et al. (2016), effectively treating aging as implicit. The 1.5-D VBS treats POA as semi-volatile and explicitly models gas-phase aging for anthropogenic and intermediate volatility precursors via OH-oxidation (Figure 2b), although this stepwise aging is disabled for biogenic precursors to prevent aerosol mass overprediction. The CMAQ model also provides alternative schemes: the established AERO7 scheme (Appel et al., 2021) and the newer CRACMM scheme (Pye et al., 2023). AERO7 utilizes a 1-D VBS framework for POA and SOA that incorporates aging primarily through particle-phase processes (Figure 2d), specifically the oligomerization of anthropogenic and biogenic precursors and the hydrolysis of organic nitrates derived from monoterpenes. CRACMM also utilizes a 1-D VBS framework for POA and SOA and simulates aging through sequential gas-phase oxidation reactions involving functionalization and/or fragmentation (Figure 2c; Pye et al., 2023). GEOS-Chem includes a "Simple" scheme that treats SOA as non-volatile with fixed yields that are linked to ambient measurements, alongside a "Complex" 1-D VBS scheme without additional aging processes (Figure 2a; Pai et al., 2020). CHIMERE's 1-D VBS scheme is notable for its comprehensive aging scheme with functionalization, fragmentation, and oligomerization (Figure 2d) where oxidation products are redistributed across volatility bins (CHIMERE, 2023). The WRF-Chem MOSAIC scheme employs a 1-D VBS for most VOCs but applies a specific stepwise gas-phase aging mechanism exclusively to IVOCs (Shrivastava et al. 2011).
Despite these structural differences, the schemes share foundational similarities, particularly in the reliance on absorptive partitioning theory by most schemes. With the exception of the GEOS-Chem Simple scheme, which assumes irreversible condensation, all models utilize either a two-product or VBS framework to describe the equilibrium partitioning of semi-volatile organic compounds. However, the treatment of aging remains the most significant source of divergence. Approaches vary from neglecting aging entirely (GEOS-Chem Complex, CAMx SOAP2) to implementing distinct mechanisms such as gas-phase oxidation (CAMx VBS, CMAQ CRACMM) versus particle-phase oligomerization (CMAQ AERO7). Additionally, the representation of IVOCs varies substantially, ranging from omission from the GEOS-Chem Simple scheme, a single lumped IVOC in most schemes, and several lumped IVOCs in the CRACMM scheme."

Second, to strengthen the research component, we added new sections "2.4 Box model tests based on different SOA schemes" and "3.4 SOA variations in box model simulations". These sections move beyond offline yield calculations to present simulated SOA concentrations at two representative locations in Texas: Dallas-Fort Worth (DFW) for an urban environment and Tyler (TYL) for a rural, biogenic-influenced environment. By applying selected SOA schemes in box model simulations, we demonstrate how the

differences in yields and aging processes identified in earlier sections translate into divergent air quality predictions under realistic conditions. The new Sections 2.4 and 3.4 are shown below in italics.

We believe these changes effectively shift the manuscript's emphasis toward the quantitative evaluation and scientific implications of model uncertainties.

2.4 Box model tests based on different SOA schemes

"We implemented three updated SOA schemes in CAMx and performed 2-layer box modeling of two locations with varied anthropogenic emissions to quantify how differences between schemes can influence predicted SOA concentrations and their response to emission changes. The alternate SOA schemes use the existing CAMx SOAP2 code with updated SOA yield parameters so that model results clearly depend on yield assumptions rather than scheme formulation or coding. Two regions of Texas were selected to capture contrasting emission environments: Dallas-Fort Worth (DFW), a major urban area dominated by anthropogenic emissions (e.g., aromatics and IVOCs), and Tyler (TYL), a rural area in Northeast Texas characterized by high biogenic activity. The box model has a surface layer and a residual layer with time-varying surface layer depth to provide a simple representation of pollutant accumulation, carry-over, and diurnal variation. Simulations were conducted over a 5-day period, utilizing meteorological inputs and initial conditions derived from the Texas Commission on Environmental Quality (TCEQ) 2019 3-D CAMx modeling platform (TCEQ, 2022).

We implemented three new SOA schemes into CAMx that emulate SOA yields produced by the CMAQ AERO7, CMAQ CRACMM and Simple schemes. Each scheme was implemented by updating the yield parameters used by the CAMx SOAP2 scheme. For the CMAQ AERO7 and CRACMM schemes, yield curves were fitted to the respective data (Figure S3) for each SOA precursor. These yields were mapped to the volatility bins defined by CAMx SOAP2 to obtain the corresponding molar-based stoichiometric coefficients (Table S11-S14). Like the GEOS-Chem Simple scheme, the CAMx Simple scheme treats SOA as non-volatile with fixed yields that are based on multi-model averages and work by Seltzer et al. (2021). Detailed descriptions of the fitting procedures, updated Simple yields, and box model configurations are provided in the Section S3 of the Supporting Information.

We further investigate the response of SOA concentrations to varying anthropogenic VOC and NOx emissions by performing a matrix of 100 simulations for each location and SOA scheme. This approach allows for a comparison of scheme performance across a wider range of atmospheric concentrations and VOC/NOx ratios. Anthropogenic emissions in the sensitivity runs were based on weekday rates, while the biogenic emissions remained unscaled and varied by date, consistent with the base case simulations. Anthropogenic VOC emissions were scaled from 0.1 to 1.0 (in increments of 0.1), while anthropogenic

NOx emissions were scaled from 0 to 9 (in increments of 1) which caused oxidant production to transition between NO-limited and VOC-limited conditions. An additional simulation with a 50% reduction in NOx emissions was conducted to examine SOA response to NOx abatement, which is a critical consideration for current and future air quality planning."

3.4 SOA variations in box model simulations

"The box model simulations reveal significant discrepancies in predicted SOA concentration and composition among the selected schemes at both the urban (DFW) and rural (TYL) locations (Figure 9). The total SOA concentrations can vary by a factor of 2–3 between schemes even under identical meteorological and emission inputs. Overall, SOA concentrations are higher at DFW than at TYL. At both locations, all schemes exhibit a consistent diurnal profile characterized by SOA accumulation throughout the day and night, followed by a sharp decline in the early morning (beginning around 06:00 LST) caused by expansion of the planetary boundary layer (PBL). At DFW, the temporal trends are similar across the four schemes; however, the magnitude varies, with Simple and AERO7 predicting the highest concentrations, while CRACMM predicts the lowest. At TYL, the inter-model spread is narrower than at DFW. Notable differences in diurnal dominance emerge: SOAP2 and CRACMM predict the highest concentrations overnight—a pattern distinct from DFW—while Simple and CRACMM produce the highest values during daytime hours. Figure 9c-d shows the maximum and minimum average SOA concentrations. At DFW, Simple and CRACMM predict the highest and lowest total SOA concentrations, respectively. Conversely, at TYL, CRACMM predicts the highest average concentration, while AERO7 predicts the lowest.

