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## **FINAL REPORT**

### **Operationalizing Exceptional Event Tools**

TCEQ Contract No. 582-19-90498  
Work Order No. 582-22-31188-008  
Revision 2.0

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## **List of Acronyms**

AIRS – Atmospheric Infrared Sounder

ARL – Application Readiness Level

NOAA ARL – NOAA Air Resources Laboratory

ASP – Aerosol Simulation Program

CAM-chem – Community Atmosphere Model with Chemistry

EEST – Exceptional Event Screening Tool

EPA – Environmental Protection Agency

FINN – Fire INventory from NCAR

MEGAN – Model of Emissions of Gases and Aerosols from Nature

MERRA – Modern Era Retrospective-analysis for Research and Application

MOZART-4 – Model for Ozone and Related chemical Tracers, version 4

NARR – North American Regional Reanalysis

NASA – National Aeronautics and Space Administration

NCAR – National Center for Atmospheric Research

NOAA – National Oceanic and Atmospheric Administration

NOAA ARL – NOAA Air Resources Laboratory

OMI – Ozone Monitoring Instrument

QAPP – Quality Assurance Project Plan

STILT – Stochastic Time Inverted Lagrangian Transport

TCEQ – Texas Commission on Environmental Quality

## Executive Summary

Previous AMEIOTS projects have developed tools for the TCEQ to demonstrate exceptional events from biomass burning and stratospheric intrusions. The Stochastic Time Inverted Lagrangian Transport model with an integrated Aerosol Simulation Program (STILT-ASP) (Brown-Steiner et al., 2019) is a trajectory-based modeling tool that allows the Air Modeling and Data Analysis Section of the TCEQ to assess the impact of certain wildfire events on ozone (O<sub>3</sub>) or fine particulate matter (PM<sub>2.5</sub>) measurements in the metropolitan areas of Texas. The Exceptional Event Screening Tool (EEST), (Lonsdale et al., 2018) allows TCEQ staff to make reasonable decision on whether to commit further resources to investigating potential O<sub>3</sub> exceedances caused by stratospheric ozone intrusions.

The purpose of this project was to update and fully integrate these tools into the TCEQ decision making process, including systems integration support and staff training. The goal was to take these tools from their current testing and validation status (Application Readiness Level (ARL) of 4) to full integration into the TCEQ's decision making process (ARL 9).<sup>1</sup>

For EEST, we made minor updates to the Docker container and source code to ensure that the container correctly downloads the needed satellite and meteorological data. We have confirmed that the EEST container can be run on the TCEQ eira machine, which allows the use of Docker. We have also confirmed that the results are identical to those generated when the container is run in AER machines, as expected.

For STILT-ASP, we again made we made minor updates to the code to ensure that the container correctly downloads the needed meteorological and emission data. We also updated the boundary condition mapping file to use CAM-Chem output for boundary conditions, as NCAR has replaces the previous MOZART-4 output with this model. We have confirmed that the STILT-ASP container can be run on the TCEQ eira machine, which allows the use of Docker. We have also confirmed that the results are identical to those generated when the container is run in AER machines, as expected.

For both models, we provided updated User's Guides to assist TCEQ in running the models and confirmed that the output met expectations.

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<sup>1</sup> <https://www.nasa.gov/sites/default/files/files/ExpandedARLDefinitions4813.pdf>

## 1. Introduction

### 1.1 Project Objectives

Previous AMEIOTS projects have developed tools for the TCEQ to demonstrate exceptional events from biomass burning and stratospheric intrusions. This project will work with the staff at TCEQ to update and fully integrate these tools into the TCEQ decision making process, including systems integration support and staff training. The goal is to take these tools from their current testing and validation status (Application Readiness Level (ARL) of 4) to full integration into the TCEQ's decision making process (ARL 9).<sup>2</sup>

The schedule of deliverables for this project is given in Table 1.

