

We thank the reviewer for the careful reading of the manuscript and for the constructive comments, which we address point by point below.

Reviewer Comment (RC): General Comments

In this manuscript the authors describe a comparison of two computational methods for simulating the gas-phase oxidation of selected volatile organic compounds (VOCs) under atmospheric conditions ranging from polluted to clean air. The Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere (GECKO-A) and the Master Chemical Mechanism (MCM) have both been widely used for many years to model complex atmospheric chemistry. Unlike the MCM, for which VOC oxidation mechanisms have been developed on more of a case-by-case basis, GECKO-A can create a mechanism for almost any compound structure using a set of fundamental reaction pathways and rate constants based on experimental data in the literature and structure-activity relationships. Mechanisms for the oxidation of butane, octane, dodecane, toluene, and alpha-pinene generated with a new open-source version of GECKO-A and the latest version of the MCM were incorporated into box models that treat processes such as inorganic species chemistry, gas-particle and gas-wall partitioning, and photolysis to compare the performance for a variety of outputs including gas- and particle-phase carbon budgets, volatility and functional group distributions, water solubility, OH reactivity, Ox production, and product molecular composition.

This is an excellent paper. The background information about the different approaches used in GECKO-A and the MCM is very useful for readers not familiar with the details of these models, and the comparisons yield valuable insights into their relative strengths and weaknesses for a wide range of calculated quantities of atmospheric interest. The paper is well-organized, the results are clearly explained and interpreted, and the authors discuss the limitations and planned future improvements. I recommend publication in GMD after the following minor comments are addressed.

Authors' Answer (AA): We thank the reviewer for this positive assessment of the work.

RC: Specific Comments

1. Page 4, line 128: Does GECKO-A include ring-closing reactions for alkoxy radicals?

AA: No, ring-closure (cyclization) reactions of alkoxy radicals onto a double bond are not included in the current version of GECKO-A. The alkoxy radical chemistry implemented in GECKO-A v1.0 follows the structure-activity relationships (SARs) of Vereecken and Peeters (2009, 2010) (as indicated on lines 115-117), which address decomposition, isomerization, and reaction with O₂ for alkoxy radicals, but not intramolecular addition onto unsaturated bonds.

Unlike the case of RO₂ radicals, for which a structure-activity relationship is available (Vereecken et al., 2021a), a systematic and validated structure-activity relationship for ring closure from an unsaturated alkoxy radical does not currently exist. This pathway has been characterized for specific systems, such as the NO₃-initiated oxidation of isoprene (Carlsson et al., 2023; Vereecken et al., 2021b) and the OH-initiated oxidation of isoprene and monoterpenes (Vereecken and Peeters, 2004, 2012). Extending the current protocol for alkoxy radicals to account for this pathway would require developing a dedicated structure-activity relationship, which is beyond the scope of the present version.

The original text (line 128) explicitly states that GECKO-A does not account for ring closure for unsaturated RO₂ radicals, but it does not mention the case of alkoxy radicals. This is a separate limitation that had not been explicitly mentioned. We have revised the text accordingly (see the change made to the manuscript below).

Manuscript change: We have revised the sentence originally at lines 127-129 as follows:

"Major limitations include the absence of H-shift isomerization reactions involving RO₂ radicals and ring-closure (cyclization) reactions for unsaturated RO₂ radicals (e.g., Bianchi et al., 2019; Crounse et al., 2013; Vereecken and Nozière, 2020; Vereecken and Peeters, 2004; Vereecken et al., 2021a), as well as ring-closure reactions of unsaturated alkoxy radicals (e.g., Carlsson et al., 2023; Vereecken and Peeters, 2004, 2012; Vereecken et al., 2021b). [...] Ring-closure reactions of unsaturated alkoxy radicals would first require a dedicated structure-activity relationship, which is not currently available."

RC: 2. *Page 4, line 140 and Conclusions: Are there any plans to include multiphase reactions that form oligomers?*

AA: The Conclusions section mentions dimer formation via RO₂ + RO₂ reactions in the gas phase (line 1101). It also indicates that preliminary work is underway to incorporate this process into a future version of GECKO-A (lines 1111-1113).

Regarding multiphase oligomerization more specifically, there are no plans to include this process in the short or medium term. A simple parameterization to represent the effect of condensed-phase dimerization is conceptually straightforward to design (for example, a bimolecular reaction between species already present in the condensed phase). However, such a parameterization requires at minimum a structure-activity relationship (SAR) to estimate the associated rate constants. To our knowledge, no such SAR is currently available with the level of generality required for implementation in GECKO-A.