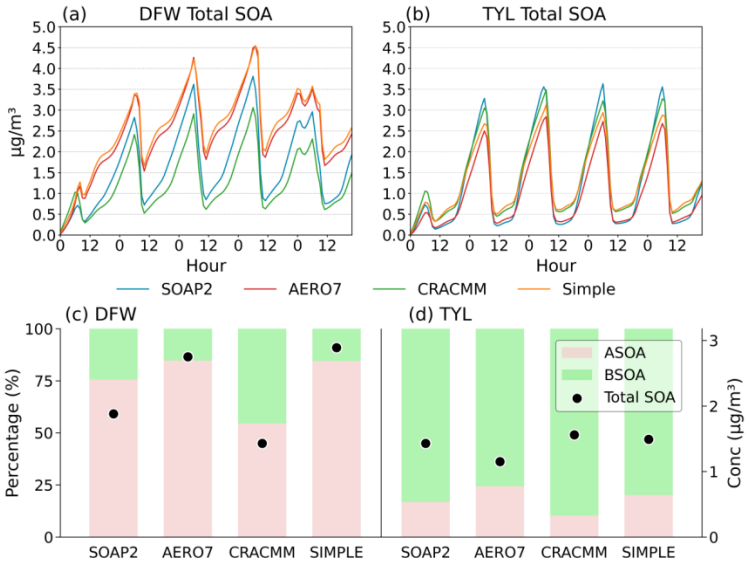


Figure 9 Diurnal profiles of total SOA (µg/m^3) from the 5-day box model base simulations at (a) DFW and (b) TYL. Average SOA concentrations (µg/m^3) over days 2

through 5 of base model simulations for each SOA scheme (circles) and average contributions of ASOA and BSOA (bars) at (c) DFW and (d) TYL.

Response surface plots for 24-hour average SOA concentrations derived from the matrix of simulations with varied anthropogenic NOx and VOC emissions are presented in Figure S4-S5. At DFW, total SOA concentrations generally decrease as anthropogenic NOx emissions increase relative to the base case (scaling factors 2–9) for all schemes, with the notable exception of CRACMM. CRACMM predicts negligible changes or a slight increase in SOA as NOx rises from low to mid scaling factors and a decrease is observed only when NOx emissions are increased by about a factor of 7 or greater. CRACMM also predicts the lowest SOA concentrations across all scaling factors. AERO7 and SIMPLE are very similar in both response surface shape and magnitude. For each scheme, SOA concentrations decrease as the anthropogenic VOC emissions decrease. At TYL, the response surfaces for AERO7, Simple, and SOAP3 are similar, with SOA concentrations remaining relatively constant at NOx scaling factors greater than 1. In contrast, CRACMM demonstrates a much stronger response, with SOA mass increasing concurrently with NOx emissions. At this biogenic-dominated site, SOA concentrations in all schemes are minimally sensitive to variations in anthropogenic VOC emissions.

Understanding how SOA responds to NOx reductions is critical for near-term air quality planning, as many regulatory strategies (e.g., cleaner vehicles, energy transition) produce substantial NOx emissions abatement (Crippa et al. 2016; EPA et al. 2017; Li et al. 2024). Table 4 summarizes the impact of a 50% reduction in NOx emissions on total SOA, ASOA, and BSOA. In all schemes, reducing NOx leads to increased ASOA concentrations, with the most pronounced increase predicted by SOAP2. SIMPLE predicts the smallest increase in ASOA at DFW, while CRACMM predicts the smallest increase at TYL. At DFW, this NOx reduction also drives an increase in BSOA concentrations across most schemes, with the notable exception of CRACMM. Consistent with the ASOA results, SOAP2 predicts the largest increase in BSOA. The distinct behavior in CRACMM is driven by its monoterpene SOA parameterization; contrary to other schemes and experimental evidence (Lane et al. 2008; Sarrafzadeh et al. 2016, Zhao et al. 2018), CRACMM predicts decreasing yields under lower NOx conditions. Consequently, the substantial reduction in BSOA predicted by CRACMM at DFW results in a net decrease in total SOA, a trend opposite to that observed in the other schemes. At TYL, all schemes predict a decrease in both BSOA and total SOA, with the most significant reductions observed in the CRACMM simulation. The dominance of biogenic emissions at TYL compared to DFW is reflected in the significantly higher BSOA concentrations. The differing SOA responses to NOx reduction between the two sites are attributable to the distinct biogenic emission regimes producing different VOC/NOx emission ratios.

Table 4 Average concentrations (μg/m^3) of anthropogenic SOA (ASOA) and biogenic SOA (BSOA) over days 2 through 5 for the base and reduced NOx model simulations. Shading indicates a decrease in SOA concentrations in the reduced NO*x* model runs compared to the base runs.

Location	Species	SOAP2			AERO7		
		Base	50% NO*x*	Diff (%)	Base	50% NO*x*	Diff (%)
DFW	ASOA	1.34	1.48	9.60%	2.34	2.38	1.90%
	BSOA	0.42	0.48	12.20%	0.41	0.42	0.40%
	Total SOA	1.76	1.96	10.30%	2.75	2.8	1.60%
TYL	ASOA	0.24	0.25	4.40%	0.28	0.31	9.90%
	BSOA	1.19	1.14	-4.10%	0.87	0.82	-6.20%
	Total SOA	1.43	1.4	-2.50%	1.16	1.14	-1.80%
Location	Species	CRACMM			Simple		
		Base	50% NO*x*	Diff (%)	Base	50% NO*x*	Diff (%)
DFW	ASOA	0.78	0.81	3.50%	2.44	2.45	0.60%
	BSOA	0.65	0.59	-10.70%	0.45	0.46	2.40%
	Total SOA	1.43	1.4	-2.50%	2.88	2.91	0.90%
TYL	ASOA	0.16	0.17	1.00%	0.3	0.32	8.50%
	BSOA	1.4	1.24	-12.60%	1.19	1.14	-4.40%
	Total SOA	1.56	1.41	-11.00%	1.49	1.46	-1.50%

2) The results and discussion, currently as written, read more as a measurement report, meaning that the values on the figures are directly discussed without really place the results from these figures into bigger context. This bigger context includes directly comparing the results from one model to another, which is sometimes done but gets lost. Also, placing the results into the context of prior research is currently not done, leading the results/discussion reading as a measurement report. To move the science beyond measurement report, if the authors want this to be a research article, I would recommend more in depth analysis (e.g., plotting the SOA yields as ratios to a model to demonstrate how much more SOA is being produced or plotting the average and spread of SOA yields across the models and what does that mean for total SOA produced for a typical urban environment and typical biogenic environment for uncertainty). Another demonstration of this is that figures are rarely referenced, esp. Fig 6, and again generally reads more as a review in that this is how model A performs, this is model B performs, etc. How much in how the model performs is surprising? E.g., if the authors compiled results of model comparisons or different model performances in a review type method, are the differences in yields and aging surprising?

Response: We appreciate the reviewer's assessment that the original results and discussion section appeared overly descriptive. While we retained Figure 6 because it provides a necessary visual comparison of how aging treatments differ among different schemes, we have implemented the following major analytical expansions to place these results into a broader context.

(1) To directly address the reviewer's suggestion of determining "what that means for total SOA produced for a typical urban/biogenic environment," we added a new section ("Section 3.4 SOA variations in box model simulations"). By implementing the different schemes in a box model for Dallas-Fort Worth (urban) and Tyler (rural) areas of Texas, we now quantify how the yield differences and aging mechanisms translate into modeled SOA concentrations. This allows us to discuss the "spread" of model predictions in a real-world context rather than just comparing offline SOA yield calculations.

(2) Within Section 3.4, we also performed a sensitivity analysis (a matrix of 100 simulations per scheme) varying anthropogenic VOC and NO*x* emissions. This analysis, now discussed in the revised manuscript, moves beyond simple comparisons to demonstrate how the response of each model to emission changes differs. For example, we find that the CRACMM scheme NO*x* sensitivity differs from other schemes and show that this difference is relevant to policy and planning.

