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Supplement of

Decadal evaluation of regional climate, air quality, and their interactions over the continental US and their interactions using WRF/Chem version 3.6.1

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1. List of Acronyms

Table S1. List of Acronyms used in the paper

Acronym	Full Name
AER/AFWA	The Atmospheric and Environmental Research Inc. and Air Force Weather Agency scheme
AERONET	The Aerosol Robotic Network
AIRS-AQS	the Aerometric Information Retrieval System– Air Quality System
AOD	Aerosol optical depth
BCs	Boundary Conditions
CAM5	The Community Atmosphere Model version 5
CASTNET	The Clean Air Status and Trends Network
CALIOP	The Cloud-Aerosol Lidar with Orthogonal Polarization
CB05	The Carbon Bond 2005
CCN	Cloud condensation nuclei
CDNC	Cloud droplet number concentration
CERES	The Clouds and the Earth’s Radiant Energy System
CESM	The Community Earth System Model
CESM_NCSU	CESM/CAM5 developed at the North Carolina State University
CLDFRA	Cloud fraction
CMAQ	The Community Multiscale Air Quality Model
CMIP5	The Coupled Model Intercomparison Project Phase 5
CONUS	Continental U.S.
COT	Cloud optical thickness
CRU	Climatic Research Unit
CWP	Cloud water path
EC	Elemental carbon
GCMs	General circulation models
GCTMs	Global chemical transport models
GLW	Longwave radiation
GPCP	Global Precipitation Climatology Project
GSW	Net shortwave radiation
ICs	Initial Conditions
IMPROVE	The Interagency Monitoring of Protected Visual Environments
IOA	Index of Agreement
IPCC	The Intergovernmental Panel on Climate Change
JFD	January, February and December
JJA	June, July, and August
LSM	Land Surface Model
LST	local standard time
LWCF	Longwave cloud forcing

MADE/VBS	The Modal for Aerosol Dynamics in Europe / Volatility Basis Set
MAM	March, April, and May
MAN	The Maritime Aerosol Network
MB	Mean bias
MEGAN2	The Model of Emissions of Gases and Aerosols from Nature version 2
MODIS	The Moderate Resolution Imaging Spectroradiometer
MSKF	The Multi-Scale Kain-Fritsch cumulus scheme
NADP	The National Atmospheric Deposition Network
NARR	The North American Regional Reanalyses
NCDC	The National Climatic Data Center
NCEP	The National Centers for Environmental Prediction
NCEP FNL	The NCEP Final Reanalyses
NEI	The National Emission Inventory
NH_4^+	Ammonium
NMB	Normalized mean bias
NME	Normalized mean error
NO_3^-	Nitrate
NO	Nitric oxide
NO_2	Nitrogen dioxide
NO_x	Nitrogen oxide
NOAH	The National Center for Environmental Prediction, Oregon State University, Air Force, and Hydrologic Research Lab
O_3	Ozone
OA	Organic aerosol
OC	Organic carbon
OMI	The Ozone Monitoring Instrument
$PM_{2.5}$ and PM_{10}	Particulate matter with diameter less than and equal to 2.5 and 10 μm
POA	Primary organic aerosol
PRECIS	Providing Regional Climates for Impacts Studies
PRISM	The Parameter-elevation Regressions on Independent Slopes Model
R	Correlation coefficient
RCMs	Regional climate models
RCP	The Representative Concentration Pathway
RH2	Relative humidity at 2-m
RRTMG	The Rapid and accurate Radiative Transfer Model for GCM
SEARCH	The Southeastern Aerosol Research and Characterization
SMOKE	The Sparse Matrix Operator Kernel Emissions model
SOA	Secondary organic aerosol
SO_2	Sulfur dioxide
SO_4^{2-}	Sulfate
SON	September, October, and November
STN	The Speciated Trends Network
SWCF	Shortwave cloud forcing
SWDOWN	Downward shortwave radiation
T2	Temperature at 2-m

TC	Total carbon, = EC + OC
WD10	Wind direction at 10-m
WRF	Weather Research and Forecasting model
WRF/Chem	The Weather Research and Forecasting model with Chemistry
WS10	Wind speed at 10-m

2. Mapping of RCP Emissions to CB05 species

Table S2 summarizes the mapping of species from RCP emissions to CB05 species for input into the model. The explanation for the mapping process can be found in the main text.

Table S2. CB05 emissions species for WRF/Chem, their associated full names, their availability in regards to the RCP emissions dataset, and the lumped RCP group species.

