Impact of RACM2, halogen chemistry, and updated ozone deposition velocity on hemispheric ozone predictions

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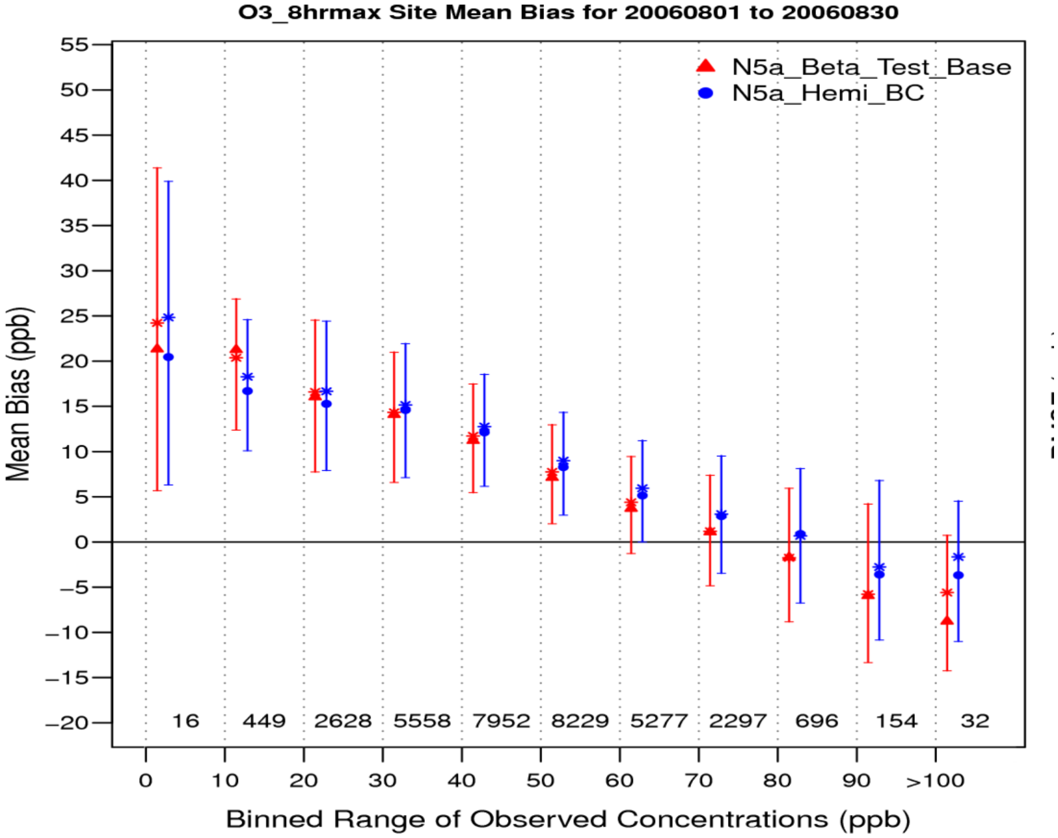
Overview of CB05TU and RACM2

- Carbon Bond mechanism has been widely used in air quality models
  - CMAQ currently uses Carbon Bond 2005 with updated toluene chemistry (CB05TU)
  - 172 reactions involving 65 species (References: Yarwood et al., 2005 and Whitten et al., 2010)
- Regional Atmospheric Chemistry Mechanism (RACM2) is a new mechanism
  - 363 reactions involving 120 species (Reference: Goliff et al., 2013)
  - There are many differences between the two mechanisms
- Examine the impact of these mechanisms on ozone over northern hemisphere
  - Motivations:
  - We use hemispheric predictions for generating LBC for continental US
  - Previous studies suggest LBCs are important for predicting ozone in the continental US
  - Mathur et al (2010, 2012) showed CMAQ over-predicts ozone in summer in the US

LBC impact on Surface O_3 Predictions

Max. 8-Hr; AQS sites; **August 2006**

CMAQ performance in CONUS domain using 12-km grids (Mathur et al., 2012)



