SOA Simulations from a New Sectional Aerosol Treatment in CAM5

Objective:

- Evaluate the radiative effects of SOAs on regional and global scales
- Explore the environmental impacts on SOA formation

Climate Relevant SOA Property(s) Investigated:

mass concentrations, size distributions, and optical properties

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Summary of progress:

- We have implemented a sectional aerosol package with comprehensive SOA formation into CAM5. Simulations by CAM5_Sect are directly comparable to observations.
- Our results demonstrate that SOAs make up a significant portion of global aerosol concentrations, and SOA formation is pronounced in tropical forested areas where the biogenic emissions of VOCs are large.
- We are in the process to account for more cutting edge aspects of SOA chemistry, including aqueous SOA formation.

Challenges or needed resources/collaborators:

- Need observations for model evaluation
- Need more lab studies for modeling SOA yields from VOCs

Features of CAM5_Sect with comprehensive SOA formation

Chemistry

- MOZART (Model for OZone And Related chemical Tracers, Emmons et al., 2009) photochemistry and sulfate chemistry (200 reactions)
- SOA chemistry (10 reactions)

  Empirical representation of SOA precursors

  Toluene + OH → c_1 TOLAER1 + c_2 TOLAER2 + OH
  Xylene + OH → c_1 XYLAER1 + c_2 XYLAER2 + OH
  Humulene + OH → HUMAER + OH
  Limonene + OH → c_i LIMAER1 + c_2 LIMAER2 + OH
  α-Pinene + OH → c_i APINAER1 + c_2 APINAER2 + OH
  α-Pinene + O3 → c_3 APINAER3 + c_4 APINAER4 + O3
  β-Pinene + OH → c_i BPINAER1 + c_2 BPINAER2 + OH
  β-Pinene + O3 → c_i BPINAER3 + c_2 BPINAER4 + O3
  β-Pinene + NO3 → BPINAER5 + NO3
  Isoprene + OH → c_i ISOPAER1 + c_2 ISOPAER2 + OH

  XXXAER1, .. XXXAER5 are the surrogate SOA precursor compounds.

  Coefficients ci for each reaction are based on smog chamber experiments
- 111 gas species

Aerosol microphysics

- MADRID 1 (Model of Aerosol Dynamics, Reaction, Ionization, and Dissolution, Zhang et al., 2004)
  - ISORROPIA for inorganic aerosols in thermodynamic equilibrium with gas phase precursors
  - Empirical gas/particle partition coefficients for condensable organic species
- 224 aerosol tracers in 8 size bins
  - 26 aerosol components (18 for SOAs)
    Na, SO_4, NH_4, NO_3, Cl, Dust, EC, POM
    14 biogenic SOAs, 4 anthropogenic SOAs
  - Aerosol water
  - Aerosol number

Interactive Biogenic VOC emissions

- MEGAN (Model of Emissions of Gases and Aerosols from Nature, Guenther et al., 2006)
- 15 VOC species from CLM