CB05 Species WRF/Chem	**Species Long name**	**RCP Species Available**	**RCP Group**
E_ALD2	Acetaldehyde	Group	Other Alkanals
E_ALDX	Higher Aldehydes	Group	Hexanes and Higher Alkanes
E_BENZENE	Benzene	Yes	
E_CH4	Methane	Yes	
E_CL2[1]	Chlorine	No	
E_CO	Carbon Monoxide	Yes	
E_ECI, E_ECJ, E_ECC	Elemental Carbon - Nuclei, Accumulation, Coarse Modes	No, Group, No	Black Carbon
E_ETH	Ethene	Yes	
E_ETHA	Ethane	Yes	
E_ETOH	Ethanol	Group	Alcohols
E_FORM	Formaldehyde	Yes	
E_HCL[1]	Hydrogen Chloride	No	
E_HONO[1]	Nitrous Acid	No	
E_IOLE	Internal Olefin Carbon Bond	Group	Other Alkenes and Alkynes
E_ISOP	Isoprene	No	
E_MEOH	Methanol	Group	Alcohols
E_NH3	Ammonia	Yes	
E_NH4I, E_NH4J[1]	Ammonium – Nuclei, Accumulation Modes	No, No	
E_NO	Nitrogen Oxides	Yes	
E_NO2[1]	Nitrogen Dioxide	No	
E_NO3I, E_NO3J[1]**, E_NO3C**	Nitrate – Nuclei, Accumulation, Coarse Modes	No, No, No	
E_OLE	Terminal Olefin Carbon Bond	Group	Other Alkenes and Alkynes
E_ORGI, E_ORGJ, E_ORGC	Organics – Nuclei, Accumulation, Coarse Modes	No, Group, No	Organic Carbon
E_PAR[1]	Paraffin Carbon Bond	No	
E_PM10	Unspeciated PM_{10}	No	
E_PM25	Unspeciated $PM_{2.5}$	No	
E_PM25I, E_PM25J[1]	Unspeciated $PM_{2.5}$ – Nuclei, Accumulation Modes	No, No	
E_PSULF[1]	Sulfuric Acid	No	
E_SO2	Sulfur Dioxide	Yes	
E_SO4I, E_SO4J,[1] **E_SO4C**	Sulfate – Nuclei, Accumulation, Coarse Modes	No, No, No	
E_TERP	Terpene	No	
E_TOL	Toluene	Yes	
E_XYL	Xylene	Yes	

[1] Emissions that were taken from 2002 NEI emissions, as well as 2006 and 2010 NEI-derived emissions

3. Observational Datasets for Model Evaluation and Operational Evaluation

Table S3 summarizes the observational databases and the variables evaluated in this work. For evaluation of chemical concentrations and meteorological variables, the surface networks include the National Climatic Data Center (NCDC) Quality Controlled Local Climatological Data (QCLCD), Clean Air Status and Trends Network (CASTNET), the Aerometric Information Retrieval System (AIRS) – Air Quality System (AQS), the Interagency Monitoring of Protected Visual Environments (IMPROVE), the Speciated Trends Network (STN), the Southeastern Aerosol Research and Characterization (SEARCH), and the National Atmospheric Deposition Network (NADP). Several aerosol-cloud-radiation variables are also evaluated against satellite retrievals including the Clouds and the Earth's Radiant Energy System (CERES) and the Moderate Resolution Imaging Spectroradiometer (MODIS).

NCDC QCLCD data contains data over 700 U.S. locations from July 1996 to December 2004, and over 1600 locations from 2005 onwards (http://www.ncdc.noaa.gov/data-access/land-based-station-data/land-based-datasets/quality-controlled-local-climatological-data-qclcd). CASTNET observations have been collected in a range of rural environments, from desert to agricultural locations, and from flat to complex terrains (http://java.epa.gov/castnet/epa_jsp/sites.jsp). It contains measurement data for meteorological variables and chemical concentrations. AIRS-AQS is the U.S. EPA's repository for ambient air quality data from over 5000 active monitors (http://www.epa.gov/ttn/airs/airsaqs/). While IMPROVE observations have been collected in protected visual environments, i.e., in National Parks and Wilderness Areas (http://vista.cira.colostate.edu/improve/), STN sites are located in a range of locations from urban to rural areas (http://www.epa.gov/ttnamti1/specgen.html). Both networks contain data for $PM_{2.5}$ and major $PM_{2.5}$ species. NADP contains precipitation data from rain gauges.

Table S3. Observational datasets and variables evaluated in this study.

