

Development and Initial Application of WRF-Chem-GHGs: Integrated Modeling of Air Quality, Carbon, and Climate

**Yang Zhang¹, Kai Wang¹, Xiao-Yang Chen¹, Daniel Schuch¹,
Eeshan Basu¹, Siqi Ma², Daniel Tong^{2,3}, and Ravan Ahmadov⁴**

¹Department of Civil and Environmental Engineering, Northeastern University

²Department of Atmospheric, Oceanic and Earth Sciences, George Mason University

³IM Systems Group

⁴CIRES, University of Colorado, Earth Prediction Advancement Division, Global Systems Laboratory, National Oceanic and Atmospheric Administration

The 20th Annual CMAS Conference (Virtual), November 1-5, 2021

Background and Objectives

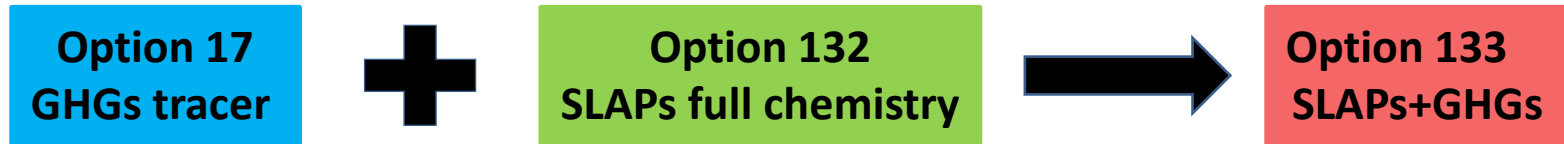
- **Background**

- Current regional/urban air quality models (e.g., CMAQ and WRF-Chem) focus on atmospheric evolution of short-lived air pollutants (SLAPs)
- Mitigation of air pollution, carbon, and climate changes requires an integrated modeling system to simulate both SLAPs and greenhouse gases (GHGs)

- **Objectives**

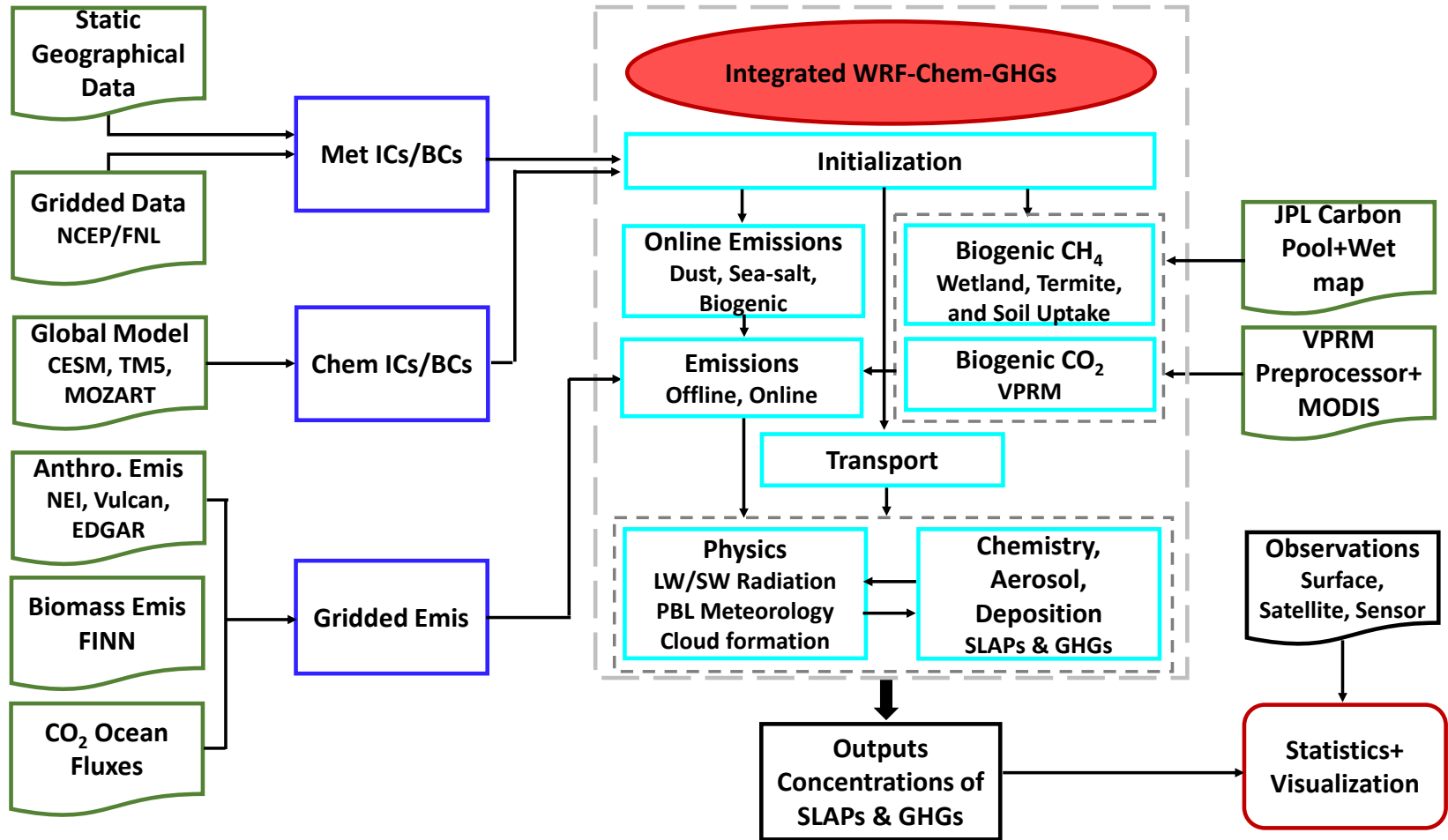
- Develop a coupled model system based on WRF-Chem to simultaneously simulate the evolution of SLAPs and GHGs and their interactions for integrated assessment and policy analysis (referred to as **WRF-Chem-GHGs**)
- Perform long-term simulations with this model under current and future scenarios in a warming climate to inform mitigation strategies that co-benefit air quality/carbon/climate change management at national/region/city scales