**Table 1. Projected Schedule for TCEQ Work Order #582-22-31188-008**

<b>Milestones</b>	<b>Planned Date</b>
<b>Task 1 - Work Plan</b>	
1.1: TCEQ-approved Work Plan	December 21, 2021
1.2: TCEQ-approved QAPP	December 21, 2021
<b>Task 2 – Progress Reports</b>	
2.1: Monthly Progress Reports	Monthly with invoice
<b>Task 3 – Cybersecurity Training</b>	
3.1: List of Individuals taking Training	December 21, 2021
3.2: Complete Cybersecurity training and submit completion certification to TCEQ Contract Manager	Within 7 days of TCEQ providing access to the training
<b>Task 4 – Operationalize the STILT-ASP model</b>	
4.1: Updated User's Guide for STILT-ASP model detailing how to successfully install and run the model on machines at the TCEQ	April 30, 2022
4.2: Copies of scripts, data files, and documentation used in the completion of Task 4	April 30, 2022
<b>Task 5 – Operationalize the EEST model</b>	
5.1: Updated User's Guide for EEST model detailing how to successfully install and run the model on machines at the TCEQ.	April 30, 2022
5.2: Copies of scripts, data files, and documentation used in the completion of Task 5	April 30, 2022
<b>Task 6 – Demonstration of Models in Relevant Environment</b>	
6.1: Updated User's Guides for the STILT-ASP and EEST models detailing how to successfully install and run the model on TCEQ machines	May 31, 2022
6.2: Copies of scripts, data files, and documentation used in the completion of Task 6	June 30, 2022
<b>Task 7 – Draft and Final Reports</b>	
7.1: Draft Report	June 15, 2022
7.2: Final Report	June 30, 2022

<sup>2</sup> <https://www.nasa.gov/sites/default/files/files/ExpandedARLDefinitions4813.pdf>

## 1.2 Background

The Stochastic Time Inverted Lagrangian Transport model with an integrated Aerosol Simulation Program (STILT-ASP) (Brown-Steiner et al., 2019) is a trajectory-based modeling tool that allows the Air Modeling and Data Analysis Section of the TCEQ to assess the impact of certain wildfire events on ozone (O<sub>3</sub>) or fine particulate matter (PM<sub>2.5</sub>) measurements in the metropolitan areas of Texas.

The Exceptional Event Screening Tool (EEST), (Lonsdale et al., 2018) allows TCEQ staff to make reasonable decision on whether to commit further resources to investigating potential O<sub>3</sub> exceedances caused by stratospheric ozone intrusions. The EEST automates: 1) the downloading of North American Regional Reanalysis (NARR) 32 km Air Resources Laboratory (ARL) format meteorological files, 2) the execution of the STILT model and 3) post-processing of STILT back- trajectories with Modern Era Retrospective-analysis for Research and Application (MERRA) potential vorticity data, Ozone Monitoring Instrument (OMI) and Atmospheric Infrared Sounder, (AIRS) satellite total ozone column data, and AIRS total integrated column of water vapor burden satellite data.

Both models have been previously implemented within Docker containers to allow easy portability. However, experience has shown the difficulty of running Docker software on Windows machines at the TCEQ due to security requirements. The goal of this project is to implement the tools on Linux machines at the TCEQ such that they can easily be used in operations by staff at the TCEQ.

## 1.3 Report Outline

This draft Final Report highlights major activities and key findings, provides pertinent analysis, describes encountered problems and associated corrective actions, and details relevant statistics including data, parameter, or model completeness, accuracy and precision. It satisfies Deliverable 7.2 of the Work Plan for Work Order No. 582-22-31188-008:

<b>Deliverable 7.2:</b>	Final Report
<b>Deliverable 7.2 Due Date:</b>	June 30, 2022

The major activities of the project are summarized in Section 2. Note that as the project was an implementation project for pre-existing software, there are no formal conclusions, just an evaluation of the models as run on TCEQ machines. Section 3 discusses the quality assurance findings for this project following the procedures from the project Quality Assurance Project Plan (QAPP). Section 4 summarizes our conclusions and Section 5 makes recommendations for future work based on the results of this project.



## **2 Operationalizing EEST and STILT-ASP on TCEQ Machines**

### **2.1 Code and User's Guide Updates**

A few code changes were made to the EEST and STILT-ASP source codes and User's Guides to ensure that they would run on the TCEQ eira machine.