Gases and PM Species			
Observational Database	**Variables Evaluated**	**Sampling Frequency**	**Number of Sites**
CASTNET	Max 1-hr and 8-hr O_3	Daily for O_3	~90
AIRS–AQS	O_3	Hourly	~1150
IMPROVE	$PM_{2.5}$, SO_4^{2-}, NO_3^-, NH_4^+, EC, OC	24-hour data. Data availability once every 3 days	~160
STN	$PM_{2.5}$, SO_4^{2-}, NO_3^-, NH_4^+, EC, TC	24-hour data. Data availability once every 3 days	~200
Meteorology			
Observational Database	*Variables evaluated*	*Temporal Resolution*	*Spatial Resolution*
NCDC QCLCD	T2, RH, WS10,WD10	Hourly	~700 before 2005 ~1600 after 2005
NADP	Precipitation	Weekly	255
Radiation and other Aerosol/Cloud variables			
Observational Database/ Satellite	*Variables evaluated*	*Temporal Resolution*	*Number of sites/ Spatial Resolution*
CERES	SWDOWN	Monthly	$1^o \times 1^o$
MODIS	AOD, CF, COT, CWP, QVAPOR, CCN	Monthly	$1^o \times 1^o$
MODIS derived based on Bennartz (2007)	CDNC	Monthly	$1^o \times 1^o$

4. Sensitivity simulations to determine precipitation and cloud bias over the Atlantic Ocean

A number of sensitivity simulations were conducted for the month of July 2005 to determine the cause of the precipitation bias, especially over the Atlantic Ocean. The sensitivity simulations consist of (i) **Base**, which is the set-up for the main simulations in this study consisting of monthly reinitialization frequency with CESM_NCSU ICs/BCs with the Grell 3D cumulus parameterization scheme; (ii) **Sen1**, which is similar to the Base case except with a 5-day reinitialization period; (iii) **Sen2**, which is similar to Base except using NCEP for the meteorological ICs/BCs; and (iv) **Sen3**, which is similar to Base except using WRF/Chem v3.7 with the MSKF cumulus parameterization, instead of Grell 3D. An additional sensitivity simulations using WRF/Chem v3.7 with both MSKF and Grell 3D and their comparison with Figure S1 showed that the differences between Sen3 and Base are mainly caused by the use of different cumulus parameterizations; other model updates between WRF/Chem v3.7 and WRF/Chem v3.6.1 only have minor contributions to such differences. A summary of the set-up of the sensitivity simulations can be found in Table S4.

The sensitivity simulations are evaluated against GPCP and PRISM data and the statistics are summarized in Tables S5 and S6, respectively. GPCP has data over the land and ocean while PRISM only has data over land. The results show that the R value for the **Base** case is the highest against both GPCP and PRISM, even though the NMB is the highest. While using more frequent reinitialization with 5-day (Sen1) reduces both the NMB and NME with slight to moderate improvements, it also reduces the R value. Using NCEP data as ICs/BCs (Sen2) also slightly-to-moderately improve the NMB and NME, indicating that using CESM_NCSU ICs/BCs contributes to the biases in precipitation. However, NCEP data are not available for future climate simulations.

Lastly, using CESM_NCSU IC/BCs with the new Multi-Scale Kain Fritsch (MSKF) scheme (Sen3) drastically reduce NMB and NME, but the correlation becomes much worse.

Table S4. Summary of set-up of sensitivity simulations

No.	Sensitivity Simulation	Reinitialization Frequency	IC/BCs	Cumulus Parameterization Scheme
1.	Base	Monthly	CESM_NCSU	Grell 3D
2.	Sen1	5-day	CESM_NCSU	Grell 3D
3.	Sen2	Monthly	NCEP	Grell 3D
4	Sen3	Monthly	CESM_NCSU	MSKF

Table S5. Statistics for sensitivity simulations against GPCP

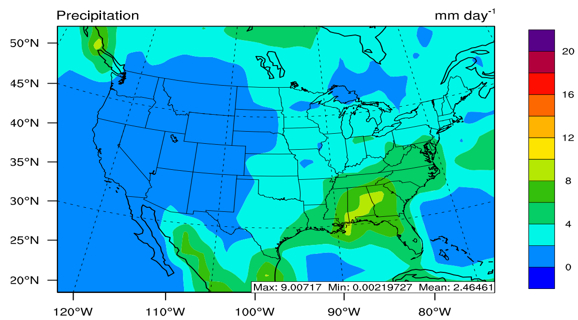
Sensitivity Simulation	Mean Obs (mm)	Mean Sim (mm)	R	NMB (%)	NME (%)
Base	2.4	5.3	0.5	121.1	150.2
Sen1	2.4	4.2	0.4	74.1	140.9
Sen2	2.4	4.5	0.5	85.1	122.4
Sen3	2.4	2.9	0.1	18.9	109.2

