Scope of Work For

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

Prepared for

Air Quality Research Program (AQRP)
The University of Texas at Austin

by

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1. STATEMENT OF WORK

1.1 Introduction

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 Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) field campaign. We will break down the contribution of emissions in specific source regions to ozone concentrations in Houston. 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 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 air pollution episode was the only time during the DISCOVER-AQ field campaign when Houston may have been influenced by transport from the north. Back trajectories calculated by the Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model reveal that Houston may have 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.

Outlook Reports located at http://www-air.larc.nasa.gov/missions/discover-aq/reports.tx2013/ describe the evolution of the air pollution episode and is briefly summarized here. 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.

This study builds upon work currently being performed with DISCOVER-AQ funding. Below we break down the work covered with DISCOVER-AQ funding and a list of tasks that will be performed with Texas AQRP funding.

1.2 Work covered under DISCOVER-AQ funding

Collaborator Pickering, the DISCOVER-AQ Project Scientist, is leading an effort to perform and evaluate Community Multi-scale Air Quality (CMAQ) Version 5.0.2 model simulations fed off-line by output from the Weather Research and Forecasting (WRF) Version 3.6 model covering the entire DISCOVER-AQ Houston field campaign with PI Loughner and Co-I Follette-Cook. The models will be run with nested domains with horizontal resolutions of 36, 12, and 4 km as shown in Figure 1. Model configuration options for the WRF and CMAQ modeling are shown in Table 1. This work involves creating all input files required to run WRF and CMAQ. The 2012 baseline anthropogenic emissions from the Texas Commission on

Environmental Quality (TCEQ) will be obtained and converted to CMAQ input files. These emissions files include the 2012 TCEQ inventory, the most up-to-date Texas emissions inventory, and a compilation of emissions estimates from Regional Planning Offices throughout the US. The model simulations will be evaluated under DISCOVER-AQ funding using ground (ozonesondes, tethered balloons, Pandora uv-vis spectrometers, AERONET sun photometers, MPLNET instruments, in-situ ground monitoring mobile labs and stationary sites), aircraft, and satellite observations. During the model-observation intercomparison analysis, we will identify air pollution plumes that entered the Houston metropolitan area and contributed to high surface ozone concentrations (i.e., elevated air pollution levels in the residual layer that mixed down to the surface). A similar analysis was done for the DISCOVER-AQ Maryland campaign in 2011. We identified an elevated reservoir of air pollutants entering the Washington, DC and Baltimore, MD metropolitan areas during an air pollution episode (He et al., 2013).