We used the `aeraqac/eest:tceq_workshop` container as our code base for EEST. Most of the issues related to running this model were due to the access permissions for the satellite data needing to be updated or corrected. Once those changes were made, the container was able to run on the TCEQ eira machine without further changes.

We used the `container_plumerise` gitlab branch of the STILT-ASP model from Brown-Steiner et al. (2019) as our code base for that model. The major code change was due to the change from MOZART-4 boundary conditions to CAM-Chem boundary conditions. While this did not require any changes to the Fortran source code of STILT-ASP, it did require changes to the species mapping files to account for the change in the aerosol species names between MOZART-4 and CAM-Chem. The changes to the mapping file are shown below in Table 2. Once those changes were made, the container was able to run on the TCEQ eira machine without further changes.

**Table 2. Changes in boundary condition mapping file to account for update to CAM-Chem.**

MOZART-4 to ASP	CAM-Chem to ASP
SO <sub>4</sub> ;(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	so4_a1; (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> ; 0.33
NH <sub>4</sub> :[UNUSED]	so4_a2; (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> ; 0.33
NH <sub>4</sub> NO <sub>3</sub> ;NH <sub>4</sub> NO <sub>3</sub>	so4_a3; (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> ; 0.33
SOA;IVOC1	soa1_a1;IVOC1;0.1
CB1;BC;0.5	soa1_a2;IVOC1;0.1
CB2;BC;0.5	soa2_a1;IVOC1;0.1
OC1;CPD3	soa2_a2;IVOC1;0.1
OC2;CBIO	soa3_a1;IVOC1;0.1
SA1;NaCl;0.25	soa3_a2;IVOC1;0.1
SA2;NaCl;0.25	soa4_a1;IVOC1;0.1
SA3;NaCl;0.25	soa4_a2;IVOC1;0.1
SA4;NaCl;0.25	soa5_a1;IVOC1;0.1
	soa5_a2;IVOC1;0.1
	bc_a1;BC;0.5
	bc_a4;BC;0.5
	pom_a1;CPD3
	pom_a4;CBIO
	ncl_a1;NaCl;0.33
	ncl_a2;NaCl;0.33
	ncl_a3;NaCl;0.33

## 2.2 Running Docker on the TCEQ eira machine

Chuhua Tian of TCEQ helped to get us access to the Docker user's group on eira. Similar access will be required for any TCEQ staff member who wants to use the codes on eira.

Both models require a Docker cloud account as well to be able to access the container repository. You can register for a Docker Cloud account at <https://cloud.docker.com/>

The instructions for running both mode docker containers are in the updated User's Guides supplied to TCEQ as part of Deliverable 6.1. The instructions are repeated here for completeness.

### 2.2.1 Docker EEST Instructions

After registering for a Docker cloud account the following commands should be entered in eira to run the EEST:

- 1) Create a project directory (eg. mkdir EEST) containing:
  - a) A site\_info.csv file with spatial and temporal information for STILT run (site name, 4-digit year, 2-digit month, 2-digit day of month, 2-digit hour, latitude, longitude, time zone, number of particles, trajectory length in hours, and elevation in meters).

Example site\_info.csv file:

```
MonitorID,year,month,day,hour,latitude,longitude,timezone,NumPart,traj_1
length,elev
ElPaso,2012,6,4,22,31.77,-106.5,Mountain,500,48,25
```

- b) Copy your NASA Earthdata login credentials from your home directory to a netrc.txt file in this directory.
- c) Create the following empty sub-directories where the EEST Tool will download satellite files and writeoutput files to. Note that these directories can be anywhere on your local machine as long as the full path is provided:

```
> mkdir SATELLITE_FILES images Stilt_OUTPUT MetFiles
```

Your project directory should now contain the following:

```
SATELLITE_FILES/Stilt_OUTPUT/ images/ Metfiles/ netrc.txtsite_info.csv
```

