Isoprene -derived secondary organic aerosols under future climate conditions

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Organic aerosol contributes substantial mass fractions of submicron aerosols



Organic aerosols are generated from multiple sources



The largest contribution to organic aerosol production is from biogenic sources ٠

VOC: Volatile

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IEPOX-SOA can contribute to total OA concentrations by as much as 36%, especially for forested regions under low NO across the globe









Simulating IEPOX-SOA formation: Explicit vs parameterization (VBS)





The widely used parameterization (VBS) scheme does not capture the response to emission changes due to simplified chemistry



Correct sensitivity to emission change is critically important for future prediction of SOA



Objective: Investigate the future IEPOX -SOA change using the explicit isoprene chemistry, and compare it with the isoprene SOA predictions by the VBS parameterization

- CESM 2.1.0 release version (CAM6-chem)
 - + detailed isoprene gas-phase mechanism (MOZART-T2 chemistry, Schwantes et al., 2020)
 - + MOSAIC thermodynamic model for aerosol pH calculation (Zaveri et al., 2020)
 - + IEPOX reactive uptake on acidic aerosols
 - + NO_x-dependent yields for the VBS parameterization
 - + reduced tropical isoprene emissions (emission factors of tropical tree PFTs are decreased by half)
- F case run
 - coupled atmosphere and land models

– prescribed SST and ice from observational dataset (present) and WACCM results for CMIP6 (future, conducted by Mike Mills)

- Under present (2005-2014) and future (2045-2054; 2091-2100) climate
- Four Shared Socioeconomic Pathways (SSPs) used SSP1-2.6, SSP2-4.5, SSP3-7.0, and SSP5-8.5



Model evaluation against global surface aerosol mass spectrometer dataset



 $R^2 = 0.65$



Factors affecting isoprene emission changes under future climate (SSP5 -8.5) Ratio (SSP5-8.5 / Present)



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Global mean IEPOX -SOA concentrations at the surface (2010s and 2090s) simulated by explicit chemistry

(a) PRESENT (2010s)

90°N

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• Without CO₂ inhibition effect



Global mean IEPOX -SOA concentrations at the surface (2010s and 2090s) simulated by explicit chemistry Without CO₂ inhibition effect Aerosol acidity ↓ IEPOX-SOA formation rate Sulfate ↓ Aerosol surface area J Sulfate aerosol ratio SO4 ratio (SSP126/PRESENT) SO4 ratio (SSP245/PRESENT) (e) SSP1-2.6 (2090s) / PRESENT (f) SSP2-4.5 (2090s) / PRESENT 90°N 90°N 90°N 90°N 60°N 60°N 60°N 60°N 30°N 30°N 30°N 30°N 0 0 0° 30°S 30°S 30°S 30°S 60°S 60°S 60°S 60°S 90°S 180° 90°S – 180° 120°E 120°W 120°E 180° 60°E 60°W 60°E 120°W 60°W 180° 120°W 60°W 60°E 120°E 180° 60°E 120°W 60°W 120°E 180° 1/5 1/2 2 1/5 1/2 (g) SSP3-7.0 (2090s) / PRESENT (h) SSP5-8.5 (2090s) / PRESENT 90°N 90°N SO4 ratio (SSP370/PRESENT) SO4 ratio (SSP585/PRESENT) 90°N 90°N 60°N 60°N 60°N 60°N 30°N 30°N 30°N 30°N 0° 0 30°S 30°S 30°S 30°S 60°S 60°S 60°S 60°S 90°5 – 180° 90°S 90°S ∟ 180° 120°W 60°W 60°E 120°E 60°E 90°S – 180° 180° 120°W 60°W 120°E 180 120°W 60°W 60°E 120°E 180° 120°W 60°W 60°E 120°E 180° 1/5 1/2 1/5 1/2 1/2 1/5 Ż 1



Global mean IEPOX -SOA concentrations at the surface (2010s and 2090s)

Without CO₂ inhibition effect •



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Simulating IEPOX-SOA formation: Explicit vs parameterization (VBS)



Volatility basis set (VBS) approach



Global tropospheric IEPOX -SOA burden under present and future climate





Global tropospheric IEPOX -SOA burden under present and future climate



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- Lower R² between IEPOX-SOA concentrations and isoprene emissions
- → There are other factors affecting IEPOX-SOA formation (e.g. chemistry) in addition to isoprene emissions
- The VBS parameterization shows nearly constant IEPOX-SOA formation efficiencies across different SSP scenarios

Summary

Organic aerosol contributes substantial mass fractions of submicron aerosols



IEPOX-SOA can contribute to total OA concentrations by as much as 36%, especially for forested regions under low NO across the globe



IEPOX-SOA formation depends on oxidants, aerosol pH and other properties



The ex for pre concentrations

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120°W

60°W

60°E

120°E

180

Detailed chemistry will be very important for aerosol simulation in future climate with different emissions