New Representations in WRF-Chem-GHGs



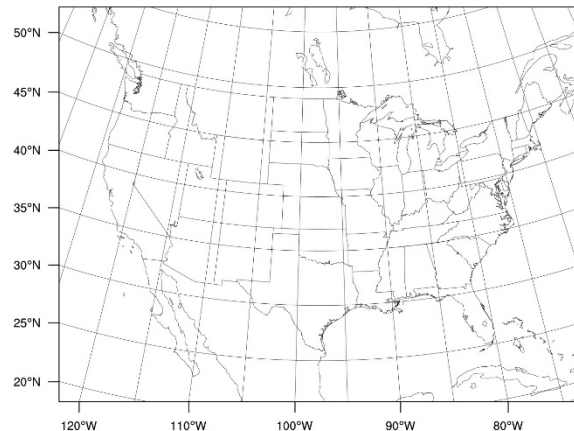
- An option to use anthropogenic and biogenic CO₂ and CH₄ emissions
- An online Vegetation Photosynthesis and Respiration Model (VPRM) that uses predicted temperature and radiation to estimate biogenic CO₂ fluxes
- The use of dynamic lateral boundary conditions (BCs) and initial conditions (ICs) for CO₂ and CH₄ based on Carbon tracker CT2019B and MOZART, respectively
- The use of time- and space-varying prognostic CO₂ and CH₄ concentrations in the RRTMG longwave and shortwave radiation schemes
- Chemical production of CO₂ from the oxidation of CO, CH₄, and volatile organic compounds (VOCs) (ongoing)