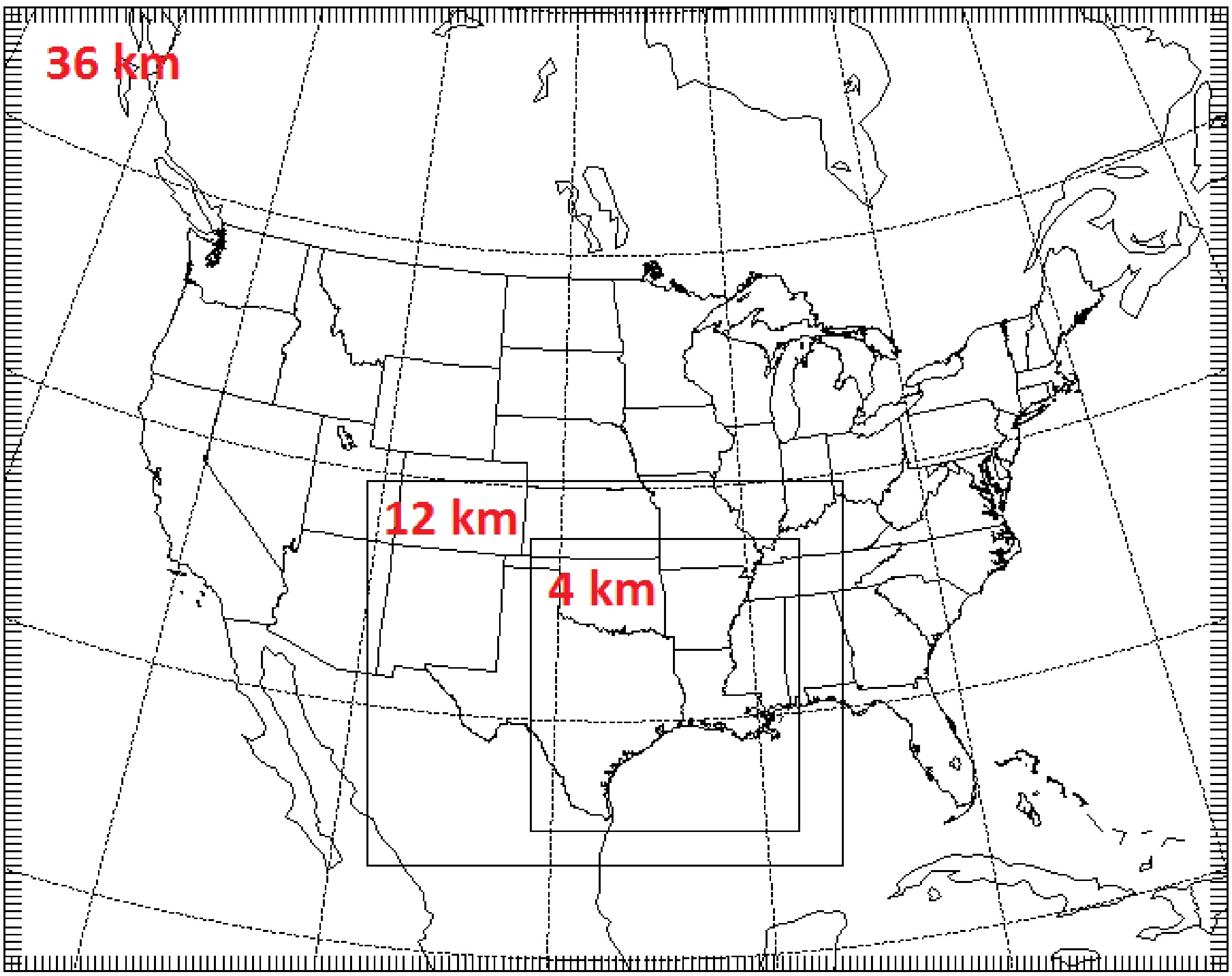

Figure 1. Location of the 36 km, 12 km, and 4 km domains that will be used in the WRF modeling. The CMAQ modeling domains will be slightly smaller than the WRF modeling domains (grid cells close to the horizontal edge of the WRF domains will not be included in the CMAQ domains).

Table 1. 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

1.3 Work covered under Texas AQRP funding

Our goal of this study is to identify and quantify the contributions of various emissions source regions to Houston's highest ozone air pollution episode in 2013 through a series of tasks.

1.3.1 Task 1: Identify air pollution emissions source regions

We will first identify the origins of the observed air pollution plumes entering the Houston metropolitan area in late September 2013 by calculating twenty four hour kinematic back trajectories from Houston during the late September air quality episode 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. Dr. Loughner will be responsible for this task and Dr. Pickering will provide guidance in performing this work.

1.3.2 Task 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 anthropogenic 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 Task 1, 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). 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 due to the model not being 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 1) to accurately simulate the temperature gradient along the coastline, which is necessary to accurately simulate the strength of sea breezes. The CMAQ simulation will be evaluated using the following statistics defined in Table 2: mean bias, normalized mean bias, normalized mean error, and root mean square error. Results from the 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. Drs. Loughner and Follette-Cook will be responsible for this task and Dr. Pickering will provide guidance in performing this work.

Table 2: 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	$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2}$

1.3.3 Task 3: Identify regional transport of pollutants with satellite observations

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, 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 viewed and analyzed qualitatively to determine if regionally the satellite observations detect air pollution plumes transported into the Houston metropolitan area. Loughner has compared CMAQ and OMI NO_2 to detect a day of the week dependence of column integrated NO_2 (Tzortziou et al., 2013). Currently, Duncan, Pickering, Loughner and Follette-Cook are involved in a project analyzing CMAQ simulations using emissions inventories from varying years and OMI observed tropospheric NO_2 throughout the lifetime of the instrument to detect the effect of NOx emissions reductions on the tropospheric NO_2 column (Loughner et al., 2013b). A recent analysis of VIIRS AOD shows aerosols from fires in the southeastern US transported over the Houston metropolitan area in mid-September, but aircraft observations made during the DISCOVER-AQ field campaign reveal these transported aerosols stayed aloft and were not mixed down to the surface impacting human health. This demonstrates the importance of combining satellite observations with in-situ observations or model simulations to gain a complete picture of what is happening in the atmosphere, which is what we plan to do in the proposed study. Drs. Loughner and Follette-Cook will be responsible for this task and Drs. Pickering and Duncan will provide guidance in performing this work.

1.3.4 Task 4: Deliverables

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, TCEQ, and other outside parties to utilize the information.

AQRP Workshop

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

1.4 Modeling

Meteorological and air quality models will be utilized to complete the above tasks.