P30, L488-L524:

"*Response surface plots illustrating 24-hour average SOA concentrations derived from the matrix of simulations with varied anthropogenic NOx and VOC emissions are presented in Figure S4-S5. At DFW, total SOA concentrations generally decrease as anthropogenic NOx emissions increase relative to the base case (scaling factors 2–9) for all schemes, with the notable exception of CRACMM. CRACMM predicts negligible changes or a slight increase in SOA as NOx rises from low to mid scaling factors and a decrease is observed only when NOx emissions are increased by about a factor of 7 or greater. CRACMM also predicts the lowest SOA concentrations across all scaling factors. AERO7 and SIMPLE are very similar in both response surface shape and magnitude. For each scheme, SOA concentrations decrease as the anthropogenic VOC emissions decrease. At TYL, the response surfaces for AERO7, Simple, and SOAP3 are similar, with SOA concentrations remaining relatively constant at NOx scaling factors greater than 1. In contrast, CRACMM demonstrates a much stronger response, with SOA mass increasing concurrently with NOx emissions. At this biogenic-dominated site, SOA concentrations in all schemes are minimally sensitive to variations in anthropogenic VOC emissions.*

Understanding how SOA responds to NOx reductions is critical for near-term air quality planning, as many regulatory strategies (e.g., cleaner vehicles, energy transition) produce substantial NOx emissions abatement (Crippa et al. 2016; EPA et al. 2017; Li et al. 2024). Table S20 summarizes the impact of a 50% reduction in NOx emissions on total SOA, ASOA, and BSOA. In all schemes, reducing NOx leads to increased ASOA concentrations, with the most pronounced increase predicted by SOAP2. SIMPLE predicts the smallest increase in ASOA at DFW, while CRACMM predicts the smallest increase at TYL. At DFW, this NOx reduction also drives an increase in BSOA concentrations across all schemes, with the notable exception of CRACMM. Consistent with the ASOA results, SOAP2 predicts the largest increase in BSOA. The distinct behavior in CRACMM is driven by its monoterpene SOA parameterization; contrary to other schemes and experimental evidence, CRACMM predicts decreasing yields under lower NOx conditions. Consequently, the substantial reduction in BSOA predicted by CRACMM at DFW results in a net decrease in total SOA, a trend opposite to that observed in the other schemes. At TYL, all schemes predict a decrease in both BSOA and total SOA, with the most significant reductions observed in the CRACMM simulation. The dominance of biogenic emissions at TYL compared to DFW is reflected in the significantly higher BSOA concentrations. The differing SOA responses to NOx reduction between the two sites are attributable to the distinct biogenic emission regimes producing different VOC/NOx emission ratios."

3) Authors state that they do not want to say use model X after this evaluation; however, from the results, it would feel like at least two models need to be used in order to better demonstrate all possible answers and uncertainty, which would be resource heavy. Could any evaluation against published chamber studies be done to provide better guidance of at least potential biases of one model vs another?

Response: We share the reviewer's assessment that relying on a single scheme seems unwise considering the large differences that we found, especially when model results may be used to guide costly policy interventions. While we acknowledge that using multiple schemes is resource-intensive, our study aims to highlight that the current spread in model results represents the uncertainty rather than a lack of model calibration. Regarding the suggestion of evaluation against published chamber studies to identify potential biases, we would like to clarify that the parameterizations of all schemes reviewed in this study were originally derived from or fitted to experimental data. Therefore, evaluating these models against the same or similar chamber studies would likely show reasonable agreement for each model within its specific experimental context, yet it would not resolve the fundamental discrepancies between different schemes. As discussed in Section 5 (now Section 4), significant challenges exist in determining "true"

experimental SOA yields. For example, traditional chamber experiments are perturbed by deposition to the chamber walls and therefore require wall adjustments that are uncertain. Oxidation flow reactor (OFR) experiments achieve high radical concentrations, and therefore short RO_2 radical lifetimes, which effectively suppress RO_2 radical autoxidation reactions that are now recognized as critical in real-world SOA chemistry. Rather than recommending a single "best" model, we provide guidance by identifying the specific processes (e.g., IVOC aging or NO*x* sensitivity) where model design most strongly impacts results.

4) The largest concern is the title does not reflect what is in the paper. After reading this, there was no evident discussion about the policy implications of these 8 different models/mechanisms. If this is important aspect the authors want to address, which I would support, more in-depth analysis, as suggested in comment 2), should be done. E.g., if a typical urban area starting with a mixture of aromatics, biogenics, IVOCs, etc., is modeled, how much total SOA is produced with the different metrics the authors discuss? How do these differences imply differences in policy strategy, such as explicit emission control (assuming most of the precursors are coming from heating or transportation or another source) vs more widespread emission control (transportation plus solvents plus . . .). What could the economic and/or public health impact be using one model that has lower total SOA vs another that has too high SOA? E.g., if the lowest performing model underpredicts the SOA for an urban area, what does that mean for the policy implications that were pursued due to using that model? If the model overpredicted, is that an economical concern?

Response: We agree with the reviewer that the "policy implications" mentioned in the title should be more explicitly supported by the analysis. While a full-scale economic or public health impact assessment is beyond the scope of this study—given that such impacts are highly sensitive to local emissions and socio-economic factors—we have significantly strengthened the discussion of policy implications by adding box model simulations (Section 3.4) for two representative scenarios in Texas: an urban site (Dallas-Fort Worth) and a rural site (Tyler). This allows us to quantify how the discrepancies in initial yields and aging mechanisms identified in the study propagate into total SOA mass predictions under real-world-like precursor mixtures. Our results show that total SOA concentrations can vary by a factor of 2–3 between schemes even under identical meteorological and emission inputs. We show that schemes can have directionally opposite responses to reducing NO*x* emissions.

Page 28, Line 453-460:
"The NOx effect on terpene-derived SOA in CRACMM is particularly noteworthy: the model predicts an eightfold increase in SOA yields under high NOx conditions compared to low NOx. This is significant given that terpenes are key SOA precursors in many

forested regions, such as the Eastern U.S., where anthropogenic NOx emissions may change due to ongoing urban development (which could increase NOx levels) or the implementation of emission control technologies (which may reduce them).”

Page 33, Line 566-571:

“For instance, discrepancies in yields lead to different precursor rankings (e.g., the relative importance of aromatics vs. IVOCs). If a model underpredicts the SOA potential of IVOCs, policy strategies might disproportionately focus on traditional VOCs (e.g., from petroleum-based solvents), potentially leading to ineffective widespread controls that miss the critical contribution of IVOCs.”

Reviewer #2

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

by Ling Huang, et al.

The article compares the SOA yields of 8 SOA schemes from 5 different chemical transport models. To remove the influence of other, model-specific differences, the SOA schemes were compared in an offline setting. Furthermore, the effect of different ageing processes on final SOA yields was also studied, depending on which ageing processes are included in the different schemes. The authors conclude that SOA yields vary widely between the different schemes (both with and without ageing), and that, on the one hand, this variety is good from a research perspective, but on the other hand causes problems when using such models in decision making. For the latter, the authors state that it may be better to use simpler schemes with well-defined SOA yields.

In principle, I find these kinds of studies useful, but I have some concerns regarding this manuscript.

Response: We appreciate the reviewer's positive comment. We provide point-by-point responses below.

First off, if I understand the text correctly, the schemes were not actually run (isolated from their host models) in a "chamber setting". Instead, the different model parameters were used in separate offline calculations to estimate the yields. I find this problematic, as there are bound to be assumptions in this approach which are not clearly lined out in the manuscript. There are references to two earlier works by Huang et al. describing this method, but I would like to see more details on the approach also here. In the end, I'm not convinced that this simple approach really reflects the actual yields obtained by the schemes. In case that I understood this part wrong, more explanation is needed in the methods section.

Response: We appreciate the reviewer's careful attention to our methodology. The reviewer is correct that the comparisons were based on offline calculations using the specific parameterizations (stoichiometric coefficients, saturation concentrations, aging mechanisms, etc.) for each model/scheme as obtained from the model documentation and confirmed in the source code. We described each scheme in detail in the original methods section, now moved to Supporting Information based on other review comments. We used this approach because isolating schemes from their host

models (i.e., extracting source code) would introduce greater uncertainties considering that schemes are not necessarily modular within their host model and that models have different coding practices. Performing our own implementation of each scheme allowed for consistent coding methods and provided us with full visibility into how each scheme operates.

