Quality Assurance Project Plan

Project 14-004
Emission source region contributions to a high ozone episode during DISCOVER-AQ

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Summary of Project

QAPP Category Number: III
Type of Project: Research or Development (Modeling)

QAPP Requirements: This QAPP includes descriptions of the project and objectives; organization and responsibilities; scientific approach; air quality modeling procedures; quality metrics; data analysis, interpretation, and management; reporting; and references.

QAPP Requirements:
Audits of Data Quality: 10% Required
Report of QA Findings: Required in final report

May 29, 2014

Distribution List

Gary McGaughey, Project Manager, Texas Air Quality Research Program

Cyril Durrenberger, Quality Assurance Project Plan Officer, Texas Air Quality Research Program

Doug Boyer, Project Liaison, Texas Commission on Environmental Quality

Chris Owen, Quality Assurance Project Plan Officer, Texas Commission on Environmental Quality

Maria Stanzione, Project Manager, Texas Air Quality Research Program

APPROVALS

The QAPP was approved electronically on June 19, 2014 by Gary McGaughey, The University of Texas at Austin

Gary McGaughey
Project Manager, Texas Air Quality Research Program

The QAPP was approved electronically on June 10, 2014 by Cyril Durrenberger, The University of Texas at Austin

Cyril Durrenberger
Quality Assurance Project Plan Officer, Texas Air Quality Research Program

1. PROJECT DESCRIPTION AND OBJECTIVES

1.1 Problem Statement

There is a need for a more quantitative understanding of the impact of regional emissions and transport versus local emissions on surface air quality. Local scale circulations and regional transport cause both local and regional air pollutants to accumulate resulting in poor air quality. Identifying and quantifying the impact of air pollution emissions source regions on surface air quality will aid air resource managers in developing air pollution emissions controls. Previous research has shown sea breeze circulations are a critical ingredient to poor air quality in Houston (Banta et al., 2005; Chen et al., 2011; Darby, 2005; Parrish et al., 2009). Sea breeze circulations were a daily occurrence during the Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) field campaign. Recent research has shown regionally transported air pollution into Houston is at its greatest concentrations when the air originates from Louisiana and the Midwest (Estes et al., 2013; Smith et al., 2013). The September 24-26, 2013 air pollution episode was the only time during the DISCOVER-AQ field campaign when Houston was influenced by transport from the north. Back trajectories calculated by the Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model reveal that Houston experienced transport from the Gulf of Mexico and Louisiana on September 24, northeastern Texas and the Great Plains states from Oklahoma to Wyoming on September 25, and northeastern Texas and Louisiana on September 26.

On September 24, air was transported from Louisiana and the Gulf of Mexico over the Houston metropolitan area. On the 25th, northerly flow brought continental air over Houston. High air pollution levels that were observed aloft in the residual layer in the morning mixed down to the surface impacting surface air quality, indicating pollution emitted on a previous day from local and/or regional sources impacted surface air quality in Houston on the 25th. In addition, a sea breeze circulation developed in the afternoon causing pollutants that were transported over the water in the morning to recirculate back inland and converge with pollutants over land at the sea breeze convergence zone. Laporte Sylvan Beach was near the sea breeze front and reported maximum 8 hr average ozone of 124 ppbv, the highest observed value in the Houston metropolitan area in 2013. On the 26th, winds were primarily from the south and southeast, resulting in maximum recorded ozone concentrations to the north and northwest of Houston.

1.2 Project Objectives

The goal of this study is to quantify the contributions of local versus regional sources to Houston's highest ozone air pollution episode in 2013 during the DISCOVER-AQ field campaign. We will break down the contribution of emissions in specific source regions to ozone concentrations in Houston.