RC: 3. *Page 4, line 158: Can partitioning of radicals also be important and included in the mechanism?*

AA: The timescale of gas-particle equilibrium in our simulations is on the order of a few minutes (line 549). The gas-phase lifetime of most organic radicals is short compared to the characteristic timescale of mass transfer from the gas phase to the particle phase. This is particularly true for alkoxy radicals, whose gas-phase lifetime is typically several orders of magnitude shorter than the gas-particle transfer timescale.

Peroxy radicals, on the other hand, can have gas-phase lifetimes close to this order of magnitude, particularly under low-NO_x conditions where bimolecular loss is slower. GECKO-A does not yet incorporate RO₂ autoxidation reactions, which are often very fast. Incorporating these reactions would reduce the effective gas-phase lifetime of RO₂, which would likely reinforce the assumption that gas-particle partitioning of RO₂ remains a relatively minor process under most conditions for most RO₂.

The development of a phase-transfer treatment for radicals in GECKO-A is also limited by the lack of vapor pressure estimates for radicals. The approach in the current model relies on an estimate of the saturation vapor pressure of each species. To our knowledge, no appropriate structure-activity relationship currently exists for estimating vapor pressures for radical species. Existing estimation methods (for example, those used in GECKO-A and listed at lines 119-120) were developed and parameterized exclusively for stable closed-shell compounds. This currently prevents representing radical partitioning with the current configuration of the model, independently of the kinetic argument raised above.

Even setting aside the question of vapor pressure, the dynamic gas-particle partitioning treatment currently implemented in GECKO-A for closed-shell species would likely not be sufficient for radicals. Radical reactivity in the condensed phase is expected to be fast, potentially faster than in the gas phase (e.g., Renbaum and Smith, 2009). Under such conditions, condensed-phase chemistry, rather than simple phase transfer, is likely what controls the net exchange of radicals between the gas and particle phases. Recent work has also shown that peroxy radicals can be efficiently taken up by certain solid surfaces

through reactive (redox) uptake rather than simple dissolution (Durif et al., 2024), and that their condensed-phase reactivity can differ from their gas-phase chemistry (for example, enhanced formation of organic nitrates from $\text{RO}_2 + \text{NO}$ in the condensed phase; Barber et al., 2024).

Modeling radical mass transfer would therefore require a description of condensed-phase radical chemistry, in addition to the mass-transfer parameterization itself. Neither of these elements is currently available at the level of generality required for implementation in GECKO-A.

RC: 4. Page 6, Table 1: *One of the impressive features of GECKO-A is its ability to simulate multigeneration chemistry. But how necessary and important is this? In their comprehensive lab study of α -pinene oxidation Isaacman-VanWertz et al. (Nat Chem, 10, 462, 2018) conclude that within about one day of atmospheric oxidation most carbon is sequestered into two long-lived reservoirs: volatile oxidized gases and low-volatility particles.*

AA: Our GECKO-A simulations are consistent with two features of the oxidation sequence described by Isaacman-VanWertz et al. (2018) for α -pinene. The first is the progressive shift from functionalization to fragmentation. Both processes compete throughout oxidation, but their balance changes as oxidation proceeds. In our simulations, early-generation species are primarily mono- and bifunctional. More heavily functionalized species only form later (lines 586-587), while fragmentation becomes progressively dominant, ultimately producing CO and CO_2 (lines 565-568). The second feature is the sequestration of low-volatility carbon in a relatively unreactive particle reservoir. Figure 3 shows that SOA concentrations reach a plateau for all hydrocarbons, including α -pinene, after approximately 1-2 days of simulated time. Isaacman-VanWertz et al. (2018) also identified a second long-lived reservoir, made of volatile oxidized organic gases. Our simulations do not reproduce such a reservoir, except marginally (e.g., through acetone formation). Non-sequestered gas-phase carbon continues to be converted to CO and CO_2 over the simulated period (Fig. 5) and does not reach a fully unreactive state within the duration of our simulation.