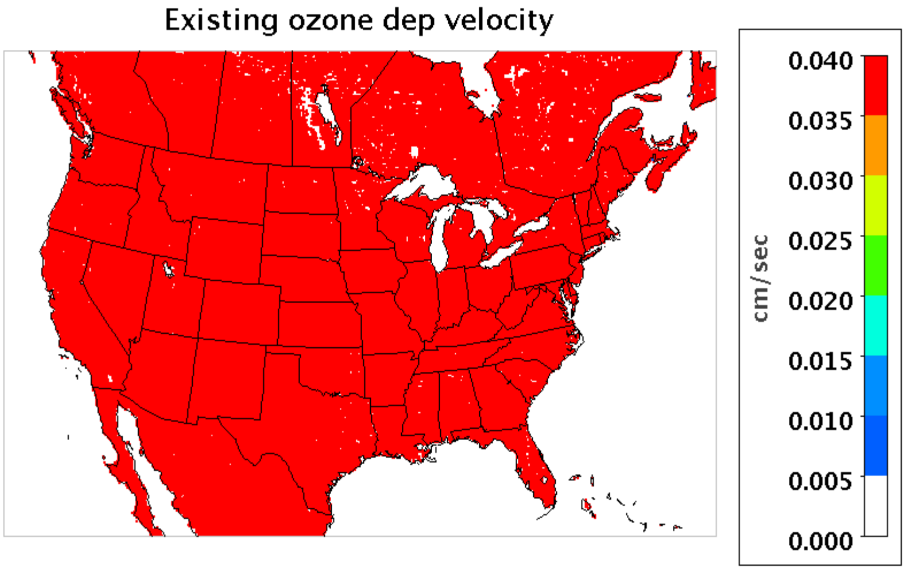
Halogen chemistry over gulfs and oceans

- Recent studies suggest halogen chemistry can destroy ozone over water
- Bromine/iodine chemistry are important
- Current CMAQ does not contain these reactions and their emissions
- Read et al. (2008) and Mahajan et al. (2010) measured O_3 in the Cape Verde archipelago in Atlantic Ocean
  - They suggested halogens can destroy ozone by ~2.0 ppbv/day
  - We developed an effective ozone loss reaction using data from Read et al. (2008) with a first order loss of 2.0×10^{-6} s^{-1} for the reaction
  - We employed it in CMAQ to account for the halogen mediated O_3 loss over the over gulfs and oceans only during day and within PBL
  - Read et al., *Nature*, 453, 1232-1235, 2008 and Mahajan et al., Atmospheric Chemistry & Physics, 2010