2. ORGANIZATION AND RESPONSIBILITIES

2.1 Personnel and Responsibilities

This project is a collaborative effort between the Dr. Loughner of the University of Maryland, Dr. Follette-Cook of Morgan State University, and Drs. Pickering and Duncan of the NASA Goddard Space Flight Center. Dr. Loughner is the Principal Investigator with overall responsibility for the research and quality assurance. The project will be overseen by the Texas Air Quality Research Program Project Manager Gary McGaughey and the Texas Commission on

Environmental Quality (TCEQ) Project Liaison Doug Boyer. Project participants and their responsibilities are provided in Table 1 below.

Table 1. List of the project participants, their affiliations and key responsibilities.

Participant (Organization)	Key Responsibilities
Dr. Christopher P. Loughner (University of Maryland)	Principal Investigator with overall responsibility, including preparing and submitting reports, performing back trajectory analysis, editing emissions input files for sensitivity CMAQ simulations, and working with Co-I Follette-Cook to perform CMAQ sensitivity simulations, analyze the model results, and analyze the satellite observations.
Dr. Melanie Follette-Cook (Morgan State University)	Work with the PI to perform CMAQ sensitivity simulations, analyze the model results, and analyze satellite observations.
Dr. Ken Pickering (NASA Goddard Space Flight Center)	Provide guidance in analyzing model results and analyzing satellite observations.
Dr. Bryan Duncan (NASA Goddard Space Flight Center)	Provide guidance in the use of satellite observations.

2.2 Schedule

As part of this project the following tasks will be performed:

Task 1) Identify air pollution emissions source regions;
Task 2) Perform a set of sensitivity CMAQ simulations with anthropogenic emissions zeroed out from particular emissions source regions;
Task 3) Identify regional transport of pollutants with satellite observations; and
Task 4) Reporting

The schedule for the specific tasks is listed in Table 2.

Table 2. Schedule of project activities.

	2014							2015					
	J	J	A	S	O	N	D	J	F	M	A	M	J
Task 1													
Task 2													
Task 3													
Task 4													

3. SCIENTIFIC APPROACH

3.1 Identify air pollution emissions source regions

We will first utilize model output from the Weather Research and Forecasting (WRF) model Version 3.6 and the Community Multi-scale Air Quality (CMAQ) model Version 5.0.2 obtained from work funded by DISCOVER-AQ to identify the origins of the observed air pollution plumes entering the Houston metropolitan area in late September 2013. These models will be run with nested domains with horizontal resolutions at 36 km, 12 km, and 4 km as shown in Figure 1. Model configuration options that will be used are shown in Table 3. Twenty four hour kinematic back trajectories from Houston during the late September air quality episode will be calculated from WRF model output using the RIP (Read/Interpolate/Plot; http://www.mmm.ucar.edu/wrf/users/docs/ripug.htm) program. The progression of these plumes over time will be investigated using CMAQ model output. We will extract ozone (O_3), carbon monoxide (CO), nitrogen oxides (NO_x), and volatile organic compounds (VOCs) along the path of the back trajectories to identify which source regions imported a significant amount of ozone and ozone precursors.