Although maxgen was set to 20 to minimize the impact of mechanism reduction on the simulated trajectories (line 387), this limit is never reached in practice. Figure 1b shows that the number of species generated reaches a plateau after approximately 6-8 generations (line 229). Furthermore, Figure S3 (updated to Fig. 17 in the revised manuscript, Sect. 6, added in response to RC25 from the first reviewer) shows that species from generations beyond the fourth contribute only marginally to the mass balance. The manuscript states that "most of the SOC mass is accounted for by species up to the fourth generation, regardless of the parent hydrocarbon or scenario considered" (lines 969-971). This corroborates the reviewer's point and suggests "significant potential for mechanism simplification in GECKO-A without major loss of chemical information" (line 971). This potential is illustrated by red-GECKO-A, a reduced configuration (maxgen=5). It is compared to GECKO-A in a new section added to the manuscript, in response to comments from the first reviewer (RC25 and RC26).

As indicated in the Conclusions (lines 1096-1113), the next version of GECKO-A will incorporate RO_2 autoxidation. This process is expected to generate multifunctional, low-volatility species as early as the first generations, whereas the current protocol requires several generations of sequential functionalization. Although this effect remains to be quantified, this process is expected to substantially increase the sequestration of organic carbon into the particle phase from the earliest stages of the simulation, likely reducing the number of generations needed to reach a given SOA yield. This point is developed further in the Conclusions, in connection with the reduced mechanism red-GECKO-A (see RC25 in review 1).

RC: 5; Page 10, line 321: *Is there a reason the parameterization for gas-wall partitioning developed by Krechmer et al. (EST, 50, 5757, 2016), which is used in GECKO-A in the study by Peng et al. (ACP, 21, 14649, 2021) is not implemented?*

AA: We thank the reviewer for this comment. We would like to clarify that gas-wall partitioning was not activated in the simulations presented in this study (`g2wfg = False`, Table 1). The description given at lines 305-321 simply documents this feature of GECKO-A, as the paper aims to present the range of options offered by the tool.

The default treatment currently documented in GECKO-A (lines 311-321) follows Matsunaga and Ziemann (2010), as implemented by La et al. (2016). This implementation uses a fixed uptake rate constant common to all species, with a default characteristic timescale of 15 minutes for wall uptake. The effective wall sorption capacity is represented by the empirical parameter ($C_w/M_w\gamma_w$), expressed as a molar concentration. For simplicity, GECKO-A uses two default values covering broad classes of compounds (hydrocarbons and oxygenated compounds, line 320). Matsunaga and Ziemann (2010) and Yeh and Ziemann (2015) reported values for several distinct compound families, however, not just two. These two values constitute a simple default parameter that users can adjust for specific applications.

In the parameterization of Krechmer et al. (2016), as used by Peng et al. (2021) in a GECKO-A-based study, the effective wall sorption capacity (C_w) itself decreases as species volatility decreases. This parameterization further links the characteristic uptake timescale to the surface-to-volume ratio of the specific chamber considered (for example, about 1000 s for the CU chamber used by Peng et al., 2021, versus the fixed, chamber-independent default value of 900 s currently used in GECKO-A).

Both parameterizations describe gas-wall partitioning as a reversible first-order process governed by an uptake rate and an equilibrium constant. Adopting the formulation of Krechmer et al. (2016) would mainly require updating the numerical values used for the uptake rate constant and the equilibrium relationship, rather than a fundamental structural change to the box model. Peng et al. (2021) show that such a substitution is feasible within the existing GECKO-A framework. More generally, the box model provides a generic framework for gas-wall mass transfer rather than a chamber-specific parameterization. Users can replace the default values with those suited to their chamber and application, as Peng et al. (2021) did.

Manuscript change: We have added the following sentences (originally after line 321):

"The values provided here define a generic framework for gas-wall mass transfer within the GECKO-A code structure. These default parameterizations are intended as a practical starting point and should be adjusted by the user to the specific chamber and compounds under consideration, for example by substituting alternative published parameterizations such as that of Krechmer et al. (2016), as illustrated by Peng et al. (2021)."