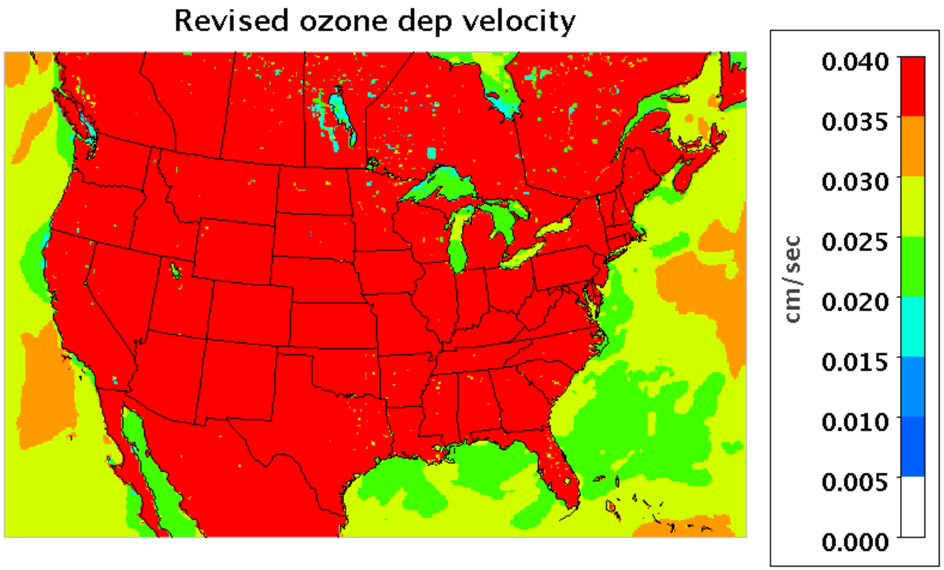
Ozone deposition velocity over water

- Helmig et al. (2012) measured ozone fluxes
  - Over Gulf of Mexico, Atlantic Ocean, and Pacific Ocean
  - Reported median ozone deposition velocity ranged 0.009-0.034 cm s^{-1}
  - Ref: Helmig et al., *JGR*, 117, D04305, 2012
- We analyzed CMAQ ozone deposition velocity over gulfs and oceans
  - CMAQ values are an order of magnitude lower than observed values
  - We revised ozone deposition treatment in CMAQ following Chang et al. (2004)
  - It enhanced ozone deposition velocity similar to the observed values over water
  - Ref: Chang et al., Atmospheric Environment, 38, 1053–1059, 2004