- 2) Run Docker or Docker Toolbox with administrative privileges initially (in Docker Toolbox, these permissions are required for, e.g., VirtualBox configuration).
  - a) When setup is complete, if a Docker terminal does not appear, open a command window. This will depend on what version and what operating system you are running.
  - b) Login to your Docker cloud account by typing `docker login` at the Docker command line.
- 3) In the command line in the Docker terminal, execute the following command to pull the EEST Docker image from Docker cloud and execute the tool at once (component details are described in further detail below). Note that in green is *your local full path* (which can change between runs), and following that in red must be *the hardcoded path in the container* (this won't change between runs). Both green and red components are needed in the docker run command when volume mounting.

```
docker run \  
-v your_FULL_PATH_to_site_info.csv:/EEST/site_info.csv \  
-v your_FILL_PATH_to_netrc.txt:/EEST/netrc.txt \  
-v your_FULL_PATH_to_Stilt_OUTPUT:/EEST/Stilt_OUTPUT \  
-v your_FULL_PATH_to_SATELLITE_FILES:/EEST/SATELLITE_FILES \  
-v your_FULL_PATH_to_images:/EEST/images \  
-v your_FULL_PATH_to_Metfiles:/EEST/Metfiles \  
aeraqac/eest:tceq_workshop
```

Optionally you can type ‘--rm’ after docker run to remove the image from your system after the run, if memory is an issue.

### **2.2.1.1 Required files and folders**

- i. “docker run” calls the “docker” command and instructs it to pull a container from Docker cloud unless there is one named locally. To see your locally stored images type “docker images”
- ii. site\_info.csv volume mount
- iii. netrc.txt volume mount
- iv. aeraqac/eest:tceq\_workshop is the name of the image on which the container run is based. This is where the Docker Cloud account is important – “aeraqac” is the Docker Cloud user name of EEST image developer, and “eest” is the name of the publicly available image in the aeraqac (AER Air Quality and Atmospheric Composition) repository (“tceq\_workshop” is the tag of the “eest” image for the workshop presentation and “latest” is the most up-to-date version of the tool).

### **2.2.1.2 Recommended files and folders**

- i. STILT\_output/ volume mount – this is the directory in which the netCDF files generated by STILT are saved.
- ii. SATELLITE\_FILES/ volume mount – the EEST downloads NARR, AIRS, MERRA2, and OMI data and utilizes them in its analysis. For every run, a check is done to ensure that the necessary files for a run exist, and if they do not, they are downloaded from the appropriate source. By mounting this directory, the user can save time in future EEST runs for time periods that have been processed in previous EEST runs.
- iii. images/ volume mount – the directory where EEST output is saved. Output is in the form of PNG files.
- iv. Metfiles/ volume mount – this is the directory in which the NARR files are downloaded to.

#### **a) Additional optional commands**

- i. rm – this Docker keyword instructs the Docker command to remove the container after it finishes (successfully or not). Otherwise, the container will still exist in the Docker environment of the user.
- ii. The convention for volume mounting is “-v FULL\_LOCAL\_PATH:CONTAINER\_PATH”
- iii. Adding a ‘-it’ command after ‘docker run’ (eg. docker run -it --rm...) and specifying an entry point and shell at the end (eg. --entrypoint /bin/csh aeraqac/eest:tceq\_workshop) will allow you to ‘interactively’ run the container. From here you will be in the main /EEST directory within the

container, and you can use basic linux commands to navigate through the directory structure. This can be helpful in understanding the contents of what the container includes and is almost identical to the directory structure of what is included in the CentOS version of the tool.

## 2.2.2 How to Run the Containerized STILT-ASP v3.1.1

### 2.2.2.1 Description of Model Inputs

After registering for a Docker cloud account, the user should have the following contents in a dedicated input directory.