Integrated WRF-Chem-GHG Modeling System



Simulation Setup and Evaluation Protocol for Initial Application

- **Period:** Jan. and Jul., 2012
- **Domain:** CONUS, 142×112 grid cells
- **Horizontal resolution:** 36 km
- **Vertical resolution:** 34 layers (up to 100 mb)
- **Emissions:**
 - **Anthropogenic:** NEI 2016(v1) for SLAPs; Vulcan, EDGAR, ODIAC, FFDAS for CO_2 & EDGAR for CH_4
 - **Biogenic emissions:** MEGAN2; **Dust:** AFWA scheme, **Sea salt:** Gong scheme for SLAPs, VPRM for CO_2
- **ICs and BCs:**
 - **Chemical:** Modified CESM/CAM5 for SLAPs; TM5 for CO_2 ; MOZART for CH_4/CO
 - **Meteorological:** NCEP/FNL
- **Chemical options**
 - **Gas-phase chemistry:** Modified CB05
 - **Aerosol module:** MADE/VBS
 - **Cloud chemistry module:** AQCHEM
- **Data for model evaluation:**
 - AQS/CASNET/IMPROVE/CSN: O_3 , $\text{PM}_{2.5}$
 - CCGG: CO_2
 - NCDC/NADP: T2, RH2, WS10, WD10, Precip



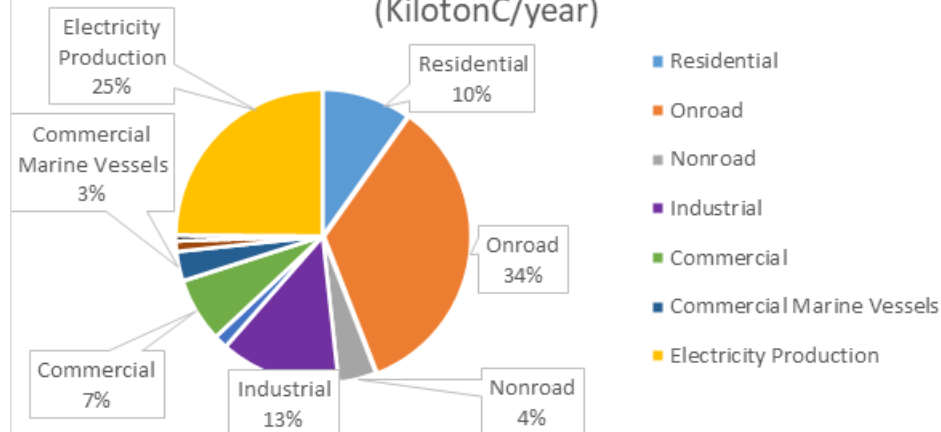
• Evaluation Protocol

- **Statistics:** Mean Bias (MB), Normalized Mean Bias (NMB), Normalized Mean Error (NME), Root Mean Square Error (RMSE), Correlation coefficient (R)
- Benchmark MBs for T2, WS10, and WD10: $\leq \pm 0.5^\circ\text{C}$, $\pm 0.5 \text{ m s}^{-1}$, and $\pm 10^\circ$, respectively
- Benchmark NMBs of $\leq \pm 15\%$, $\pm 30\%$, and $\pm 5\%$; NMEs of $< 25\%$, 50% , and 5% , for O_3 , $\text{PM}_{2.5}$, CO_2 , respectively
- **Spatial distribution:** overlay, MB, NMB
- **Temporal variation:** diurnal and time series plots