To provide full transparency regarding our calculation method, we have added a step-by-step working example in Section S2 of the Supporting Information. We also provide calculation details of the SOA yields for CMAQ CRACMM in Section S3 of the Supporting Information. We have released the calculation spreadsheet publicly at https://doi.org/10.5281/zenodo.19019177, allowing readers to observe the calculations directly. The calculation spreadsheets for other schemes are available upon request. The new Sections S2 and S3 are shown below in italics

Section S2 An example of offline calculation for the SOA yields

"As an illustrative example, we present the calculation of non-aged SOA yields from benzene (BENZ) under high NOx conditions for the CAMx SOAP2 and CMAQ AERO7 schemes. For CAMx SOAP2, the effective saturation concentration (C^* = 0.31, 14 μg/m^3) listed in Table S1 are defined at 300K. These values were adjusted to a standard temperature of 298 K using the Clausius-Clapeyron equation:

$$C_i^* = C_{i,0}^* \frac{T_0}{T} exp\left[\frac{\Delta H_i^{vap}}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$

where C_i^* and $C_{i,0}^*$ are the saturation concentrations for volatility bin i at T and T_0 (=298 K), respectively. R is the universal gas constant, and ΔH_i^{vap} denotes the enthalpy of vaporization for volatility bin i.

Subsequently, using Eq. 1 and the stoichiometric coefficients from Table S1, the SOA yield from BENZ at C_{OA} of 10 μg/m^3 was calculated as:

$$Y = \frac{0.391}{1 + 0.21/10} + \frac{0.248}{1 + 10.31/10} = 0.505\ g/g$$

The CMAQ AERO7 scheme parameterizes SOA yields from BENZ using a VBS framework. The molar yields listed in Table S3 were converted to mass yields using the molecular of BENZ (=78.1 g/mol) and the oxidation product. Utilizing Eq.2, the SOA yield from BENZ at C_{OA} of 10 μg/m^3 was calculated as:

$$Y = \frac{0.0779}{1 + 1/10} + \frac{0}{1 + 10/10} + \frac{0.793}{1 + 100/10} + \frac{0}{1 + 1000/10} = 0.143\ g/g$$

These calculations were repeated over a C_{OA} range of 0.1 μg/m^3 to 50 μg/m^3 to generate the yield curves presented in Figure 3. A spreadsheet demonstrating these example calculations is available at https://doi.org/10.5281/zenodo.19019177.

Calculation data for other species and schemes are available from the corresponding authors upon request."

Section S3 Offline calculation of SOA yields in CMAQ CRACMM

"In this section, we show how SOA yields from benzene and α-pinene are calculated under high and low NOx conditions in CMAQ CRACMM. All the relevant reactions and parameters (Table S1) are obtained from Table B1 and Table S1 of Pye et al. (2023).

S3.1 SOA yields from benzene

Under high-NOx conditions, the following reactions take place that form SOA from benzene (BENZ). For clarity, only the relevant species involved in SOA formation are listed.

$$BENZ + HO \rightarrow 0.470\ BENP + 0.530\ PHEN + \ldots \qquad R17\ (k = 1.22\times10^{-12})$$

$$BENP + NO \rightarrow 0.001\ VROCP4OXY2 + 0.001\ VROCN1OXY6 + 0.499\ FURANONE + \ldots \qquad R18\ (k = 9.03\times10^{-12})$$

$$FURANONE + HO \rightarrow 0.040\ ASOATJ + \ldots \qquad R19\ (k = 4.4\times10^{-11})$$

$$PHEN + HO \rightarrow 0.152\ ASOATJ + \ldots \qquad R20\ (k = 2.63\times10^{-11})$$

Under low-NOx condition, SOA formation from BENZ follows the following reactions:

$$BENZ + HO \rightarrow 0.470\ BENP + 0.530\ PHEN + \ldots \qquad R21\ (k = 1.22\times10^{-12})$$

$$PHEN + HO \rightarrow 0.152\ ASOATJ + \ldots \qquad R22\ (k = 2.63\times10^{-11})$$

$$BENP + HO_2 \rightarrow 0.398\ VROCN1OXY6 + \ldots \qquad R23\ (k = 2.28\times10^{-11})$$

In our calculation, we assumed $[OH]=3.0\times10^{6}$ *molecules/cm*^{3}, $[NO]=100$ *ppt, and* $[HO_2]= 1.5\times10^{8}$ *molecules/cm*^{3} $(=[OH]\times 50)$ *for the calculation of reaction rates. The saturation concentration* (C^*) *for the species VROCP4OXY2, VROCN1OXY6 and ASOATJ is* 10^4, 10^{-1} *and* 10^{-9} *μg/m*^{3}, *respectively. With an ambient OA concentration* (C_{OA}) *of 10 μg/m*^{3}, *the gas fractions of the three species are 100%, 1%, and 0%. VROCP4OXY2 and VROCN1OXY6 participate in further reactions with OH, resulting in products that exhibit either increased or decreased* C^*, *as outlined in Table S1 below (derived from the reactions labeled under "ROCOXY" in Table B1 of Pye et al. (2023)). In contrast, ASOATJ is characterized as non-volatile and non-reactive.*

Calculations are stepped through time to simulate aging. At each time step, denoted as t, the total SOA mass is the sum of ASOATJ and the particle fraction of semi-volatile species:

$$SOA_t = [ASOATJ]_t + (f_{particle}^{VROCP4OXY2} \times [VROCP4OXY2]_t + f_{particle}^{VROCN1OXY6} \times [VROCN1OXY6]_t + f_{particle}^{VROCN1OXY1} \times [VROCN1OXY1]_t + \cdots) \qquad Eq.\ S1$$

Where $f_{particle}^{species}$ *is the particle fraction of each semi-volatile species and* $[species]_t$ *represents the mass of species (i.e. VROCP4OXY2, VROCN1OXY6) at time t. The mass of ASOATJ at time t is further calculated as:*

$$[ASOATJ]_t = [ASOATJ]_{t-1} + \sum_n \{[species]|_{t-1}^{j} \times f_{gas}^{j} \cdot (1\text{-}e^{-k_{OH}^{j} * [OH] * \Delta t}) \times \alpha_j^{ASOATJ}\} \qquad Eq.\ S2$$

j represents all the species that, when oxidized by OH, can form ASOATJ and α_j^{ASOATJ} *is the corresponding molar yield of ASOATJ. Similarly, the mass of semi-volatile species at time t, taking VROCP4OXY2 as an example, is calculated as:*

$$[VROCP4OXY2]_t = [VROCP4OXY2]_{t-1} \times (f_{particle}^{VROCP4OXY2} + f_{gas}^{VROCP4OXY2} \cdot e^{-k_{OH} * [OH] * \Delta t}) +$$

$$\sum_n \{[species]|_{t-1}^{j} \times f_{gas}^{j} \cdot (1\text{-}e^{-k_{OH}^{j} * [OH] * \Delta t}) \times \alpha_j^{VROCP4OXY2}\} \qquad Eq.\ S3$$

The mass of VROCP4OXY2 at time t consists of three components: (1) the particle-phase of VROCP4OXY2 at time t-1, (2) the remaining gas-phase of VROCP4OXY2 after OH oxidation, and (3) the additional mass gained from OH oxidation of other species, characterized by molar yields as $\alpha_j^{VROCP4OXY2}$ *(as shown in Table S10). We started the calculation from t=0 to t=24 hr and progress with a time step Δt of 0.2 hr. Figure S1a shows the SOA yields from benzene as a function of the aging time. Under both high and low NOx conditions, the SOA yields increase sharply during the initial six hours, after which the increase is negligible. With a 24-hour aging period, the SOA yield from benzene is 0.23 g/g under high NOx conditions and 0.67 g/g under low NOx conditions, respectively.*