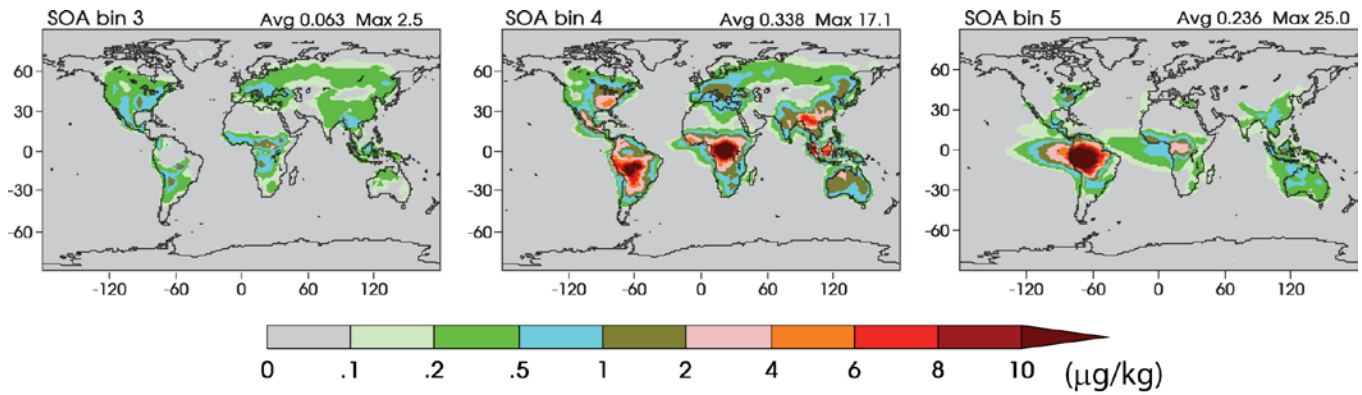
  Isoprene (C_5H_8), α-Pinene ($C_{10}H_{16}$), β-Pinene ($C_{10}H_{16}$), Limonene ($C_{10}H_{16}$), Humulene ($C_{15}H_{24}$), Methanol (CH_3OH), Acetone (CH_3COCH_3), Acetaldehyde (CH_3CHO), Formaldehyde (CH_2O), Carbon monoxide (CO), Ethane (C_2H_6), Propane (C_3H_8), Ethene (C_2H_4), Propene (C_3H_6), Ethanol (C_2H_5OH)

Results

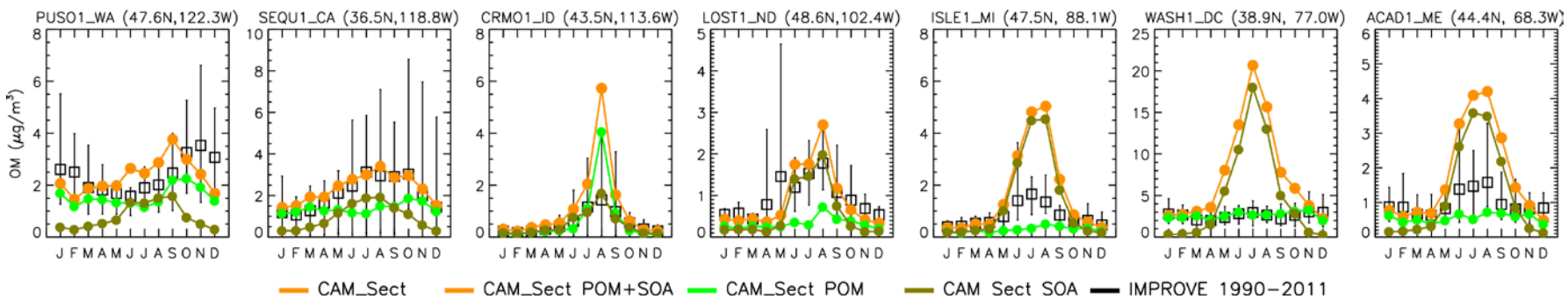
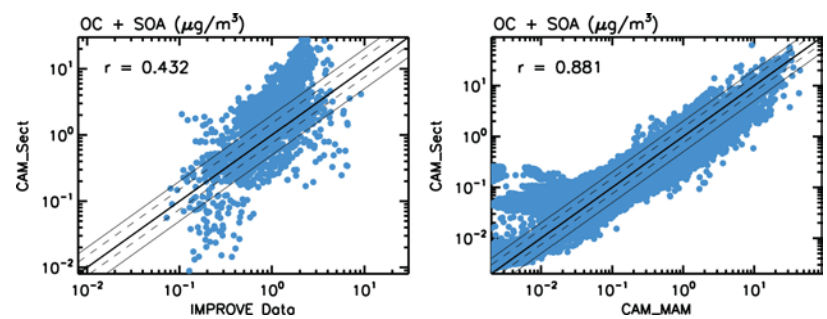
Annual SOAs at surface for size bins 3 - 5

8 size bins (in diameter)

bin1: 0.022 - 0.046 µm
bin 2: 0.046 - 0.10
bin 3: 0.10 - 0.22
bin 4: 0.22 - 0.46
bin 5: 0.46 - 1.0
bin 6: 1.0 - 2.2
bin 7: 2.2 - 4.6
bin 8: 4.6 - 10



Comparison of seasonality of simulated OC with IMPROVE data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