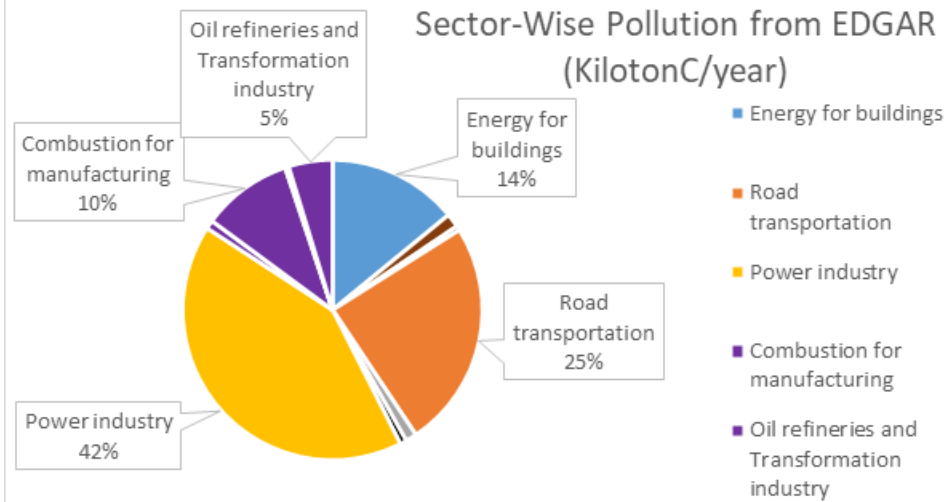
Anthropogenic CO₂ Emission Datasets

Dataset	Temporal Resolution	Spatial Resolution	Year	kilotonC/year	Million metrictonCO ₂ /year	EIA (million metrictonCO ₂ /year)	Relative Difference with respect to EIA (%)
EDGAR	Annual	0.1°	2012	1376813.00	4579.76	5229	14.18
VULCAN	Hourly	1-km	2012	1515675.00	5041.66		3.72
ODIAC	Monthly	1°	2012	1302459.00	4332.43		20.69
FFDAS	Annual	0.1°	2012	1359665.00	4522.71		15.62

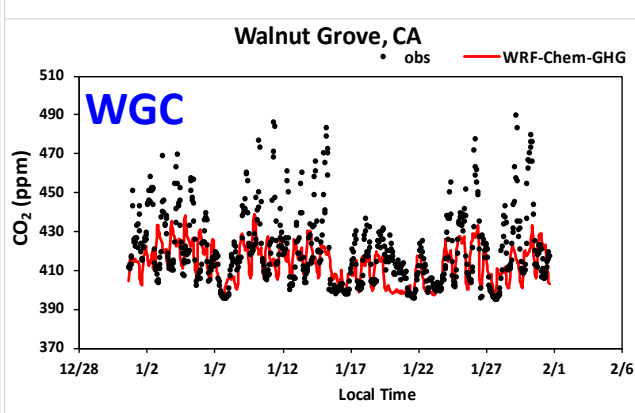
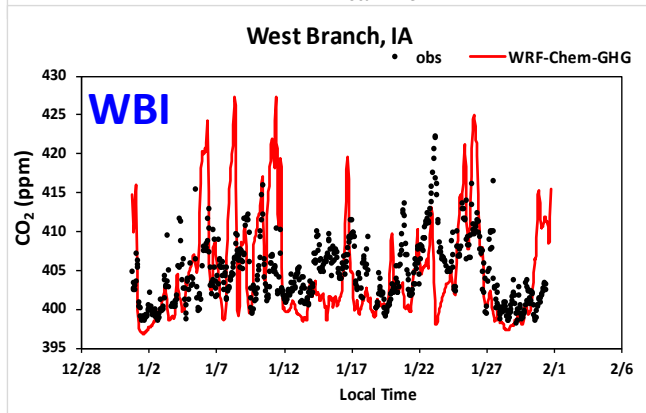
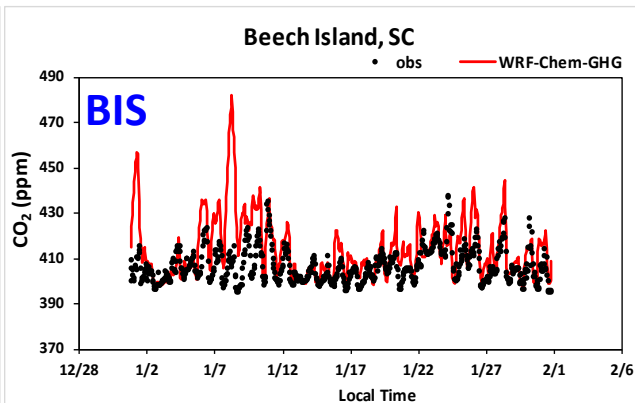
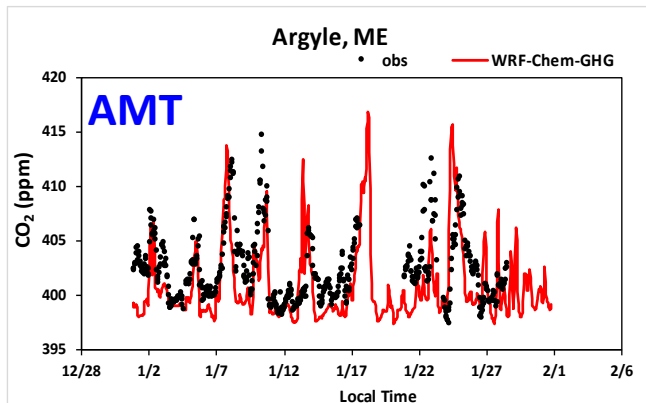
Sector-Wise Pollution from VULCAN
(KilotonC/year)