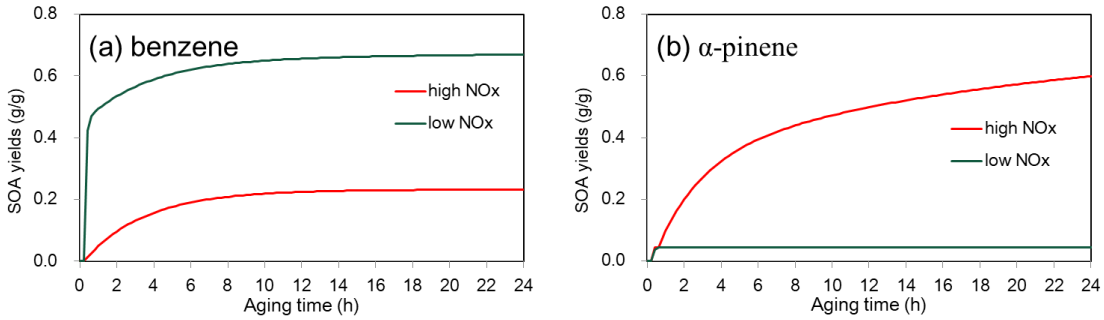


Figure S1 Effect of OH-oxidation aging on SOA yield (g/g) from (a) benzene and (b) α-pinene as a function of aging time in CMAQ CRACMM.

Table S1 *Stoichiometric yields of L/S/IVOC oxidation by OH (adopted from Table B1 from Pye et al. 2023)*

Species	VROCN2 OXY8	VROCN2 OXY4	VROCN2 OXY2	VROCN1 OXY6	VROCN1 OXY3	VROCN1 OXY1	VROCP0 OXY4	VROCP0 OXY2	VROCP1 OXY3	VROCP1 OXY1	VROCP2 OXY2	VROCP3 OXY2	VROCP4 OXY2	VROCP5 OXY1	VROCP6 OXY1	OP3
C* ($\mu g/m^3$)	0.01	0.01	0.01	0.1	0.1	0.1	1	1	10	10	100	1000	10000	100000	1000000	10
k_{OH}	5.90E-11	6.07E-11	5.54E-11	5.63E-11	5.46E-11	4.50E-11	5.17E-11	4.73E-11	4.50E-11	3.80E-11	3.93E-11	3.52E-11	3.12E-11	2.40E-11	2.05E-11	4.69E-11
VROCN2OXY8	0.085	0.464	0.104	0.204	0.279	0.007	0.282	0.066	0.178	0.002	0.044	0.032	0.012			0.119
VROCN2OXY4		0.198	0.564	0.007	0.403	0.119	0.117	0.458	0.192	0.134	0.173	0.076	0.017	0.01		0.001
VROCN2OXY2			0.214		0.009	0.726		0.116	4.00E-04	0.335	0.01	0.001		0.001		
VROCN1OXY6		0.012	0.015		0.032	0.012	0.032	0.033	0.074	0.008	0.051	0.053	0.048	0.009	0.006	0.039
VROCN1OXY3		0.015	0.03		0.008	0.03	0.018	0.066	0.045	0.119	0.112	0.049	0.025	0.015	0.005	
VROCN1OXY1			0.01			0.007		0.005		0.076	0.001					
VROCP0OXY4		0.062	0.019		0.019	0.029	0.001	0.031	0.063	0.029	0.134	0.155	0.088	0.07	0.022	0.011
VROCP0OXY2			0.046		0.01	0.045		0.002	0.001	0.077	0.04	0.015		0.015		
VROCP1OXY3		0.039	0.031		0.051	0.023		0.04	0.001	0.028	0.051	0.105	0.092	0.104	0.05	
VROCP1OXY1			0.02		0.007	0.035		0.021		0.012	0.007	0.001	0.007	0.003	0.002	
VROCP2OXY2		0.049	0.046		0.051	0.062	0.066	0.054	0.023	0.065	0.024	0.053	0.097	0.165	0.088	
VROCP3OXY2		0.04	0.045		0.046	0.052	0.053	0.052	0.059	0.071	0.029	0.009	0.046	0.157	0.138	
VROCP4OXY2		0.018	0.045		0.051	0.051	0.025	0.052	0.065	0.067	0.073	0.043	0.002	0.072	0.146	
VROCP5OXY1			0.033		0.014	0.035		0.037	0.017	0.042	0.052	0.058	0.048	0.006	0.043	
VROCP6OXY1			0.037			0.075		0.042		0.091	0.059	0.066	0.074	0.14	0.096	
OP3		0.031	0.003			0.016		0.011	0.015	0.007	0.004	0.051	0.061	0.022	0.032	

S3.2 SOA yields from α-pinene

Under high-NOx conditions, the following reactions occur, leading to the formation of SOA from α-pinene (API).

$API + HO \rightarrow 0.975\ APIP1 + 0.025\ APIP2 + \ldots$	R24 ($k = 5.29\times10^{-11}$)
$APIP1 + NO \rightarrow 0.820\ PINAL + 0.180\ TRPN + \ldots$	R25 ($k = 4.00\times10^{-12}$)
$APIP2 + NO \rightarrow HOM + \ldots$	R26 ($k = 4.00\times10^{-11}$)
$PINAL + HO \rightarrow 0.230\ PINALP + \ldots$	R27 ($k = 3.89\times10^{-11}$)
$PINALP + NO \rightarrow 0.050\ TRPN + \ldots$	R28 ($k = 9.03\times10^{-12}$)
$PINALP \rightarrow HOM$	R29 ($k = 1.0\ s^{-1}$)
$TRPN + HO \rightarrow HOM$	R30 ($k = 4.80\times10^{-11}$)

HOM is the final non-volatile SOA product while other products (APIP1, APIP2, TPRN, PINAL, etc.) are all volatile. Similar to benzene case, we assumed $[OH]=3.0\times10^{6}$ molecules/cm^3, [NO]=100 ppt, and $[HO_2]= 1.5\times10^{8}$ molecules/cm^3 (=[OH] × 50) for the calculation of reaction rates. The SOA mass yield, specifically HOM, from API at time t is calculated as follows:

$$SOA_t = [HOM]_{t-1} + [TRPN]_{t-1} \cdot (1\text{-}e^{-k_{TRPN+OH}*[OH]*\Delta t}) \cdot \alpha_{TRPN}^{HOM} + [APIP2]_{t-1} \cdot (1\text{-}e^{-k_{APIP2+NO}*[NO]*\Delta t}) \cdot \alpha_{APIP2}^{HOM} + [PINALP]_{t-1} \cdot (1\text{-}e^{-k'_{PINALP\rightarrow HOM}*\Delta t}) \cdot \alpha'_{PINALP\rightarrow HOM} \quad \text{Eq. S4}$$

PINALP will either react with NO (R10, $k=9.03\times10^{-12}$ cm^3·molecule^{-1}·s^{-1}) or undergo auto-oxidation (R11, $k=1\ s^{-1}$). With [NO]=100 ppt, the reaction rate of R10 is equal to 0.02 s^{-1}. We combine these two reactions to get:

$$k'_{PINALP\rightarrow HOM} = \frac{k_{auto-oxidation}}{k_{PINALP\rightarrow HOM} + k_{auto-oxidation}} \quad \text{Eq. S5}$$

$$\alpha'_{PINALP\rightarrow HOM} = \alpha_{auto-oxidation} \times \frac{k_{auto-oxidation}}{k_{PINALP\rightarrow HOM} + k_{auto-oxidation}} \quad \text{Eq. S6}$$

Figure S2a shows the yields of PINAL, TRPN, PINALP, and HOM as a function of aging time. As expected, both PINAL and PINALP undergo rapid reactions to produce TRPN, which subsequently leads to the formation of HOM. The SOA yields (i.e. HOM) experiences a significant increase during the initial six hours, after which the rate of increase becomes negligible. With a 24-hour aging period, the SOA yield from API is 0.599 g/g under high NOx conditions.