CMAQ estimated O_3 deposition velocity



Ozone deposition velocity with the existing treatment



Ozone deposition velocity with the revised treatment

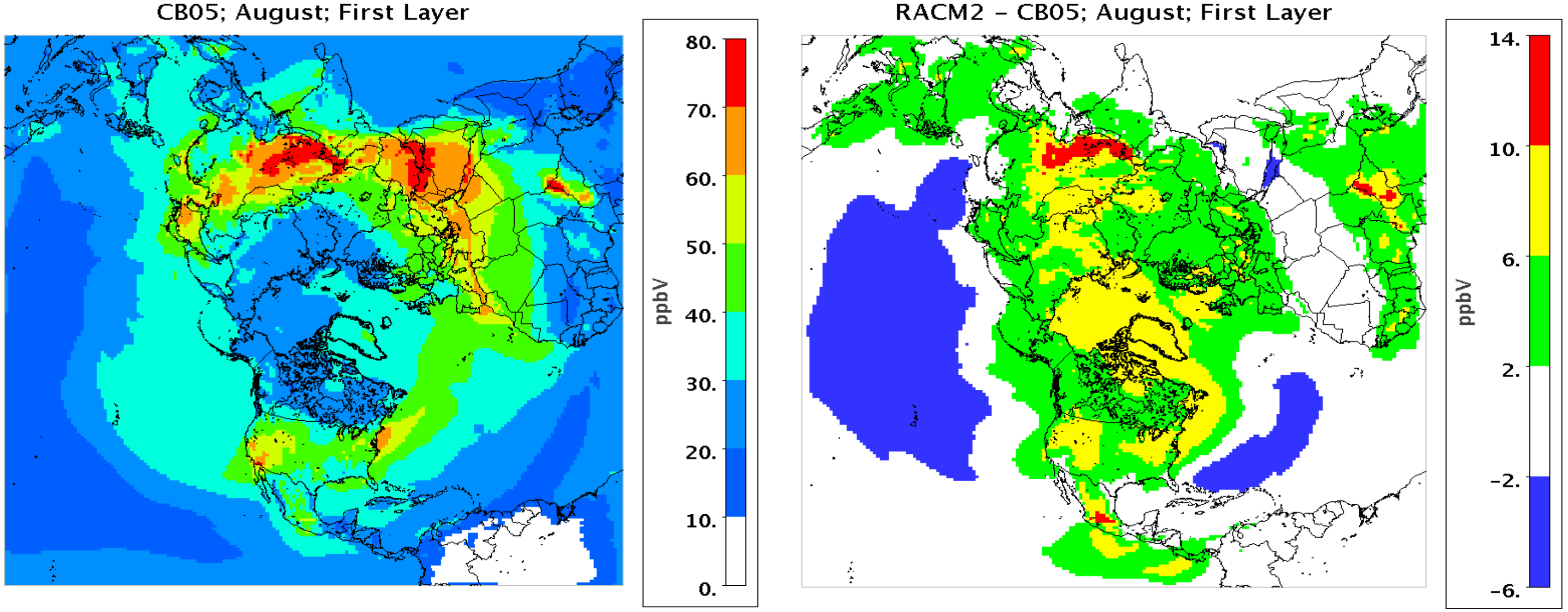
Modeling details

- Community Multiscale Air Quality (CMAQv50) hemispheric model
  - WRF-CMAQ coupled model
  - Modeling domain: northern hemisphere
  - Horizontal grid size: 108-km
  - Vertical resolution: 44 layers from surface to 50 mbar (20-m surface layer)
- Model-ready emissions were developed using
  - Emissions Database for Global Atmospheric Research (EDGAR)
- IC – Results from a previous hemispheric CMAQ annual simulation
- BC – Clean air profiles along the equator (Mathur et al., 2010 and 2012)
- Simulation period
  - Three months: June, July, August, 2006
  - Spin-up period: One-month (May, 2006)

Modeling details

- Three different model simulations were performed
  - CB05TU
  - RACM2
  - RACM2 + halogen reaction + revised O_3 deposition treatment
- Compare model predictions with observations from several field campaigns
  - 2006 TexAQS - Texas Air Quality Study 2006
  - IONS-06 - INTEX Ozonesonde Network Study
  - SHADOZ - Southern Hemisphere ADditional OZonsondes

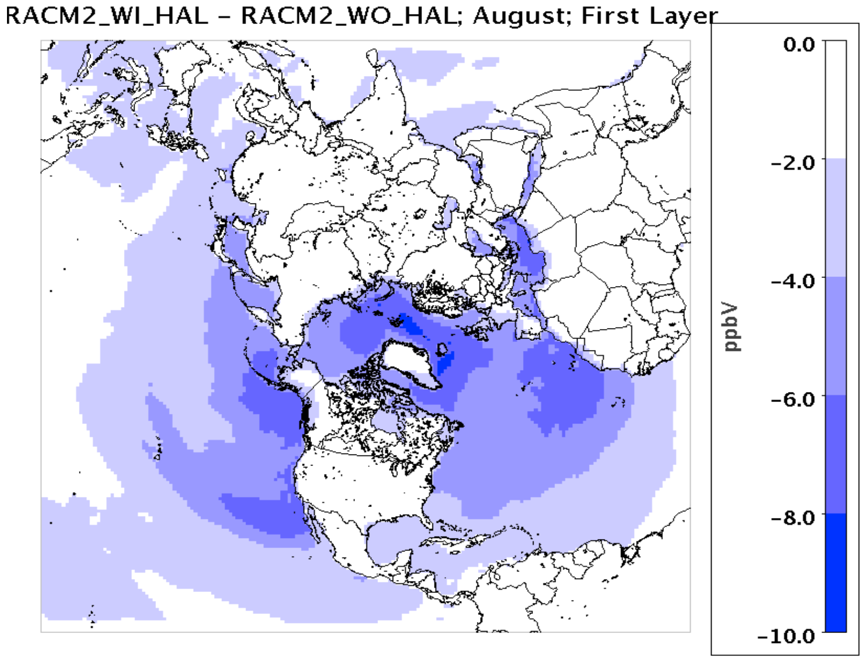
CB05TU predicted mean surface ozone and differences between RACM2 and CB05TU predictions



RACM2 enhances ozone in polluted areas while decreasing it in remote areas
Changes occur due to greater NO_x recyling and active organic chemistry in RACM2