Sector-Wise Pollution from EDGAR
(KilotonC/year)

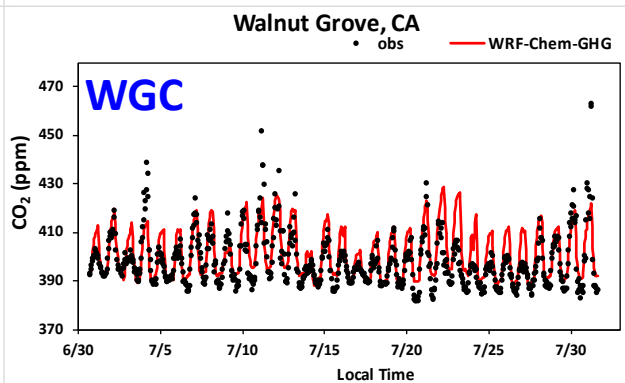
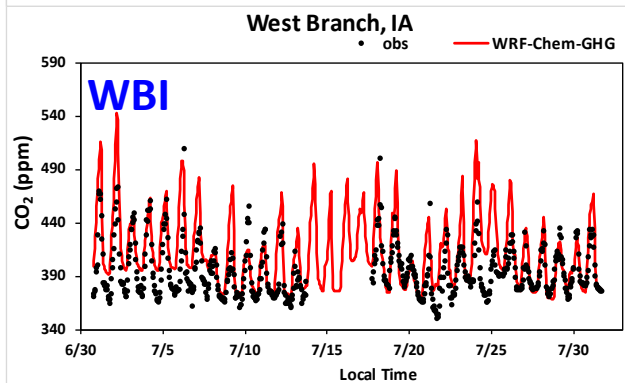
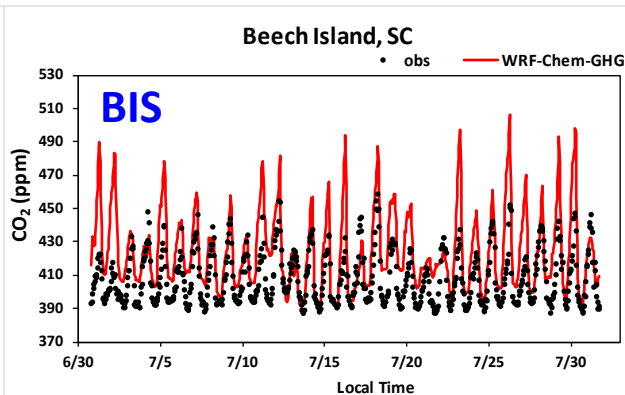
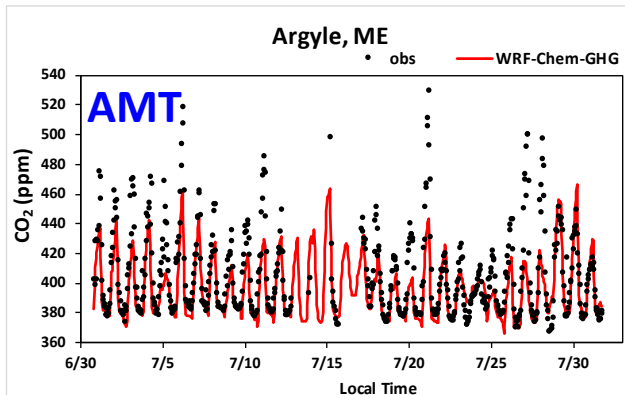


WRF-Chem-GHG: CO₂ Mixing Ratio, Jan 2012



- Temporal variation of CO₂ is well captured for most days at all sites except WGC
- Underpredictions of may be associated with uncertainties in anthropogenic emissions at WGC