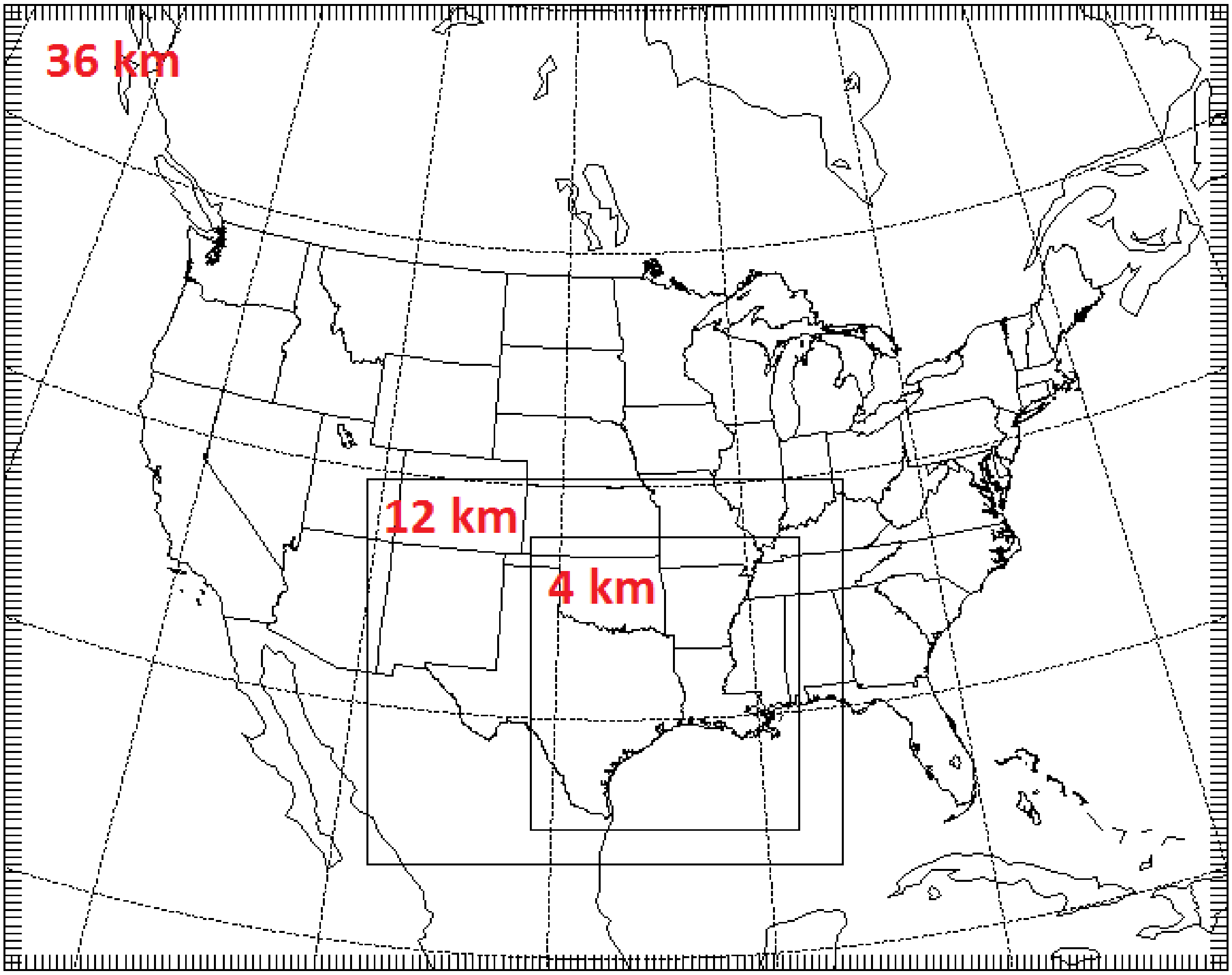

Figure 1. Location of the 36 km, 12 km, and 4 km domains that will be used in the WRF modeling. The CMAQ modeling domains will be slightly smaller than the WRF modeling domains (grid cells close to the horizontal edge of the WRF domains will not be included in the CMAQ domains).

Table 3. WRF and CMAQ configuration options.

