Response to reviewer #1' comments

General comment

This manuscript presents an evaluation of the model CMAQ for three chemical mechanisms with respect to $PM_{2.5}$ concentration. It complements a comparable evaluation for the model performance in simulating ozone. Model predictions are sensitive to the chemical scheme used. Additionally, the benefit of accounting for evaporation (and reactions) of semivolatile compounds from POA is shown. The manuscript is well written and deserves publication. I recommend that the issue I raise in my main comment below is addressed satisfactorily.

We thank the reviewer for dedicating time to a thorough review of our manuscript and for providing constructive comments and valuable suggestions. Our point-by-point responses are listed below. The reviewer's comments are presented in *Italic*, followed by our responses (in blue) and the corresponding revisions made to the manuscript, highlighted in red.

Major comments

-The authors rightly acknowledge the limitations and uncertainties stemming from emissions-to-species mapping. However, for the limitations related to mapping L/S/IVOC emissions the authors refer only to Chang et al. (2022) without elaborating how their own choice of the 15 CRACMM species and Emission strengths might affect the results. A discussion on this aspect is needed in my opinion.

We agree that uncertainties associated with the mapping of L/S/IVOC emissions to CRACMM species warrant additional clarification beyond citing Chang et al. (2022). We have revised the manuscript to explicitly discuss the mapping uncertainties between 2D-VBS and CRACMM, and L/S/IVOC emission strengths. We added the mapping rules between 2D-VBS and CRACMM in the methodology section, please refer to Page 10.

Lines 261-281: In this study, all species mapped from the full-volatility inventory (implemented using the two-dimensional VBS (2D-VBS) framework) to CRACMM are classified into two lumped categories: (1) an alkane-like ROC group, (2) 15 CRACMM mechanism species representing oxygenated S/IVOCs. Since all species exist in both the particle and gas phases, the same mapping rules are applied. The mapping rules for the gas phase are summarized in

Table S8.

For eight new alkane-like ROC species with high OA formation potential spanning the L/S/IVOC range and are grouped by $log_{10}(C_i^*)$ into ROCN1ALK, ROCP0ALK, VROCP1ALK, ROCP2ALK, ROCP3ALK, ROCP4ALK, ROCP5ALK, and ROCP6ALK. They are mapping from CSM1O2C00P, CS00O2C00P, CS01O2C00P, CS02O2C00P, CS03O2C00P, CS04O2C00P, CS05O2C00P and CS06O2C00P species in full-volatility emission inventory used in the 2D-VBS mechanism where numbers after CS indicate the negative(M) or positive (0) $log_{10}(C_i^*[\mu g/m^3])$ value and the number after 2C means $10 \times nO{:}nC$ (e.g., CS05O2C00P is $C_i^* = 10^{-5}$ μg/m^3 with $nO : nC = 0$).

For oxygenated L/S/IVOC, the species in 2D-VBS mechanism were lumped into 15 CRACMM mechanism species, spanning C_i^* values of 10^{-2} to 10^{6} μg/m^3 and $nO : nC$ of 0.1 to 0.8: ROCN2OXY2, ROCN2OXY4, ROCN2OXY8, ROCN1OXY1, ROC N1OXY3, ROCN1OXY6, ROCP0OXY2, ROCP0OXY4, ROCP1OXY1, ROCP1OXY3, ROCP2OXY2, ROCP3OXY2, ROCP4OXY2, ROCP5OXY1, and ROCP6XY1. 2D-VBS products of known nC and nO were mapped to the available CRACMM model species, first by interpolating to the two nearest species in nO: nC space, and then to the two nearest species $log_{10}(C_i^*)$ points.

The mapping uncertainties between 2D-VBS and CRACMM and L/S/IVOC emission strengths are added in lines 722-738.

For the species which can be mapped on a one-to-one basis in Table S8, the associated uncertainty is assumed to be zero. For species mappings involving similar $log_{10}(C_i^*)$ values, such as VROCP1OXY1, VROCP0OXY4, and VROCN2OXY4, some uncertainty may be introduced due to the proximity in volatility space. Anthropogenic L/S/IVOC emission inventories for China (Figure S4) contains (a) particle-phase emissions with full volatility coverage and (b) gas-phase emission inventories (Chang et al., 2022). Based on uncertainties of activity data and emission factors for each sector, the uncertainty of OA emissions can be quantified using a Monte Carlo method. According to Chang et al.(2022), the overall uncertainties at the 95% confidence interval for LVOC, SVOC, IVOC and VOC are (-40%, +43%), (-35%, 38%), (-33%, +33%) and (-21%, +28%), respectively. The overall uncertainty for L/S/IVOC is (-25%, +30%). Uncertainties across sectors tend to partially offset each other, resulting in a total emission uncertainty that is often smaller than that of the individual sectors.

S/IVOC emissions from domestic Volatile Chemical Products (VCPs) have the largest uncertainties (-81%, +143%), followed by open biomass burning (-58%, +81%) and industrial VCPs (-50%, +65%). Although the emission factors are based on local experiments, emissions from domestic fossil fuel and biomass burning still have considerable uncertainties (-38%, +62%) and (-38%, +51%), respectively.

