What's new in CRACMM2

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What is CRACMM?

- The Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM) is designed to integrate modeling of ozone, secondary organic aerosol (SOA), and toxic air pollutants
- CRACMM development is led by EPA ORD scientists in collaboration with partners from NOAA and academia
- CRACMM1 was released in CMAQv5.4 (Pye et al. 2023; Place et al. 2023)
- An updated version, CRACMM2, has now been released in CMAQv5.5 (Skipper et al. 2024)
- Want to learn more about CRACMM?
  - The CRACMM homepage has more information about CRACMM development efforts
  - The CRACMM github site includes files needed for 0-D box modeling (and much more!)

Background

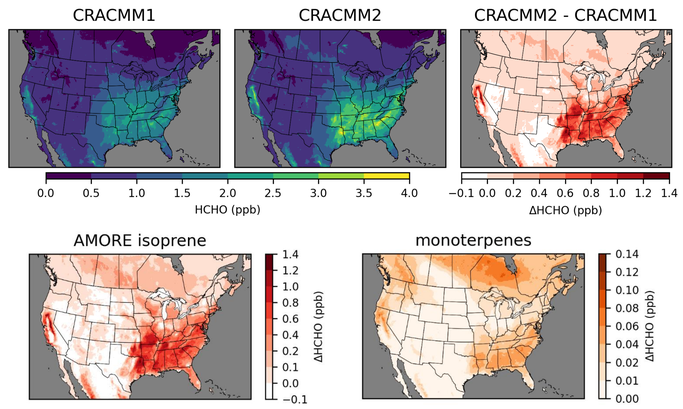
- In CMAQv5.4, two versions of CRACMM were included with different isoprene chemistry
  - CRACMM1 used isoprene chemistry from RACM2 plus additional IEPOX chemistry
  - CRACMM1AMORE used isoprene chemistry based on the AMORE isoprene condensation of a detailed isoprene degradation mechanism (Wiser et al. 2023)
- CRACMM2 updates the isoprene chemistry to a new version of the AMORE isoprene condensation and merges the CRACMM and CRACMM-AMORE development lines
- Development of CRACMM2 was primarily focused on improving the representation of secondary formaldehyde (HCHO) which was too low in CRACMM1
- HCHO has direct health effects as a HAP, so model-based estimates of HCHO cancer risk may be too low
- HCHO can be used in inverse modeling applications to constrain emission of isoprene and other reactive organic carbon (ROC) species using satellite-based HCHO observations, so underestimated secondary HCHO could bias inverse analyses

Chemistry updates

Name	Description
AMORE isoprene	Improve isoprene degradation chemistry; Increase HCHO production; Improve SOA precursors
ECH4	Track effects of locally emitted methane in addition to global background
heterogeneous	Add heterogeneous uptake of HO_2 and NO_3 radicals for effects on ozone
aromatics	Add two new explicit HAP species (styrene and ethylbenzene); Update xylene isomer emission mapping
monoterpenes	Add β-pinene products to API (previously just α-pinene products); Update HCHO production
MT nitrates	Update NOx recycling and aerosol formation
MT aldehydes	Reduce autoxidation rates of monoterpene aldehyde peroxy radicals; Update peroxy radical product from monoterpene ozonolysis

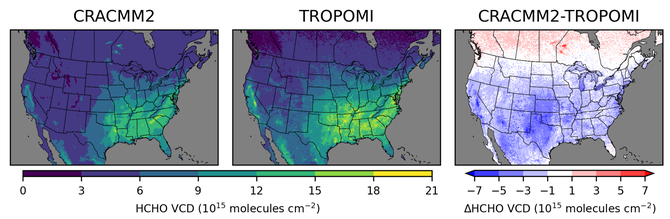
Implications for HCHO

CMAQ surface concentrations



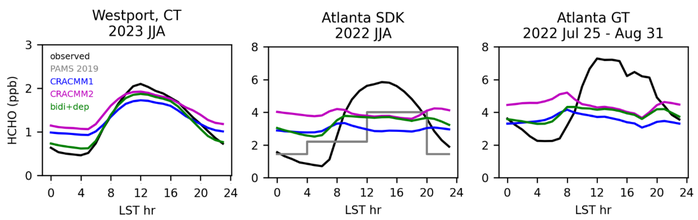
June-August 2019 CMAQ-simulated average HCHO during peak photochemical production (11am-3pm) with CRACMM1 and CRACMM2 (top) and the changes due to updates in the isoprene and monoterpene systems (bottom)

Satellite-based observations



June-August 2019 CMAQ-simulated HCHO vertical column density (VCD) compared to TROPOMI. CRACMM2 is improved compared to CRACMM1 but still lower than TROPOMI across the CONUS, particularly in western US oil and gas producing regions and parts of California.