RC: 6. Page 23, Figure 7 and page 32, Figure 11: *It appears that the reactions of butane, octane, and dodecane do not form ether groups at any oxidation timescale. Are the authors aware of recent computational chemistry results from Arathala et al. (JPCA, 125, 5963, 2021) that indicate that the timescale for cyclization of 1,4-hydroxycarbonyls in the gas phase to form cyclic hemiacetals can be on the order of seconds to minutes due to catalysis by HO₂ or HNO₃, respectively. For example, the calculated timescale is ~30 min under the range of HO₂ concentrations used here and ~10 s for 2 ppb of HNO₃. For alkanes this can have a major impact on the chemistry, since 1,4-hydroxycarbonyls are ~60% of the first-generation products and the corresponding cyclic hemiacetals have a tertiary H atom with an alpha-ether group that will greatly enhance (~10x) the rate of abstraction by OH and drive much of the subsequent secondary reactions through this pathway. The authors could comment on how*

this might impact the results presented here and could also consider adding this rather simple feature as an option to their alkane models.

AA: We thank the reviewer for pointing us to Arathala et al. (2021), which we were not aware of. GECKO-A can include a pathway forming cyclic hemiacetals (and subsequently dihydrofurans, DHFs) from 1,4-hydroxycarbonyls, but this pathway is currently implemented only as a heterogeneous, condensed-phase process as described in La et al. (2016). This process was not included in the mechanisms generated for this study, as only gas-phase chemistry was considered here (line 400), and for consistency with the MCM, which does not include this chemistry either. This option (dhffg) is not among the parameters listed in Table 1, but can be activated by adding it to the "process" section of the mechanism-generation namelist.

Arathala et al. (2021) present ab initio calculations showing that cyclization of 1,4-hydroxycarbonyls to form the corresponding hemiacetal may also occur in the gas phase via catalysis by species such as HO₂ or HNO₃, becoming atmospherically relevant. As noted by the reviewer, 1,4-hydroxycarbonyls account for a major fraction of first-generation alkane oxidation products. Their gas-phase cyclization could therefore affect the subsequent oxidation of alkanes, independently of particle or wall partitioning.

GECKO-A's mechanism-generation architecture is well suited to test this kind of sensitivity, as it allows alternative reaction protocols to be activated selectively and compared systematically. However, since the rate constants reported by Arathala et al. (2021) currently rest on theoretical (ab initio) calculations for a single prototype compound, without experimental kinetic validation or a generalized SAR applicable across 1,4-hydroxycarbonyl structures, we prefer to await further development before incorporating this pathway into GECKO-A's default protocol.

Manuscript change: We have added the following sentences after line 249 (Sect. 2.4):

"In addition to the parameters summarized in Table 1, the namelist can include further options, allowing users to activate additional, optional reaction pathways that are not enabled by default. This includes, for example, the heterogeneous formation of cyclic hemiacetals and dihydrofurans (DHFs) from 1,4-hydroxycarbonyls (Lim and Ziemann, 2009). This option is activated with the dhffg flag, to be added in the "process" section of the namelist (see the user documentation of GECKO-A v1.0 in Aumont et al., 2026)."

RC: 7. *I understand that this paper describes a model-model comparison, but it would be useful to include some comments about how well they have been shown to simulate experimental results.*

AA: The primary objective of this study is to present the newly released open-source version of GECKO-A (v1.0) and to explore in detail the oxidative trajectories, chemical budgets, and volatility distributions it produces under a range of environmental conditions. The comparison with MCM is used here as a benchmark to position GECKO-A relative to an established reference mechanism (see also the detailed responses to Reviewer 1).

Earlier versions of GECKO-A have been evaluated against experimental observations in several dedicated studies. As noted at lines 335-337, the GECKO-A box model has previously been evaluated against laboratory chamber data (La et al., 2016; McVay et al., 2016; Peng et al., 2021) as well as against complex, realistic VOC mixtures representative of urban, forested, and outflow environments (Lee-Taylor et al., 2011, 2015; Mouchel-Vallon et al., 2020). Valorso et al. (2011), cited at line 110 of this manuscript, similarly evaluated GECKO-A-simulated SOA formation from α -pinene photooxidation against chamber measurements.

A systematic evaluation of GECKO-A would require a benchmark dataset for routinely testing successive versions of the model. Developing and maintaining such a dataset would be valuable but is beyond the scope of the present paper.

Manuscript change: We have revised the sentence at lines 335-337 to explicitly note that these applications included evaluation against experimental data: "Examples of box model applications include evaluation against laboratory chamber data (e.g., La et al., 2016; McVay et al., 2016; Peng et al., 2021; Valorso et al., 2011) as well as simulations of realistic, complex VOC mixtures in urban and forested environments and outflow plumes (e.g., Lee-Taylor et al., 2011, 2015; Mouchel-Vallon et al., 2020)."

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