Table S8 Mapping rules between 2D-VBS species and CRACMM S/IVOC species in the gas phase

2D-VBS	CRACMM
CSM1O2C00P	VROCN1ALK
CS00O2C00P	VROCP0ALK
CS01O2C00P	VROCP1ALK
CS02O2C00P	VROCP2ALK
CS03O2C00P	VROCP3ALK
CS04O2C00P	VROCP4ALK
CS05O2C00P	VROCP5ALK
CS06O2C00P	VROCP6ALK
CS06O2C01P	VROCP6OXY1
CS05O2C01P CS04O2C01P	VROCP5OXY1
CS03O2C01P CS02O2C01P CS01O2C01P CS00O2C01P CSM1O2C01P	VROCP1OXY1
CSM1O2C02P	VROCN2OXY2
CS00O2C02P	VROCP0OXY2
CS01O2C02P CS02O2C02P	VROCP2OXY2
CS03O2C02P	VROCP3OXY2
CS04O2C02P	VROCP4OXY2
CS06O2C04P CS05O2C04P CS04O2C04P CS03O2C04P CS02O2C04P	VROCP0OXY4
CS01O2C04P CS00O2C04P CSM1O2C04P	VROCN2OXY4

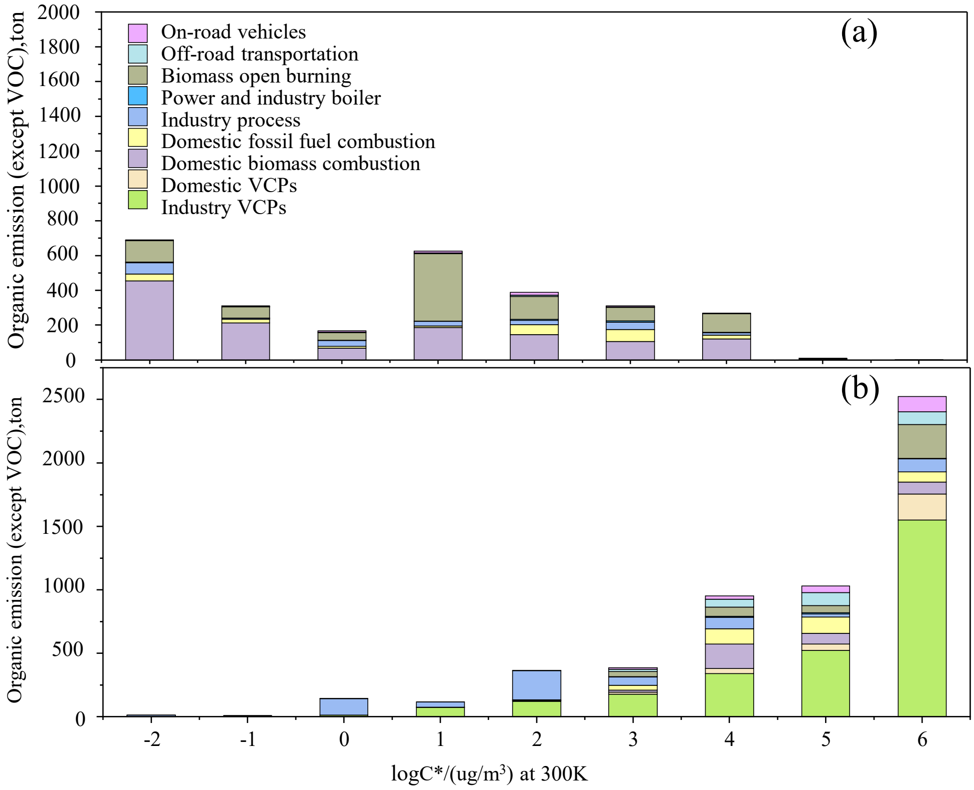

Figure S4 Anthropogenic L/S/IVOC emission inventory for China, binned by volatility: (a) particle-phase emissions, (b) gas-phase emissions.

We also added the following sentence in lines 285-287 of the revised manuscript.

The anthropogenic L/S/IVOC emission inventory using a volatility-binned approach with full coverage of both particle and gas phases was shown in Figure S4.

Sect. 2.2.2

It is not clear how the mapping of LVOC, SVOC and IVOC to CRACMM is done. Also in the Supplement no information is given regarding how the Emission strengths of species are assigned. Both Woody et al. (2016) and Chuang et al. (2022) provide emissions by source category, at least in the main text. This lack of information affects the reproducibility of the results.

We appreciate the constructive comments. Detailed mapping approaches for the emission species corresponding to LVOCs, SVOCs and IVOCs have been incorporated into the

Methodology section, with Table S8 and Figure S4 additionally added to the Supplement file. Table S8 shows the mapping rules between L/S/IVOC and CRACMM species. The source category dependent emission strengths were provided in Figure S4. These additions are intended to ensure that the results can be fully reproduced by other researchers.

- in Table 1 "Full volatile inventory" but somewhere else "Full volatility inventory". Is it volatile or volatility?

The correct term is “full-volatility inventory”, as it refers to an inventory covering the full range of compound volatilities. We have carefully revised the manuscript to ensure consistent use of this term throughout the text, figures, and tables.

Chang, X., Zhao, B., Zheng, H., Wang, S., Cai, S., Guo, F., Gui, P., Huang, G., Wu, D., Han, L., Xing, J., Man, H., Hu, R., Liang, C., Xu, Q., Qiu, X., Ding, D., Liu, K., Han, R., Robinson, A. L., and Donahue, N. M.: Full-volatility emission framework corrects missing and underestimated secondary organic aerosol sources, One Earth, 5, 403-412,doi: 10.1016/j.oneear.2022.03.015, 2022.