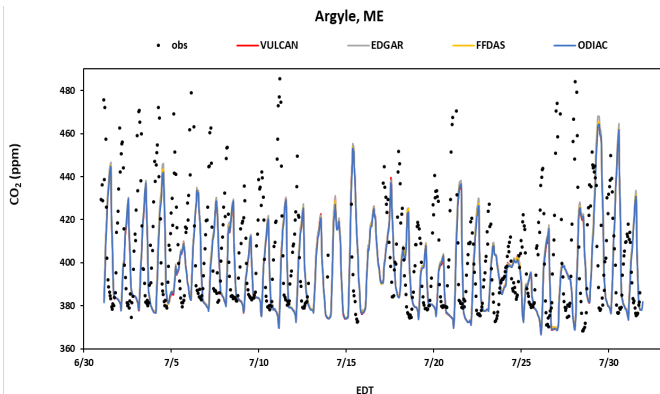
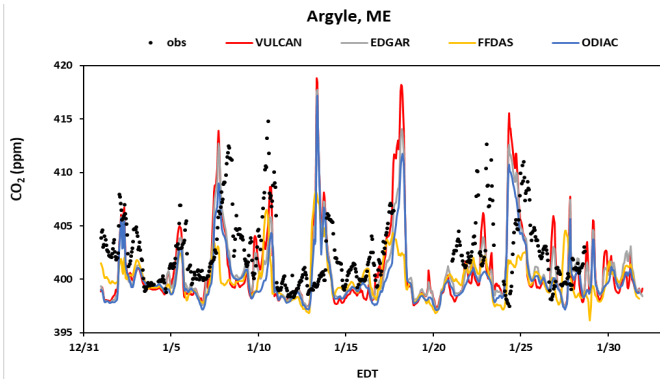
WRF-Chem-GHG: CO₂ Mixing Ratio, Jul 2012



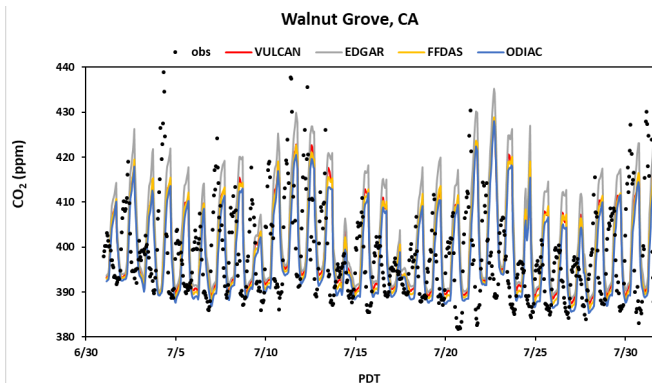
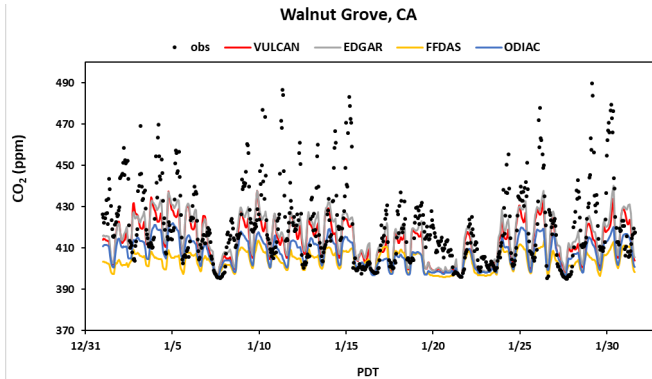
- Temporal variation of CO₂ is well captured for most days at all sites
- Underpredictions may be associated with uncertainties in biogenic emissions at AMT, and firework and wildfire emissions at WGC