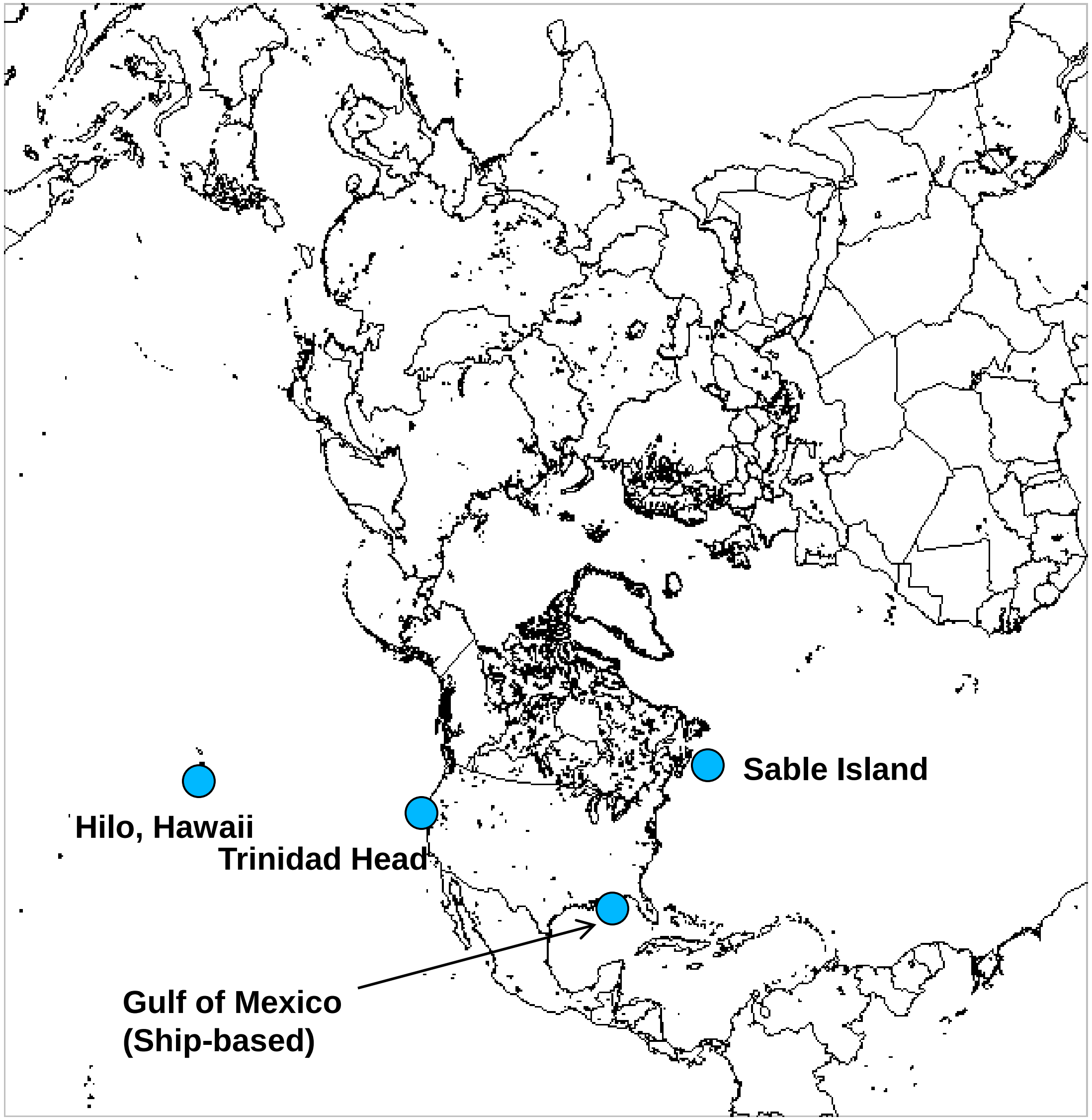
Effect of the halogen reaction and the updated ozone deposition velocity on ozone predictions