Additionally, we examined the sensitivity of SOA yields after a 24-hour aging period due to variations in NO concentration and the auto-oxidation rate. As illustrated by Figure S2b, SOA yield remains relatively stable until [NO] > 1000 ppt.

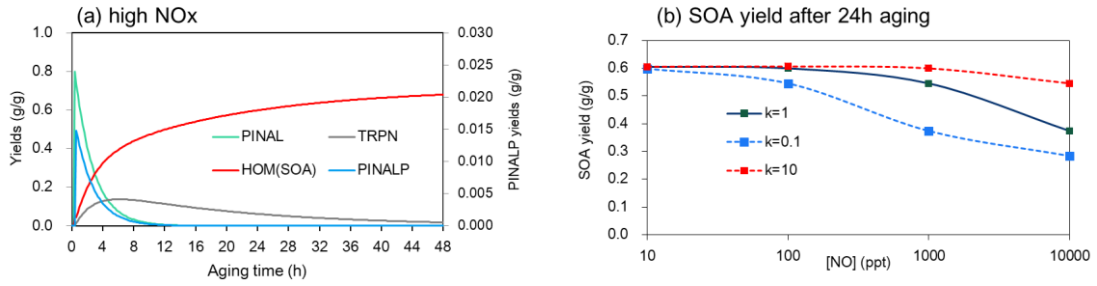


Figure S2 (a) Yields of different species from API + OH as a function of aging time under high NOx conditions and (b) sensitivity of SOA yields to different [NO] and auto-oxidation rate.

Under low NOx conditions, SOA formation from API follows the following reaction:

$$API + HO \rightarrow 0.975\ APIP1 + 0.025\ APIP2 + \ldots \qquad R31\ (k = 5.29\times10^{-11})$$

$$APIP1 + HO2 \rightarrow OPB \qquad R32\ (k = 1.50\times10^{-11})$$

$$APIP2 + HO2 \rightarrow HOM \qquad R33\ (k = 1.50\times10^{-11})$$

In this case, the SOA yield rapidly reaches a maximum value of 0.05 g/g after 1-hour and stays the same afterwards (Figure S1b).”

The methods section in particular is very hard to follow. The detail given for the different models and schemes varies a lot and feels slightly random. For instance, in some places chemical reactions treated in a model are explicitly given, which I find unnecessary. Instead of listing the working principles of the different models on by one, it would be much more helpful to describe how the models differ from each other. This could be done, for instance, by merging some part of the very detailed Introduction (especially the figures) with the methods section. Some sort of table would also be really helpful.

Response: We appreciate the reviewer’s helpful feedback regarding the organization and readability of the Methods section. To address this, we have significantly streamlined the text by moving the detailed, model-by-model parameterizations (formerly Section 3) to the Supporting Information. In line with the reviewer's suggestion to focus on how the models differ rather than listing their working principles sequentially, the revised Methods section now provides a high-level synthesis. We discuss the schemes in terms of their conceptual similarities and differences. Furthermore, to address the request for a helpful overview, we have moved the comprehensive summary table (formerly Table S1) to the main text (now Table 1), which serves as a concise reference for the subsequent quantitative analysis.

Revised text in Section 2.1:

“A comparative overview of the SOA schemes is presented in Table S1 while

comprehensive details regarding their specific parameterizations can be found in Section S1 of the Supporting Information.

The review of these SOA schemes reveals diverse parameterizations ranging from simplified, non-volatile assumptions to complex, multi-dimensional volatility basis sets. CAMx offers two distinct approaches: the SOAP2 scheme (based on Strader et al., 1999) and the 1.5-D VBS (Koo et al., 2014). SOAP2 has non-volatile POA and a two product SOA scheme (Figure 1) with yields fitted to the aged VBS scheme of Hodzic et al. (2016), effectively treating aging as implicit. The 1.5-D VBS treats POA as semi-volatile and explicitly models gas-phase aging for anthropogenic and intermediate volatility precursors via OH-oxidation (Figure 2b), although this stepwise aging is disabled for biogenic precursors to prevent aerosol mass overprediction. The CMAQ model also provides alternative schemes: the established AERO7 scheme (Appel et al., 2021) and the newer CRACMM scheme (Pye et al., 2023). AERO7 utilizes a 1-D VBS framework for POA and SOA that incorporates aging primarily through particle-phase processes (Figure 2d), specifically the oligomerization of anthropogenic and biogenic precursors and the hydrolysis of organic nitrates derived from monoterpenes. CRACMM also utilizes a 1-D VBS framework for POA and SOA and simulates aging through sequential gas-phase oxidation reactions involving functionalization and/or fragmentation (Figure 2c; Pye et al., 2023). GEOS-Chem includes a "Simple" scheme that treats SOA as non-volatile with fixed yields that are linked to ambient measurements, alongside a "Complex" 1-D VBS scheme without additional aging processes (Figure 2a; Pai et al., 2020). CHIMERE's 1-D VBS scheme is notable for its comprehensive aging scheme with functionalization, fragmentation, and oligomerization (Figure 2d) where oxidation products are redistributed across volatility bins (CHIMERE, 2023). The WRF-Chem MOSAIC scheme employs a 1-D VBS for most VOCs but applies a specific stepwise gas-phase aging mechanism exclusively to IVOCs (Shrivastava et al. 2011).

Despite these structural differences, the schemes share foundational similarities, particularly in the reliance on absorptive partitioning theory by most schemes. With the exception of the GEOS-Chem Simple scheme, which assumes irreversible condensation, all models utilize either a two-product or VBS framework to describe the equilibrium partitioning of semi-volatile organic compounds. However, the treatment of aging remains the most significant source of divergence. Approaches vary from neglecting aging entirely (GEOS-Chem Complex, CAMx SOAP2) to implementing distinct mechanisms such as gas-phase oxidation (CAMx VBS, CMAQ CRACMM) versus particle-phase oligomerization (CMAQ AERO7). Additionally, the

representation of IVOCs varies substantially, ranging from omission from the GEOS-Chem Simple scheme, a single lumped IVOC in most schemes, and several lumped IVOCs in the CRACMM scheme."