1. The input directory should be created and contain the following files and subfolders:

```
> mkdir STILTASP_IN  
> cd STILTASP_IN  
> mkdir BC CAMx Fire MEGAN NARR
```

Contents of this directory include:

- a. **site\_info.csv** file with spatial and temporal information for a containerized STILT-ASP v3.1.1 run (site name, 4-digit year, 2-digit month, 2-digit day of month, 2-digit hour, latitude, longitude, time zone (eg. 'Central'), number of particles (eg. 500), length of back-trajectory (in hours), elevation). The file should have the following column names: MonitorID, year, month, day, hour, latitude, longitude, timezone, NumPart, traj\_length, elev
- b. **rda\_ucar.txt** file containing the user's login information to download the UCAR NCAR NARR data for a MEGAN model simulation.
- c. **BC/** - CAM-Chem data for boundary conditions can be downloaded from the NCAR website <https://www.acom.ucar.edu/cam-chem/cam-chem.shtml>. The web form requires that you fill in your name, affiliation, address, email, and phone number. You should then request data for a North latitude of 50°, a South latitude of 0°, a West longitude of 360°, and an East longitude of 0°. The data range should cover from 6 days before the UTC date of the earliest receptor in your simulation to the UTC date of the latest receptor in your simulation. The data file will be emailed to you by NCAR after they are processed, and the emailed files should be placed in this directory.
- d. **CAMx/** - CAMx emissions are currently only compatible with NARR meteorology data. CAMx gridded emissions from the 2012 Modeling Episode Base Case (<https://www.tceq.texas.gov/airquality/airmod/data/tx2012>) may be used as input in STILT-ASP. These emissions contain data from a variety of emission sources, including those of biogenic origin, which are subtracted

- out by the model and replaced with the MEGAN biogenic emissions generated by the container.
- e. **Fire/** - Fire emission FINN files contain daily fire emission products for inclusion into models such as MOZART and GEOS-Chem in ASCII comma-separated (CSV) form. The containerized STILT-ASP v3.1.1 has the automated capability to regrid FINN files for a simulation, provided the user provides a yearly fire inventory FINN file. These files are currently available for the years 2002 to 2016 from UCAR at <http://bai.acom.ucar.edu/Data/fire/> or upon request from AER.
  - f. **MEGAN/** - The MEGAN model produces biogenic emission files. The containerized STILT-ASP v3.1.1 has the automated capability to produce these files, including acquiring the required NARR meteorological inputs, if an NCAR UCAR Research Data Archive account credentials are provided in the rda\_ucar.txt file. If the user already contains STILT-ASP produced files, the pre-processor will not commence.
  - g. **NARR/** - The containerized STILT-ASP v3.1.1 supports only ARL-formatted meteorology data; other formats such as GRIB are not compatible. The Air Resources Laboratory (ARL) provides documentation and utilities as to how to convert GRIB files to ARL format; see [Meteorology Data Conversion Utilities](#) for more information in Brodowski et al., (2017). The containerized STILT-ASP v3.1.1 currently supports monthly files using the NARR grid (32 km resolution) downloaded from the FTP sites documented in Brodowski et al., (2017). The containerized STILT-ASP v3.1.1 has the automated capability to download the necessary ARL format NARR files for the requested STILT-ASP simulation. These files are large and take a considerable time to download, thus if these files are already downloaded by the user, the automated downloading will not commence.

### ***2.2.2.2 Running the STILT-ASP v3.1.1 Container***

1. Run Docker or Docker Toolbox with administrative privileges initially (in Docker Toolbox, these permissions are required for, e.g., VirtualBox configuration).
  - When setup is complete, if a Docker terminal does not appear, open a command window. This will depend on what version and what operating system you are running.
  - Login to your Docker cloud account by typing docker login at the Docker command line.
2. In the command line in the Docker terminal, execute the following command to pull the desired STILT-ASP v3.1.1 Docker image from Docker cloud and execute the tool

at once (component details are described in further detail below)<sup>3</sup>. Note that in blue is *your local full path* (which can change between runs), and following that in red must be *the hardcoded path in the container* (this won't change between runs). Both **blue** and **red** components are needed in the docker run command when volume mounting.

```
docker run \
-v FULL_PATH_to_STILTASP_OUT:/STILT-ASP/modelRun/TestArchives/
  2013/ \
-v FULL_PATH_to_STILTASP_IN:/STILT-ASP/inputVolume \
-v FULL_PATH_to_MEGAN_OUT:/STILT-ASP/MEGAN/Output \
-v FULL_PATH_to_MEGAN_INTERMED:/STILT-ASP/MEGAN/Input/MGN
  MET \
aeraqac/stilt-aspv3.1.1
```