Difference in monthly-mean ozone

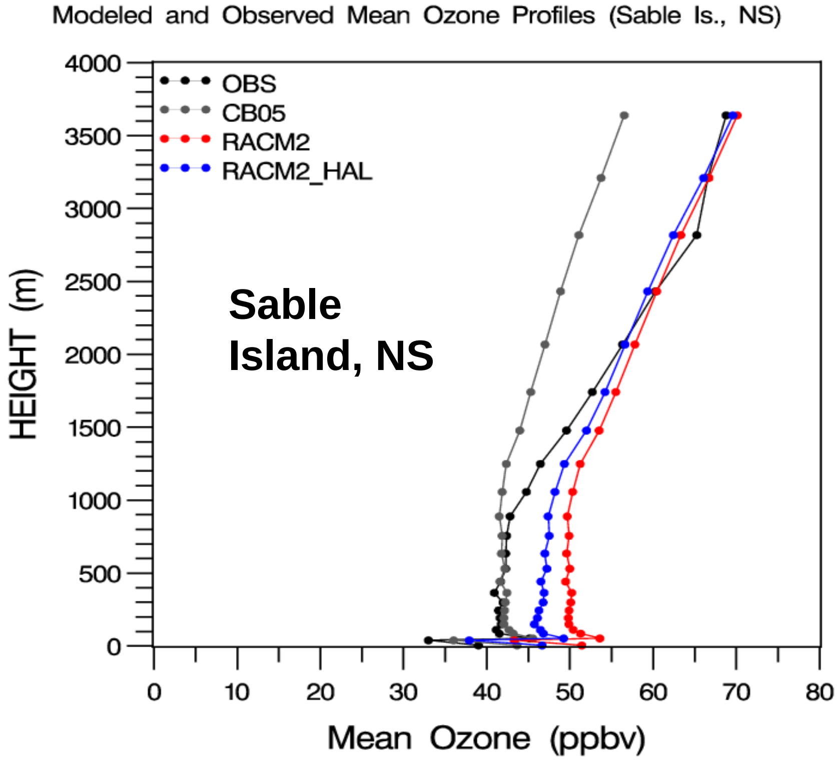


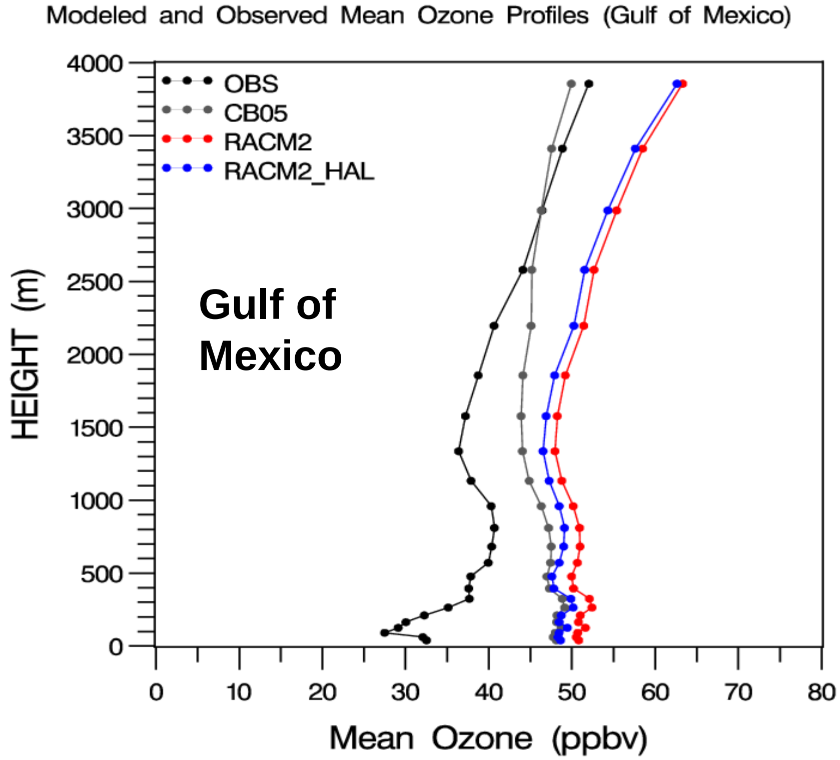
The halogen reaction and the enhanced deposition velocity decrease O_3 over water. Most of the decreases occur due to the halogen reaction.