WRF Model Options	
Radiation	LW: Rapid Radiative Transfer Model (RRTM) SW: Goddard
Surface Layer	Pleim-Xiu
Land Surface Model	Pleim-Xiu
Boundary Layer	Asymmetric Convective Model Version 2 (ACM2)
Cumulus	Kain-Fritsch (none for 1 km domain)
Microphysics	WRF Double-Moment 6-class (WSM-6)
Nudging	Observational and analysis nudging
Damping	Vertical velocity and gravity waves damped at top of modeling domain
Initial and Boundary Conditions	North American Regional Reanalysis (NARR)
SSTs	Multi-scale Ultra-high Resolution (MUR) sea surface temperature analysis (~1 km resolution)
CMAQ Model Options	
Chemical Mechanism	Carbon Bond 05 (CB05)
Aerosols	Aerosols with aqueous extensions version 5 (AE5)
Dry Deposition	M3DRY (Pleim et al., 2001)
Vertical Diffusion	ACM2
Chemical Initial and Boundary Conditions	Model For Ozone And Related Chemical Tracers (MOZART) Chemical Transport Model (CTM)
Biomass Burning Emissions	Fire Inventory from NCAR Version 1 (FINNv1)
Lightning Emissions	Calculated within CMAQ
Anthropogenic Emissions	2012 inventory supplied from TCEQ
Biogenic Emissions	Biogenic Emissions Inventory System (BEIS) calculated within CMAQ

3.2 Perform an ozone source apportionment CMAQ simulation

We will perform an ozone source apportionment CMAQ simulation with the 4 km domain to quantify how emissions from various source regions contributed to Houston's poor air quality. Anthropogenic emissions source regions will be identified to investigate the contribution of ozone concentrations in the Houston metropolitan area from each region. Based on a preliminary HYSPLIT analysis, we will tentatively split emissions source regions up as follows:

1) Houston metropolitan area
2) Dallas metropolitan area
3) Beaumont/Port Arthur
4) Lake Charles, LA
5) State of Oklahoma
6) Remaining areas in 4 km domain

After completing the back trajectory analysis, we will propose a refinement of the source regions in collaboration with the Project Manager and TCEQ Liaison. Our WRF calculated back trajectories will provide a more accurate picture of the transport path than the HYSPLIT trajectories calculated with the North American Mesoscale (NAM) model due to the use of observational and analysis nudging that will be performed in the simulation. In addition, WRF simulations performed under DISCOVER-AQ funding will be run at a higher resolution (4 km) than the NAM model (12 km), which is what was used to calculate the HYSPLIT back trajectories. Previous research has shown that model simulations performed at a horizontal resolution of 4 km are able to capture sea breeze circulation, but simulations performed at 12 km are not able to simulate a strong enough temperature gradient along the coastline in order to initialize the local scale sea breeze circulation (Loughner et al., 2011). In addition, high resolution sea surface temperatures will be incorporated in the WRF simulation (Table 3) to accurately simulate the temperature gradient along the coastline, which drives sea breeze circulations. The CMAQ ozone source apportionment simulation will use the same input files and model options as the base case simulation performed with DISCOVER-AQ funding. Results from the ozone source apportionment CMAQ simulation will allow us to quantify the impact of various emissions source regions on ozone concentrations in Houston in late September 2013.

3.3 Identify regionally transported pollutants with satellite observations

In addition, we will analyze satellite observations [Ozone Monitoring Instrument (OMI) tropospheric nitrogen dioxide (NO_2), OMI ozone (O_3) profiles, Measurement Of Pollution In The Troposphere (MOPITT) carbon monoxide (CO), and Moderate Resolution Imaging Spectrometer (MODIS) and Visible Infrared Imaging Radiometer Suite (VIIRS) aerosol optical depth (AOD)] to determine if they were able to track regional transport of pollution and buildup of pollution in the Houston metropolitan area. We will produce a time series of maps, covering south central US, of the satellite retrieval products using Interactive Data Language (IDL) software, from a week prior to the air pollution episode through the episode itself. Maps that will cover the entire area of the 12 km modeling domains shown in Figure 1 will be created twice daily for MODIS AOD observations and once daily for the remaining satellite observations. The maps will be analyzed to determine if regionally transported air pollution can be detected from current space-based instruments.

4. QUALITY METRICS

The U.S. Environmental Protection Agency (EPA) has not specified specific data quality requirements for this work, nor is it expected that the EPA will evaluate this specific application.