- “**docker run**” calls the “docker” command and instructs it to pull a container from Docker cloud unless there is one named locally. To see your locally stored images type “docker images”
- ‘**FULL\_PATH\_to\_STILTASP\_OUT**’ should be the STILT-ASP output volume mount directory. This should contain the full path location of where the user would like the final STILT-ASP trajectory files and figures written to.
- ‘**FULL\_PATH\_to\_STILTASP\_IN**’ should be the STILT-ASP Input volume mount directory. This is the full path location of the directory structure and files described in Section 3.1.
- ‘**FULL\_PATH\_to\_MEGAN\_OUT**’ should be a path to an intermediate location to the MEGAN output file first gets written.
- ‘**FULL\_PATH\_to\_MEGAN\_INTERMED**’ should be a path to an intermediate location where MEGAN intermediate files get written to.

**aeraqac/stilt-aspv3.1.1** is the name of the image on which the container run is based. ***This is where the Docker Cloud account is important*** – “aeraqac” is the Docker Cloud username of stilt-aspv3.1.1 image developer, “stilt-aspv3.1.1” is the name of the publicly available image in the aeraqac (AER Air Quality and

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<sup>3</sup> When running docker in either standard mode or interactive mode, there might be issues associated with mount volume permissions. One way to circumvent this is by appending the flag “--privileged=true” immediately after the docker run or docker run -it command. **\*\*WARNING\*\***: this approach gives root permissions to the user which can be dangerous! It is strongly recommended that you discuss this with your system administrator before adding this flag.



Atmospheric Composition) repository. Since no tag is specified, the run will use the latest version of the image.

### 2.2.2.3 Interactive command line execution instructions

The STILT-ASP model can be run in interactive mode which can be useful for an “under-the-hood” view of the model. To run the containerized STILT-ASP v3.1.1 in a CENTOS virtual, interactive setting, a user can enter the following command, which will them into a bash shell environment that contains all scripts, source code and specified volume mounts connected needed to run STILT-ASP v3.1.1. An example interactive docker container call is shown below.

```
% docker run -it --rm --privileged=true --name=STILT_ASP \
-v FULL_PATH_to_STILTASP_OUT:/STILT-ASP/modelRun/TestArchives/
  2013/ \
-v FULL_PATH_to_STILTASP_IN:/STILT-ASP/inputVolume \
-v FULL_PATH_to_MEGAN_OUT:/STILT-ASP/MEGAN/Output \
-v FULL_PATH_to_MEGAN_INTERMED:/STILT-ASP/MEGAN/Input/MGN
  MET \
--entrypoint '/bin/csh' aeraqac/stilt-aspv3.1.1
```

- i. “-it” requests interactive mode.
- ii. “--rm” (recommended) removes the container upon completion and prevents container build-up in your environment.
- iii. “--privileged=true” (OPTIONAL!) Be careful with this flag. Only add this if you have permissions errors. Consult your system administrator if you are unsure about this. See footnote 1.
- iv. “--name” (recommended) enables you to provide a customized name. In the absence of a name, a random name will be provided for your running container.
- v. “--entrypoint” can be a shell of preference, not necessarily ‘/bin/csh’ (e.g., ‘/bin/bash’)

The user can then move around the directory structure, examine and make any source code changes they would like, and execute the STILT-ASP v3.1.1 model by typing the command below. **Note that any changes to the source cannot be saved in this interactive mode and will be deleted once the container is exited** (type ‘exit’ to quit the container). To run the model, at the command line prompt inside the container’s main /STILT-ASP/ directory, type:

```
% python stiltasp_wrapper.py
```

### 3 Quality Assurance

The EEST container was run for a single site on May 31, 2011. The site\_info.csv parameters used were:

MonitorID	year	month	day	hour	latitude	longitude	timezone
PAL190	2011	5	31	9	34.88061	-101.6647	Central

An example output plot is given in Figure 1. The results were identical on eira and AER machines, and the output was consistent with the previous performance of the model. This evaluation satisfies the requirement for 10% of all model calculations to be reviewed.