Table S6. Statistics for sensitivity simulations against PRISM

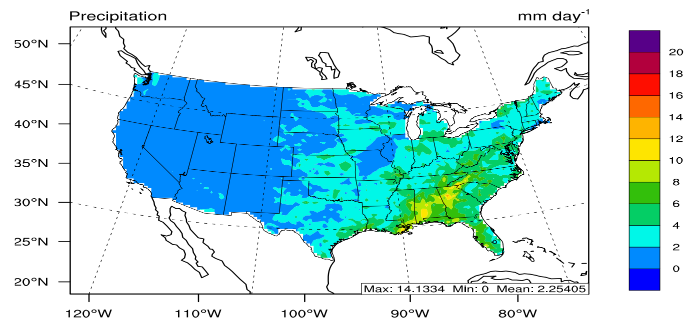
Sensitivity Simulation	Mean Obs (mm)	Mean Sim (mm)	R	NMB (%)	NME (%)
Base	2.3	4.0	0.7	77.8	96.5
Sen1	2.3	2.5	0.3	11.5	102.8
Sen2	2.3	3.6	0.5	60.9	105.0
Sen3	2.3	2.2	-0.2	-2.1	111.9

Figure S1 compares the spatial plots of the simulated precipitation with daily average observational precipitation data from GPCP and PRISM for July 2005. The high precipitation over the Atlantic ocean shown in all sensitivity simulations particularly in Sen1 and Sen2 does not exist in the GPCP observational data. The 5-day reinitialization case (Sen1) does not help to reduce the high precipitation over the ocean. Using NCEP data (Sen2) helps to reduce the precipitation over the ocean slightly. Using the MSKF scheme (Sen3) completely reduces the precipitation over the ocean, however it does not capture well precipitation over the southeastern U.S. The comparison of Sen3 and Base illustrates a very high sensitivity of the simulated precipitation to different cumulus parameterizations, which warrants future study.

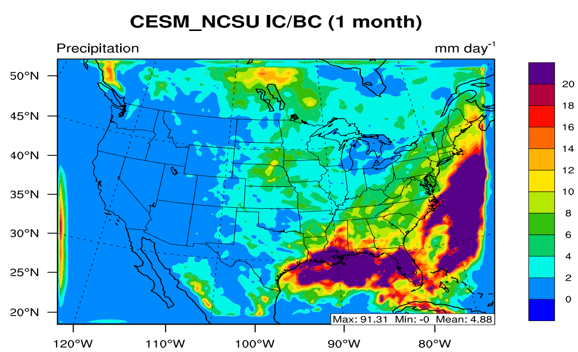
GPCP Obs



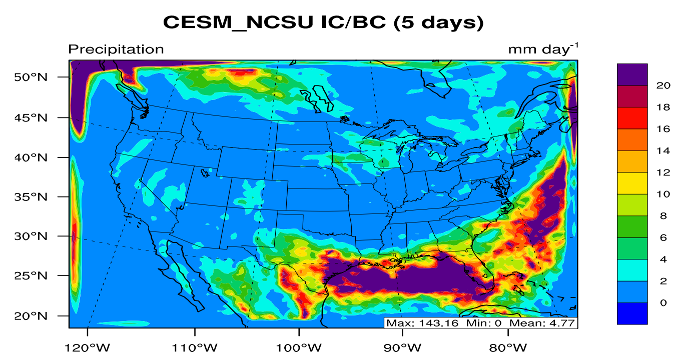
PRISM Obs



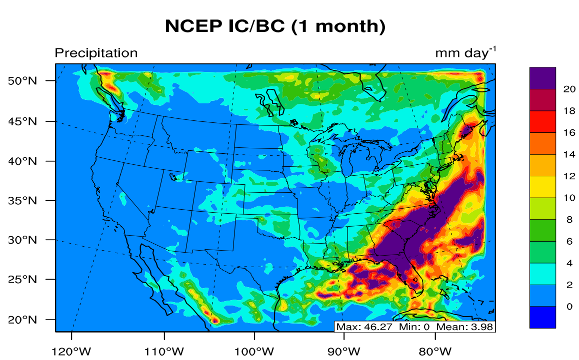
Base



Sen1



Sen2



Sen3

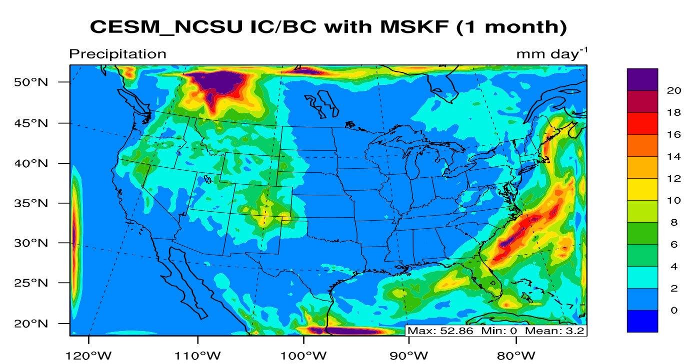


Figure S1. Spatial plots of average daily precipitation for GPCP and PRISM and sensitivity simulation cases for July 2005.

References

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