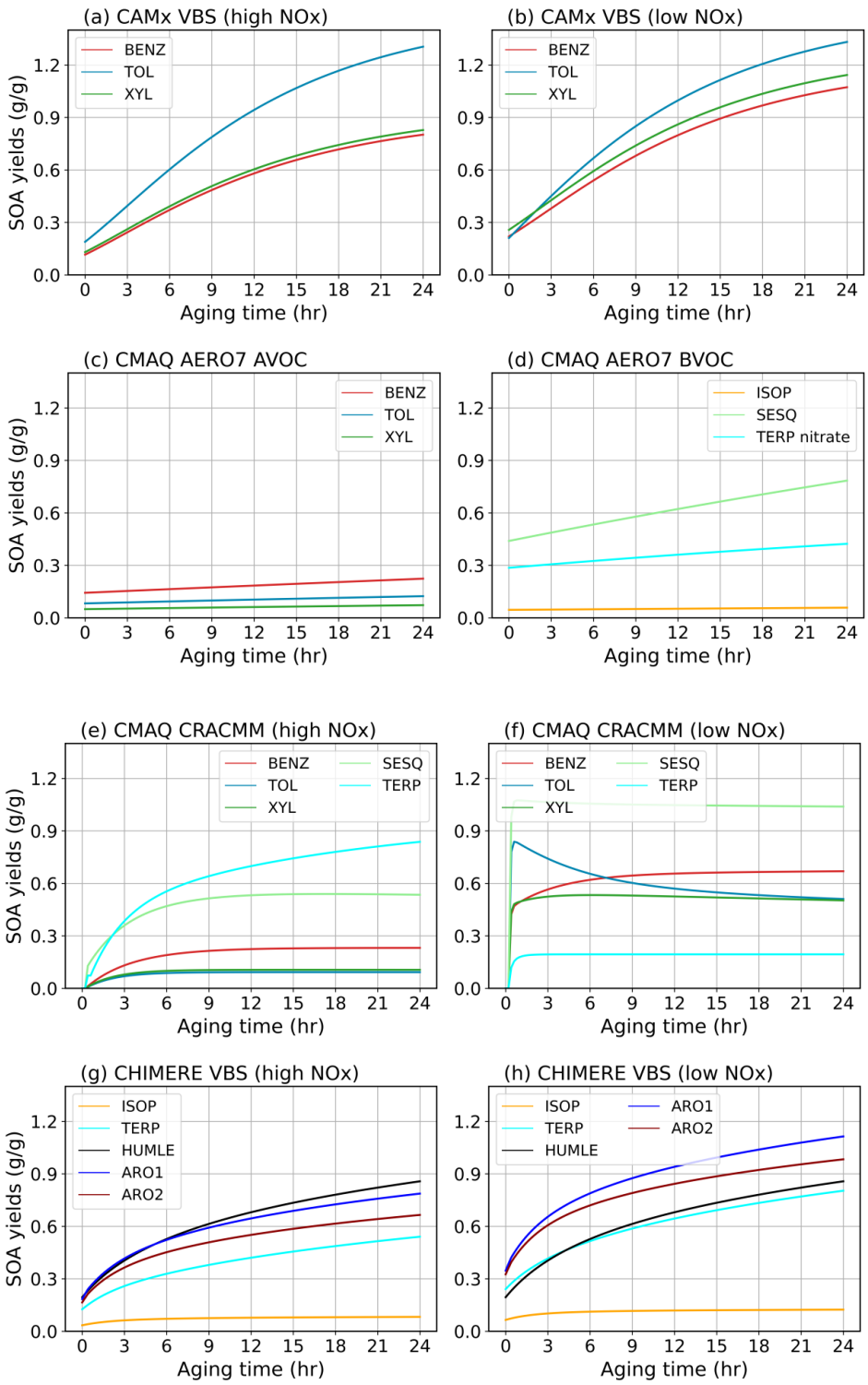
The Results section is well structured and informative. I'm having problems with the term "initial SOA yield" denoting SOA yield without considering ageing. How about something more descriptive like "non-ageing SOA yield" or some such?

Response: We thank the reviewer for this helpful suggestion. While the reviewer suggested "non-aging SOA yield", we have opted to use the term "non-aged SOA yield" throughout the revised manuscript. We believe "non-aged" more accurately describes the state of the aerosol (i.e., at time t=0, before the simulated aging processes are applied), whereas "non-aging" might be misinterpreted as a static physical property of the aerosol itself. We hope the reviewer agrees that this term provides the intended clarity for the comparative analysis.

Figure 7 is hard to comprehend in the sense that for some schemes model yield is shown as function of time, while others are shown as function of OH exposure. How can these be compared to each other? If the horizontal axes cannot be unified, it might be better to split the figures.

Response: We acknowledge the reviewer's concern regarding the inconsistency of the horizontal axes in Figure 7. Comparing OH exposure with aging time can indeed be confusing without a standardized reference. To address this and ensure a direct comparison across all schemes, we have unified the x-axes for all panels in Figure 7 (and Figure 8) to represent "Aging time (hours)". For schemes that parameterize aging as a function of OH-oxidation (e.g., CAMx VBS and CHIMERE VBS), we converted OH exposure to aging time by assuming a constant atmospheric OH concentration of 3×10^6 molecules/cm^3, which is a typical daytime value used in such comparative studies.

Revised figure:



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117 **Figure 7** Effect of aging on SOA yields (g/g) from different precursors as a function
118 of OH exposure or aging time in different schemes. (a-b) CAMx VBS; (c-d) CMAQ
119 AERO7; (e-f) CMAQ CRACMM; and (g-h) CHIMERE VBS. The numbers in the
120 brackets indicate the relative change of SOA yields at hour 24 to hour 0.

121

Also, in most of the figures in the result section, the vertical axes depicting SOA yield has different ranges in different panels of the same figure. This makes it quite hard to compare the different schemes.

Response: We appreciate the reviewer's suggestion to improve the comparability of the figures. We have carefully reviewed the axis scaling across the manuscript and implemented the following strategy to balance cross-scheme comparison with data legibility:

- For Figures 3 through 6, we maintained precursor-specific y-axis ranges for each panel. This is because the non-aged SOA yields differ by orders of magnitude between precursors—for example, ranging from approximately 0.05 g/g for isoprene to over 1.0 g/g for sesquiterpenes. Using a single unified y-axis for all precursors would compress the data for lower-yield species (like isoprene), making it impossible to discern the significant discrepancies between the eight different modeling schemes. Since all schemes for a specific precursor are already plotted on the same panel, direct comparison between models remains straightforward.

- For Figures 7 and 8, which illustrate the evolution of yields over time, we have unified the y-axis ranges where appropriate to better highlight the relative magnitude of aging effects across different schemes.

To assist the reader, we have also ensured that all figure captions explicitly note when different scales are used.

For the Implications and Conclusion settings, it would also be interesting to know whether the models/schemes have been compared in directly (i.e., by running the entire model and comparing results). If so, it would be nice to see these comparisons put into context with the findings here, as it may give indications of how other parts and processes of the models may affect modelled SOA concentrations.

Response: We appreciate the reviewer's interest in seeing a direct comparison of the modeled results. As mentioned in our manuscript, running full 3-D simulations for every model system (e.g., CMAQ vs. CAMx vs. GEOS-Chem) introduces confounding variables—such as differences in transport, deposition, and meteorological drivers—that can obscure the specific effects of the SOA mechanisms.

To address this request, we added a new section "3.4 SOA variations in box model simulations" in the revised manuscript. This section moves beyond offline yield calculations to present simulated SOA concentrations at two representative locations

in Texas: Dallas-Fort Worth (DFW) for an urban environment and Tyler (TYL) for a rural, biogenic-influenced environment. By applying selected SOA schemes in box model simulations, we demonstrate how the differences in yields and aging processes identified in earlier sections translate into divergent air quality predictions under real-world-like conditions. We also performed a sensitivity analysis (a matrix of 100 simulations per scheme) varying VOC and NO*x* emissions. This analysis moves beyond simple comparisons to demonstrate how the response of each model to emission changes differs.

3.4 SOA variations in box model simulations

"The box model simulations reveal significant discrepancies in predicted SOA concentration and composition among the selected schemes at both the urban (DFW) and rural (TYL) locations (Figure 9). The total SOA concentrations can vary by a factor of 2–3 between schemes even under identical meteorological and emission inputs. Overall, SOA concentrations are higher at DFW than at TYL. At both locations, all schemes exhibit a consistent diurnal profile characterized by SOA accumulation throughout the day and night, followed by a sharp decline in the early morning (beginning around 06:00 LST) caused by expansion of the planetary boundary layer (PBL). At DFW, the temporal trends are similar across the four schemes; however, the magnitude varies, with Simple and AERO7 predicting the highest concentrations, while CRACMM predicts the lowest. At TYL, the inter-model spread is narrower than at DFW. Notable differences in diurnal dominance emerge: SOAP2 and CRACMM predict the highest concentrations overnight—a pattern distinct from DFW—while Simple and CRACMM produce the highest values during daytime hours. Figure 9c-d shows the maximum and minimum average SOA concentrations. At DFW, Simple and CRACMM predict the highest and lowest total SOA concentrations, respectively. Conversely, at TYL, CRACMM predicts the highest average concentration, while AERO7 predicts the lowest.