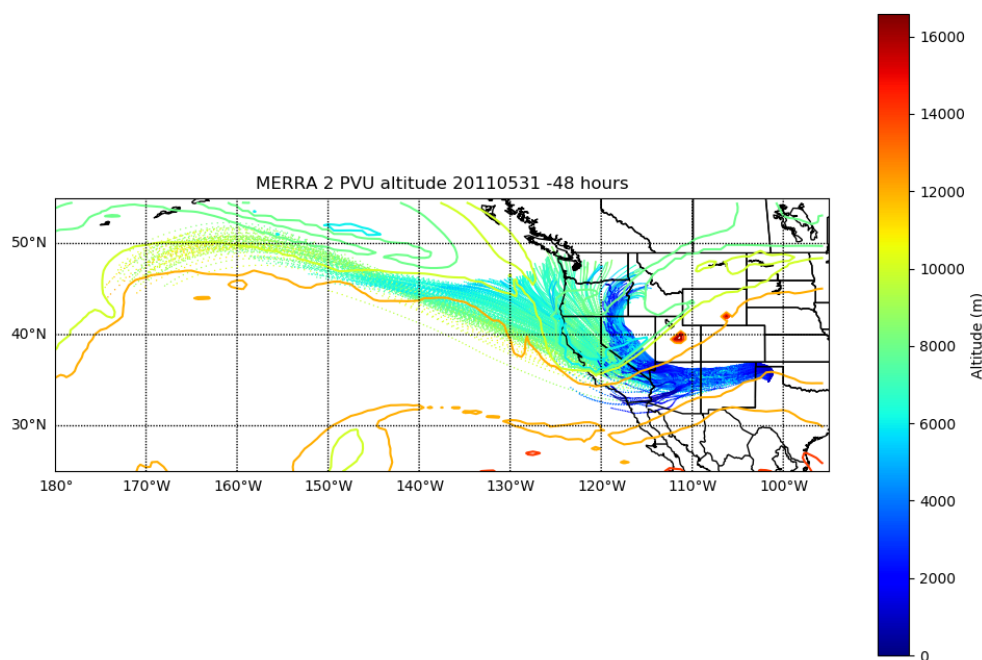


Figure 1. 48 hour back trajectories and MERRA 2 PVU altitudes for the EEST base described in the text. Cases where the contours and trajectories have the same color indicate potential stratospheric influence.

The STILT-ASP container was tested for a single El Paso case from June 4, 2012. The site\_info.csv parameters used were:

MonitorID	year	month	day	hour	latitude	longitude	timezone	NumPart	traj_length	elev
ElPaso	2012	6	4	22	31.77	-106.5	Mountain	500	48	25

The ozone output figure for the non-fire case is shown in Figure 2. The results were identical on eira and AER machines, and the output was consistent with the previous performance of the model. This evaluation satisfies the requirement for 10% of all model calculations to be reviewed.