Sensitivity to CO₂ Emissions, Jan/Jul 2012

AMT

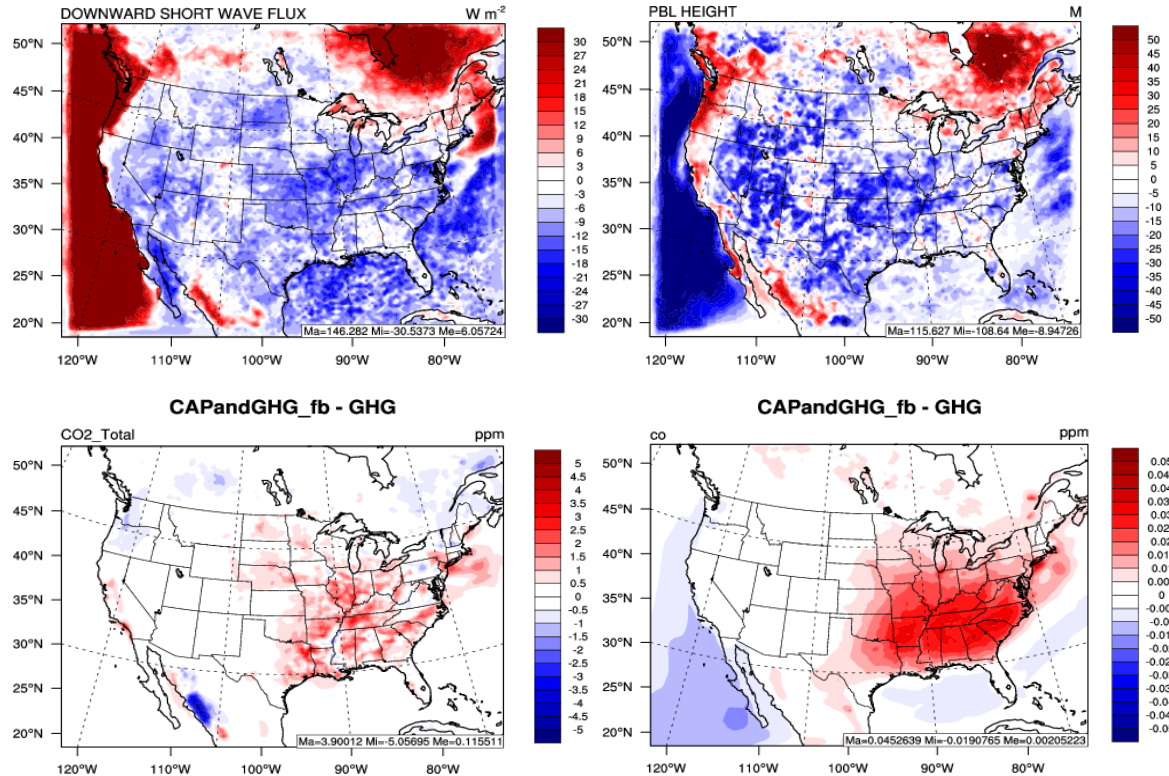


WGC



- CO₂ predictions are sensitive to different emission datasets in both months except at AMT in Jul
- VULCAN/EDGAR give the highest CO₂ in Jan/Jul, respectively

Chemistry and CO₂ Feedbacks, Jul 2012



- Prognostic CO₂ in RRTMG predicts slightly stronger shortwave radiation, which is compensated by the reduction due to chemistry feedback, leading to a net decrease in shortwave radiation, temperature, and PBL height.
- Lower T2 can increase biogenic CO₂, thus total CO₂. Lower PBLH can increase CO.

Summary of Preliminary Results and Future Work

- **WRF-Chem-GHGs is operational with overall good skill in reproducing observed CO₂. Underpredictions are mainly attributed to uncertainties in CO₂ emissions**
- **WRF-Chem-GHGs can simulate SLAPs and CO₂ feedbacks to boundary layer meteorology, radiation, and cloud formation, which in turn affect their concentrations and distributions**
- **Future work:**
 - Implement chemical production of CO₂
 - Account for CH₄ biogenic emissions from wetland, termite, and soil uptake
 - Evaluate for multi-year (2012-2017) at three grid resolutions (36-, 6- and 1-km) to establish baseline for future scenarios
 - Apply for 2047-2052 under future energy, climate, and land use change scenarios

Acknowledgements

- This project is sponsored by NOAA Office of Climate AC4 Program (NA20OAR4310293)
- Other project team members: Matthew Eckelman and Kaixin Huang, Northeastern University; Dan Loughlin, US EPA
- Collaborators: Thomas Koch, University of Jena, Germany, for providing VPRM preprocessor, Thomas Nehrkorn and Archana Dayalu from AER, Inc. for helpful discussions on VPRM and CH4 emissions
- High performance computing was support by the Stampede XSEDE high performance computing support under the NSF ACI 1053575 and Cheyenne (ark:/85065/d7wd3xhc) of NCAR's CISL, sponsored by the NSF