This project will utilize base case WRF and CMAQ model output that will be performed under DISCOVER-AQ funding. WRF and CMAQ model descriptions can be found on their respective webpages: www.wrf-model.org and www.cmaq-model.org. The WRF model will be driven by the North American Regional Reanalysis (NARR; http://rda.ucar.edu/datasets/ds608.0/) and Multi-scale Ultra-high Resolution (MUR) sea surface temperature analysis (http://podaac.jpl.nasa.gov/Multi-scale_Ultra-high_Resolution_MUR-SST). The CMAQ model will utilize chemical initial and boundary conditions from the Model for Ozone and Related Chemical Tracers (MOZART) chemical transport model (CTM) (https://www2.acd.ucar.edu/gcm/mozart). The ozone source apportionment CMAQ simulation will use the same model inputs as the base case simulation. The WRF and CMAQ simulations, including the ozone source apportionment CMAQ simulation, will be evaluated under DISCOVER-AQ funding using ground and aircraft observations obtained during the field campaign and archived on the DISCOVER-AQ website (http://www-air.larc.nasa.gov/missions/discover-aq/discover-aq.html). The following statistics will be calculated to evaluate the model and are shown in Table 4: mean bias, normalized mean bias, normalized mean error, and root mean square error. Comparisons between the model and observations and overall model evaluation will be used to ascertain why model errors and uncertainties exist (i.e., errors in the emissions, chemistry, and/or transport processes).

The following satellite observations will be analyzed to determine if current space-based observations detected regional air pollution transport into the Houston metropolitan area in late September 2013:

1) OMI tropospheric NO2 (http://disc.sci.gsfc.nasa.gov/Aura/data-holdings/OMI/omno2_v003.shtml);
2) MOPITT CO (https://www2.acd.ucar.edu/mopitt);
3) MODIS AOD (http://modis.gsfc.nasa.gov/);
4) VIIRS AOD (http://viirsland.gsfc.nasa.gov/index.html).

Only quality-assured un-flagged satellite observations will be used in this analysis. A time series of maps of the satellite observations will be created. These maps will be viewed and analyzed qualitatively to determine if the satellite observations detect air pollution plumes transported into the Houston metropolitan area.

Table 4: Statistics that will be calculated for performing the model evaluation. In these equations M represents the model results, O represents the observations, and N is the number of data points.

Statistic	**Equation**
Mean Bias	$MB = \frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)$
Normalized Mean Bias	$NMB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i} \times 100\%$
Normalized Mean Error	$NME = \frac{\sum_{i=1}^{N}\lvert M_i - O_i\rvert}{\sum_{i=1}^{N} O_i} \times 100\%$
Root Mean-Square Error	$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2}$

5. DATA ANALYSIS, INTERPRETATION, AND MANAGEMENT

Twenty four hour kinematic back trajectories from Houston during the late September air quality episode will be calculated from WRF model output using the RIP program. The IDL software package will be used for creating graphics and calculating differences in daily maximum 8 hr average ozone concentrations, corresponding to anthropogenic emissions contributions in the emission source regions.

5.1 Audits of Air Quality

At least 10% of the CMAQ model input and output files, scripts, and analysis products (i.e., trajectories, maps of satellite observations, maps of maximum 8 hr average ozone concentrations corresponding to anthropogenic emissions contributions in various emission source regions) will be reviewed for quality assurance purposes by Drs. Follette-Cook and Loughner. Results from the audits will be reported in the final report.

Model inputs and outputs, model evaluation statistics, back trajectories, and graphics generated for this project will be stored for at least three years after the completion of the project at NASA GSFC. In addition, all model inputs, outputs, and post-processing analyses will be sent to the University of Texas after the completion of the project.