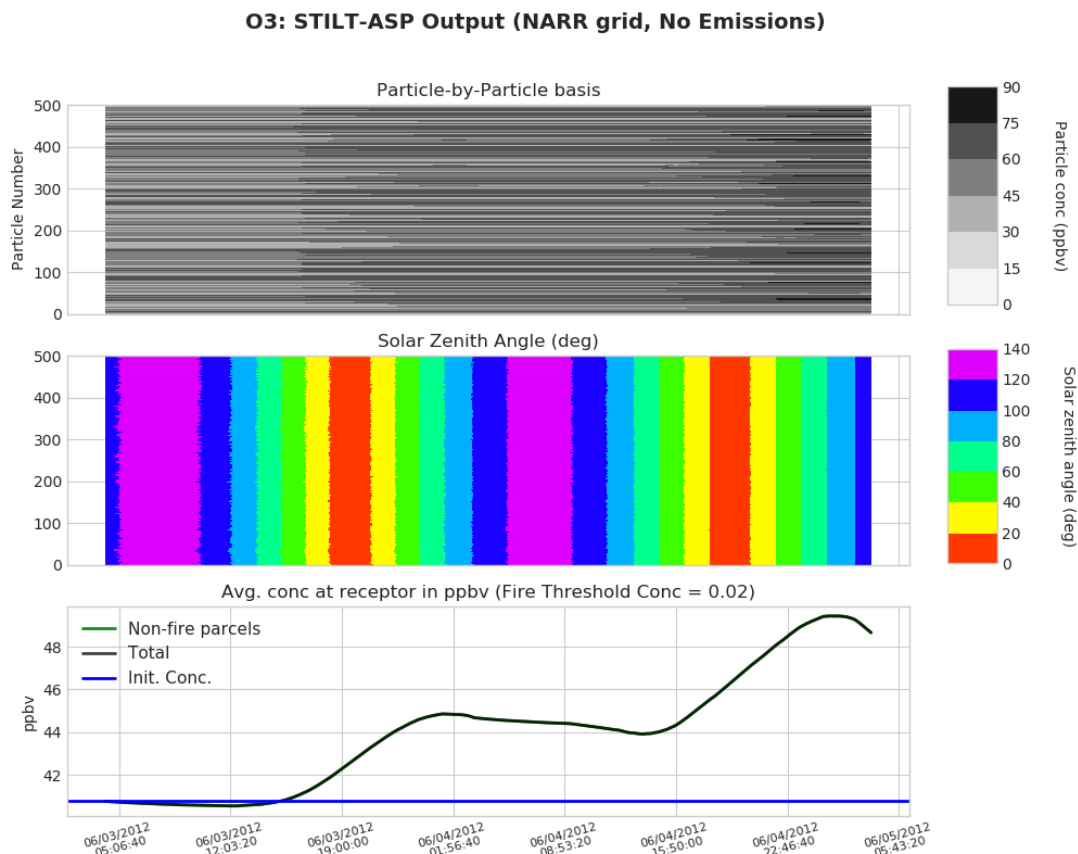


Figure 2. STILT-ASP O<sub>3</sub> output figure for the case described in the text without fire emissions.

As the quality of the information, including secondary data, has not been evaluated by EPA, the below disclaimer applies to all project deliverables:

*Disclaimer: The information contained in this report or deliverable has not been evaluated by EPA for this specific application, i.e. the identification of brown carbon aerosols and biomass burning smoke.*

#### **4 Conclusions**

Here we summarize the conclusions of our project, with reference to the corresponding report section.

- The EEST Docker container is now able to run on the TCEQ eira machine. The container downloads the relevant meteorological and satellite data, performs the STILT model run, and produces the expected figures and output. The results are identical to those run on AER machines (Section 2.2)
- The STILT-ASP Docker has been updated to use CAM-Chem boundary condition files. The container is now able to run on the TCEQ eira machine. The results are identical to those run on AER machines (Section 2.2).

#### **5 Recommendations for Further Study**

Based on the results of this work, we make the following recommendations for further study:

- TCEQ staff should use the model tools and report any errors or other issues to AER. AER will investigate any errors as time permits and push revisions back to TCEQ.
- If TCEQ agrees, access to a github repository for the code can be arranged so that TCEQ and AER staff can work on developing the codes in tandem, creating branches as needed.

## 6 References

- Brown-Steiner, B., A. Dayalu, and M. Alvarado (2019), *Uncertainty analysis and improvement of STILT-ASP for determining O<sub>3</sub> formation from biomass burning*, Final Report to Texas Commission on Environmental Quality (TCEQ) for Work Order No. 582-19-92805-03 under TCEQ Contract No. 582-19-90498, June 30.
- Lonsdale, C. R., M. Alvarado, R. Pernak and J. Henderson (2018), *Investigating Stratospheric and Wildfire Impacts on Urban Ozone Using an Automated Screening Tool and a Lagrangian Chemical Transport Model*, presented at the 2018 AGU Fall Meeting, Abstract # A23M-1798, Washington, DC, Dec. 12- 14.