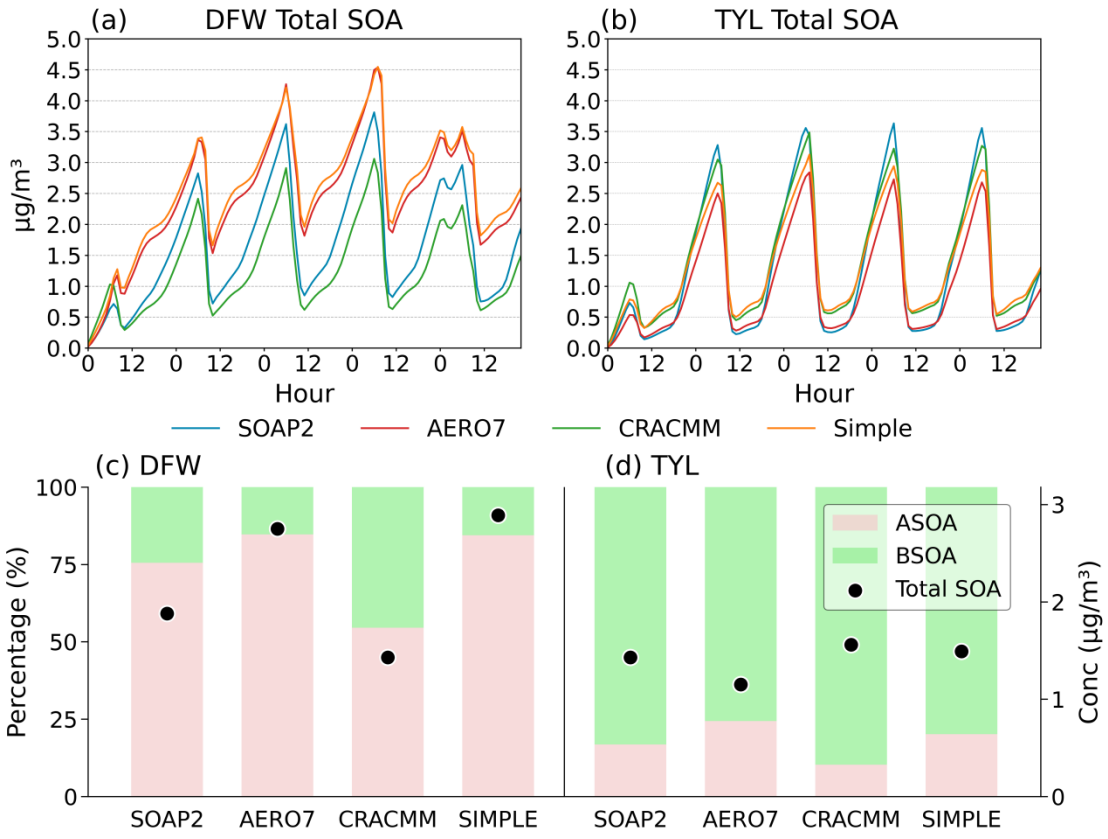

Figure 9 *Diurnal profiles of total SOA (µg/m^3) from the 5-day box model base simulations at (a) DFW and (b) TYL. Average SOA concentrations (µg/m^3) averaged over days 2 through 5 of base model simulations for each SOA scheme (circles) and average contributions of ASOA and BSOA (bars)*

Response surface plots for 24-hour average SOA concentrations derived from the matrix of simulations with varied anthropogenic NOx and VOC emissions are presented in Figure S4-S5. At DFW, total SOA concentrations generally decrease as anthropogenic NOx emissions increase relative to the base case (scaling factors 2–9) for all schemes, with the notable exception of CRACMM. CRACMM predicts negligible changes or a slight increase in SOA as NOx rises from low to mid scaling factors and a decrease is observed only when NOx emissions are increased by about a factor of 7 or greater. CRACMM also predicts the lowest SOA concentrations across all scaling factors. AERO7 and SIMPLE are very similar in both response surface shape and magnitude. For each scheme, SOA concentrations decrease as the anthropogenic VOC emissions decrease. At TYL, the response surfaces for AERO7, Simple, and SOAP3 are similar, with SOA concentrations remaining relatively constant at NOx scaling factors greater than 1. In contrast, CRACMM demonstrates a

much stronger response, with SOA mass increasing concurrently with NOx emissions. At this biogenic-dominated site, SOA concentrations in all schemes are minimally sensitive to variations in anthropogenic VOC emissions.

Understanding how SOA responds to NOx reductions is critical for near-term air quality planning, as many regulatory strategies (e.g., cleaner vehicles, energy transition) produce substantial NOx emissions abatement (Crippa et al. 2016; EPA et al. 2017; Li et al. 2024). Table 4 summarizes the impact of a 50% reduction in NOx emissions on total SOA, ASOA, and BSOA. In all schemes, reducing NOx leads to increased ASOA concentrations, with the most pronounced increase predicted by SOAP2. SIMPLE predicts the smallest increase in ASOA at DFW, while CRACMM predicts the smallest increase at TYL. At DFW, this NOx reduction also drives an increase in BSOA concentrations across most schemes, with the notable exception of CRACMM. Consistent with the ASOA results, SOAP2 predicts the largest increase in BSOA. The distinct behavior in CRACMM is driven by its monoterpene SOA parameterization; contrary to other schemes and experimental evidence (Lane et al. 2008; Sarrafzadeh et al. 2016, Zhao et al. 2018) , CRACMM predicts decreasing yields under lower NOx conditions. Consequently, the substantial reduction in BSOA predicted by CRACMM at DFW results in a net decrease in total SOA, a trend opposite to that observed in the other schemes. At TYL, all schemes predict a decrease in both BSOA and total SOA, with the most significant reductions observed in the CRACMM simulation. The dominance of biogenic emissions at TYL compared to DFW is reflected in the significantly higher BSOA concentrations. The differing SOA responses to NOx reduction between the two sites are attributable to the distinct biogenic emission regimes producing different VOC/NOx emission ratios."

Table 4 *Average concentrations (µg/m^3) of anthropogenic SOA (ASOA) and biogenic SOA (BSOA) over days 2 through 5 for the base and reduced NOx model simulations. Shading indicates a decrease in SOA concentrations in the reduced NOx model runs compared to the base runs.*

Location	Species	SOAP2			AERO7		
		Base	50% NOx	Diff (%)	Base	50% NOx	Diff (%)
DFW	ASOA	1.34	1.48	9.60%	2.34	2.38	1.90%
	BSOA	0.42	0.48	12.20%	0.41	0.42	0.40%
	Total SOA	1.76	1.96	10.30%	2.75	2.8	1.60%
TYL	ASOA	0.24	0.25	4.40%	0.28	0.31	9.90%
	BSOA	1.19	1.14	-4.10%	0.87	0.82	-6.20%
	Total SOA	1.43	1.4	-2.50%	1.16	1.14	-1.80%
Location	Species	CRACMM			Simple		
		Base	50% NOx	Diff (%)	Base	50% NOx	Diff (%)
DFW	ASOA	0.78	0.81	3.50%	2.44	2.45	0.60%
	BSOA	0.65	0.59	-10.70%	0.45	0.46	2.40%
	Total SOA	1.43	1.4	-2.50%	2.88	2.91	0.90%
TYL	ASOA	0.16	0.17	1.00%	0.3	0.32	8.50%
	BSOA	1.4	1.24	-12.60%	1.19	1.14	-4.40%
	Total SOA	1.56	1.41	-11.00%	1.49	1.46	-1.50%