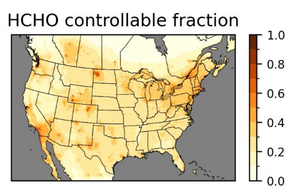
Surface observations



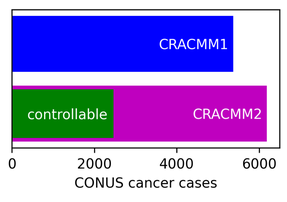
PAMS 2019: 8-h canister samples at Atlanta South DeKalb (SDK) photochemical assessment monitoring station (PAMS)
bidi+dep: results using CRACMM2 chemistry with updates to add HCHO bidirectional flux and increase nocturnal deposition

- Surface observations from field deployments (2023 STAQS; 2022 Atlanta from Mouat et al. 2024) in different years due to lack of observations in 2019 modeling year
- Averaged to diurnal cycle for qualitative comparison
- Diurnal variability improved with chemistry and deposition updates; more work needed in the southeastern US

Controllable HCHO and cancer risk

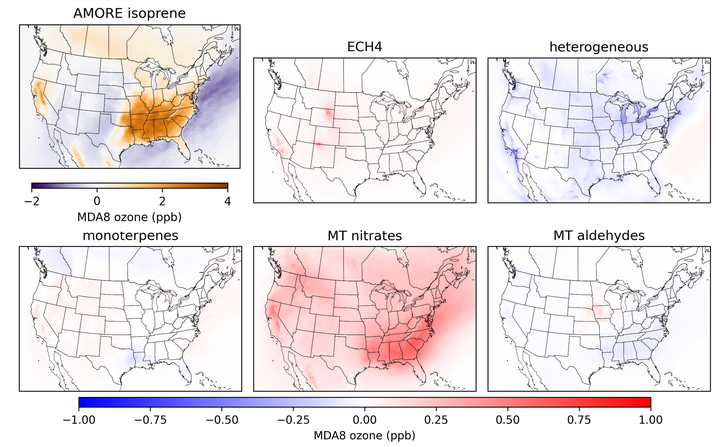


Controllable HCHO: HCHO from anthropogenic NOx and ROC emissions

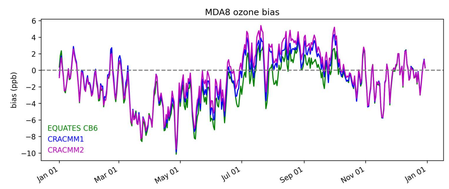


Estimated 6200 lifetime cancer cases with 40% from controllable HCHO (9000 cases for all ambient air toxics in 2019 AirToxScreen)

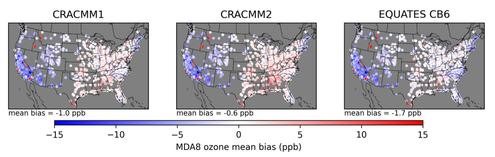
Effects on ozone



June-August average of incremental impacts on MDA8 ozone



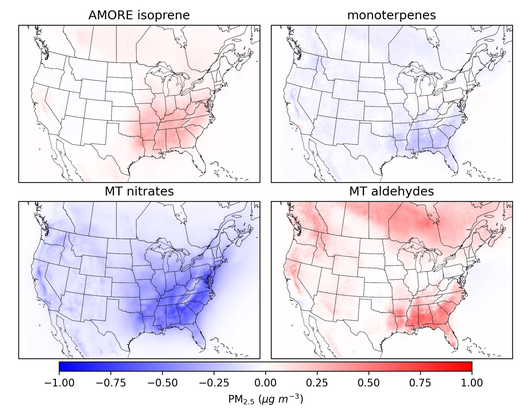
Averaged across sites, negative bias in spring and positive bias in summer (improvements in spring coming in CRACMM3 with aerosol nitrate photolysis)



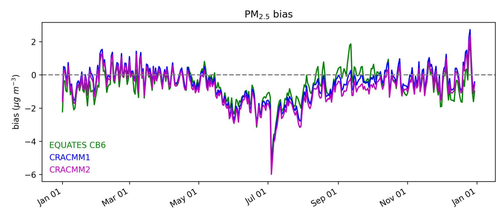
Averaged over the year, offsetting east/west biases (ozone in west will increase with aerosol nitrate photolysis)

EQUATES: EPA's Air Quality Time Series (Foley et al. 2023)

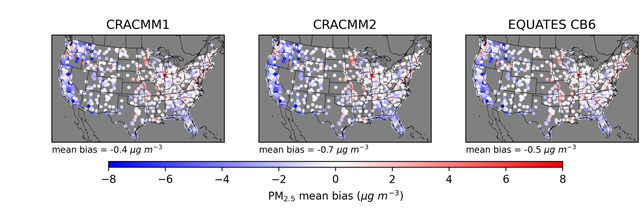
Effects on $PM_{2.5}$



June-August average of incremental impacts on $PM_{2.5}$. Some chemistry updates not shown as they had negligible impacts on $PM_{2.5}$.



Low bias in summer with contributions from several species (including OC, EC, SO_4, NO_3, NH_4)



Potential for future improvements in sulfate to also contribute to increased IEPOX uptake to improve OC

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References: Pye et al. ACP (2023) https://doi.org/10.5194/acp-23-5043-2023; Place et al. ACP (2023) https://doi.org/10.5194/acp-23-9173-2023; Skipper et al. EGUsphere (2024) https://doi.org/10.5194/egusphere-2024-1680; Wiser et al. GMD (2023) https://doi.org/10.5194/gmd-16-1801-2023; Mouat et al. AMT (2024) https://doi.org/10.5194/amt-17-1979-2024; Foley et al. DiB (2023) https://doi.org/10.1016/j.dib.2023.109022