1.4.1 Regional Meteorological Modeling

Meteorological model simulations will be performed under DISCOVER-AQ funding with the WRF model using nested domains with horizontal spatial resolutions of 36, 12, and 4 km. Since model runs at 36 and 12 km resolution are too coarse to simulate sea breeze circulations (Loughner et al., 2011), the nested 4 km simulation will be performed in order to capture these local-scale circulations, which occurred daily during the DISCOVER-AQ field campaign and are known to degrade air quality and impact transport processes along the Gulf Coast (Banta et al., 2005; Chen et al., 2011; Darby, 2005; Parrish et al., 2009). The WRF model output used to drive the CMAQ simulations will be used to calculate back trajectories to identify emissions source regions that impacted air quality in the Houston metropolitan area during the September 24-26 air pollution episode (Task 1). WRF model output will be used to drive the base case CMAQ air quality model simulation performed under DISCOVER-AQ funding. The sensitivity CMAQ runs will be performed under Texas AQRP funding (Task 2).

1.4.2 Air Quality Modeling

The base case CMAQ simulation will be performed under DISCOVER-AQ funding and the CMAQ simulation with source apportionment will be performed under Texas AQRP funding. The source apportionment simulation will be initialized on September 19 to allow for adequate model spin-up. Output from the base case simulation will be used as initial conditions for the source apportionment simulation. Results from the base case simulation will be used to examine how plumes that entered the Houston metropolitan area evolved along their trajectory into the region (Task 1). The source apportionment simulation will be analyzed to reveal how various emissions source regions impacted surface ozone concentrations in the Houston metropolitan area in late September 2013 (Task 2).

1.5 Observations

A combination of ground-, aircraft-, and space-based observations will be used during this project and are briefly described below.

1.5.1 Ground- and Aircraft-based Observations

Ground and aircraft observations will be used to evaluate the base case CMAQ simulation under DISCOVER-AQ funding. The base case simulation will be evaluated using surface meteorological data collected by the National Weather Service (NWS) and air quality data collected by the University of Houston, state and local air quality agencies, and the DISCOVER-AQ team. During the DISCOVER-AQ field experiment, additional meteorological and air quality data were collected by ground- and aircraft -based in-situ and remote sensing instruments and ground-based balloon soundings. Ground-based observations from NASA's AERONET (AErosol RObotic NETwork) and MPLNET (Micro-Pulse Lidar Network) instruments and aircraft observations from the High Spectral Resolution Lidar (HSRL) will be used to obtain aerosol optical properties. The MPLNET and HSRL retrievals will also be used to determine the planetary boundary layer height. Measurements from a network of twelve Pandora spectrometer instruments (Herman et al., 2009; Tzortziou et al., 2012) will be used to determine the spatial and temporal (every 40 seconds) distribution of column NO_2 and O_3 in addition to resolving the altitude profiles in the troposphere (at 2 sites). Aircraft in-situ data will be useful in representing the three dimensional distribution of chemical species, while ozonesondes will provide information on the vertical distribution of the ozone mixing ratios in the troposphere. Biases in the model will be identified through comparisons between these data and model output.

1.5.2 Satellite Observations

In addition to using satellite observations to evaluate the CMAQ base case simulation under DISCOVER-AQ funds, they will be analyzed to determine if they were able to detect regional transport into and buildup of pollution in the Houston metropolitan area under Texas AQRP funding (Task 3). Extensive aerial coverage for species such as CO, O_3, NO_2, and aerosols is available from space-based observations (Table 2). CO is observed globally by the MOPITT instrument on NASA's Terra satellite. The first MODIS instrument is also on Terra providing information on aerosol optical depth (AOD). An additional MODIS instrument is on NASA's Aqua satellite. The Terra satellite has an overpass time in the morning while Aqua has an overpass time in the afternoon. The Suomi National Polar-orbiting Partnership (NPP) includes high resolution AOD observations by the Visible Infrared Imaging Radiometer Suite (VIIRS). An AOD product is also available from GOES satellite observations. NASA's Aura satellite was launched in 2004 and hosts OMI. OMI provides observations of column O_3, SO_2, and NO_2. Xiong Liu's OMI O_3 profile product will be available to evaluate CMAQ. In order to compare model output with the satellite data, averaging kernels will be applied to the model data. The averaging kernel ensures that the model data is representing the atmosphere in the vertical in the same way that the satellite instrument is sensing the various atmospheric layers.

Table 2. Satellite products we plan to use in this project.

Observation	**Satellite Sensors**	**Resolution (at nadir)**	**Products**
Aerosols	MODIS; VIIRS; GOES	3km; 0.75km; 4 km	Aerosol optical depth (AOD)
Tropospheric gases	MOPITT	22km	Tropospheric CO
Trace gases	OMI	24km x 13km	NO_2 tropospheric and total column, O_3 profiles

2. TIMELINE

The key milestones and expected progress of the proposed work are described below and assumes that technical work will begin in June 2014.

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

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