Observation sites for model comparison



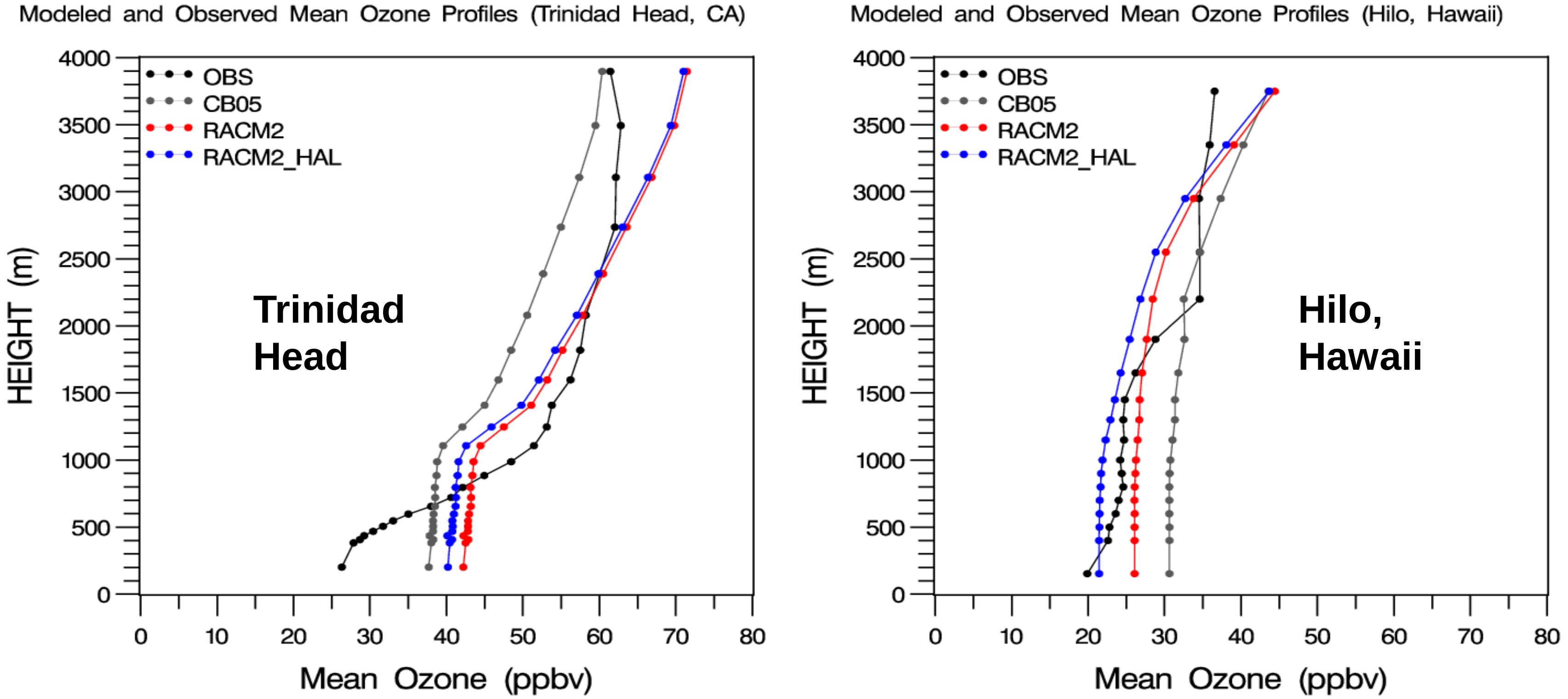
Comparison with observed data at Sable Island and Gulf of Mexico





RACM2 over-predicts ozone compared to observations near surface
Mixed performances aloft
The halogen reaction and revised ozone deposition improve the comparison

Comparison with observations at Trinidad Head and Hilo, Hawaii



At Trinidad Head, both over-predict near surface but RACM2 is better ~1000-3000-m

At Hilo, RACM2 predictions compare better

The halogen reaction and revised ozone deposition improve the comparison

Summary

- RACM2 enhances O_3 in polluted areas while decreasing it in remote areas
  - RACM2 over-predicts surface O_3 compared to observed data in polluted areas
  - RACM2 improves aloft O_3 predictions in some cases in polluted areas
  - RACM2 predictions compare better with observed data in remote areas (Hilo)
- Incorporated an effective halogen reaction/updated O_3 deposition treatment
  - They reduce O_3 predictions over water bodies
  - The majority of the reduction occurs due to the halogen reaction
  - Model O_3 predictions with these treatments compare better with observed data
- Future plans
  - Further revise the halogen reaction and ozone deposition treatment
  - Perform additional simulations and generate BC for continental US
  - Perform simulations with these boundary conditions for continental US