6. REPORTING

Several reports will be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

Executive Summary

At the beginning of the project, an Executive Summary will be submitted to the Project Manager for use on the AQRP website. The Executive Summary will provide a brief description of the planned project activities, and will be written for a non-technical audience.
Due Date: Friday, May 30, 2014

Quarterly Reports

The Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Word doc file. It will not exceed 2 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	June, July, August 2014	Friday, August 30, 2014
Quarterly Report #2	September, October, November 2014	Monday, December 1, 2014
Quarterly Report #3	December 2015, January & February 2015	Friday, February 27, 2015
Quarterly Report #4	March, April, May 2015	Friday, May 29, 2015
Quarterly Report #5	June, July, August 2015	Monday, August 31, 2015
Quarterly Report #6	September, October, November 2015	Monday, November 30, 2015

Technical Reports and Data Deliverables

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP FY14-15 MTR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start - July 31, 2014	Friday, August 8, 2014
Technical Report #2	August 1 - 31, 2014	Monday, September 8, 2014
Technical Report #3	September 1 - 30, 2014	Wednesday, October 8, 2014
Technical Report #4	October 1 - 31, 2014	Monday, November 10, 2014
Technical Report #5	November 1 - 30 2014	Monday, December 8, 2014
Technical Report #6	December 1 - 31, 2014	Thursday, January 8, 2015
Technical Report #7	January 1 - 31, 2015	Monday, February 9, 2015
Technical Report #8	February 1 - 28, 2015	Monday, March 9, 2015
Technical Report #9	March 1 - 31, 2015	Wednesday, April 8, 2015
Technical Report #10	April 1 - 28, 2015	Friday, May 8, 2015
Technical Report #11	May 1 - 31, 2015	Monday, June 8, 2015
Project Data (model inputs, outputs, and analysis products)	June 1, 2014 – June 30, 2015	July 30, 2015

Financial Status Reports

Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the AQRP FY14-15 FSR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start - July 31, 2014	Friday, August 15, 2014
FSR #2	August 1 - 31, 2014	Monday, September 15, 2014
FSR #3	September 1 - 30, 2014	Wednesday, October 15, 2014
FSR #4	October 1 - 31, 2014	Monday, November 17, 2014
FSR #5	November 1 - 30 2014	Monday, December 15, 2014
FSR #6	December 1 - 31, 2014	Thursday, January 15, 2015
FSR #7	January 1 - 31, 2015	Monday, February 16, 2015
FSR #8	February 1 - 28, 2015	Monday, March 16, 2015
FSR #9	March 1 - 31, 2015	Wednesday, April 15, 2015
FSR #10	April 1 - 28, 2015	Friday, May 15, 2015
FSR #11	May 1 - 31, 2015	Monday, June 15, 2015
FSR #12	June 1 - 30, 2015	Wednesday, July 15, 2015
FSR #13	Final FSR	Wednesday, August 15, 2015

Draft Final Report

A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Due Date: Monday, May 18, 2015

Final Report

A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Due Date: Tuesday, June 30, 2015

Project Data

All project data including but not limited to QA/QC measurement data, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion. The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information.

AQRP Workshop

A representative from the project will present at the AQRP Workshop in June 2015.

7. REFERENCES

Banta, R., C.J. Senff, J. Nielsen-Gammon, L. Darby, T. Ryerson, R. Alvarez, P. Sandberg, E. Williams, and M. Trainer, 2005. A bad air day in Houston, Bulletin of the American Meteorological Society, 86, 657-669, doi: 10.1175/BAMS-86-5-657.

Chen, F., S. Miao, M. Tewari, J.-W. Bao, and H. Kusaka, 2011. A numerical study of interactions between surface forcing and sea breeze circulations and their effects on stagnation in the greater Houston area, Journal of Geophysical Research, 116, D12105, doi:10.1029/2010JD015533.

Darby, L.S., 2005. Cluster analysis of surface winds in Houston, Texas, and the impact of wind patterns on ozone, Journal of Applied Meteorology, 44, 1788-1806, doi:10.1175/JAM2320.1.

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Pleim, J.E., A. Xiu, P.L. Finkelstein, and T.L. Otte (2001), A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes, Water, Air, and Soil Pollution: Focus, 1, 243-252.

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