An Exceptional Event Screening Tool to Estimate Natural Impacts on Ozone Exceedances

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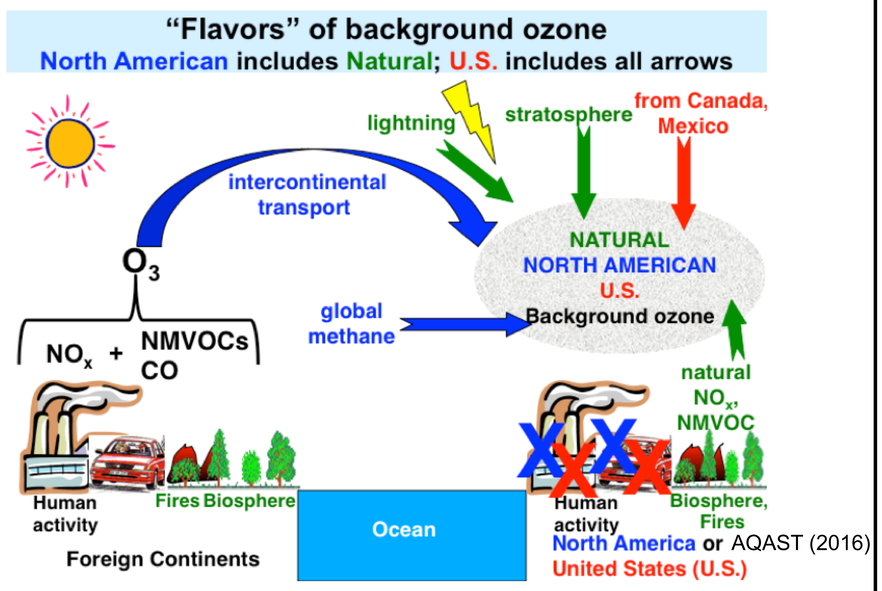
Motivation



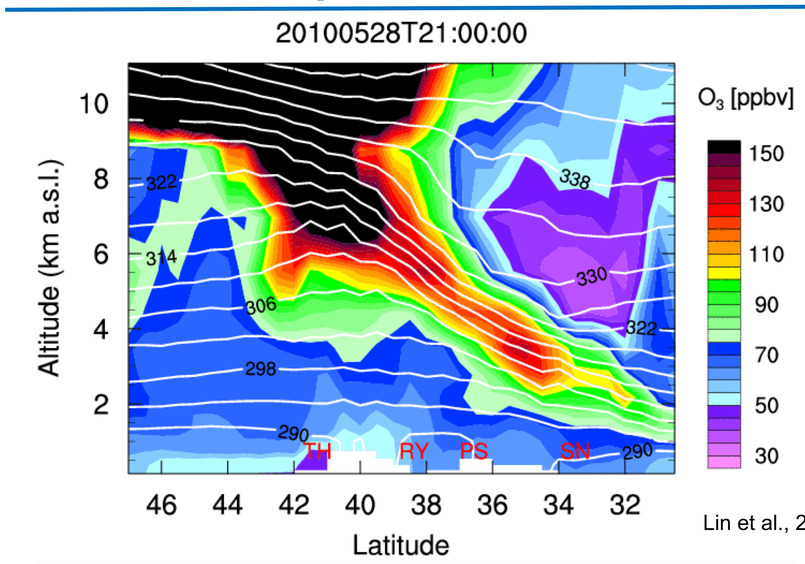
AQAST (2016)

The EPA Exceptional Event Rule

"A State may request that the EPA exclude measurement data related to exceedances or violations of a NAAQS if directly due to an exceptional event"

A detailed Exceptional Event Demonstration Report must quantitatively show that without impact from the *Exceptional Event*, **NO** exceedance would have occurred

Stratospheric Intrusions



Lin et al., 2012 JGR

A deep stratospheric ozone intrusion over the U.S. West Coast simulated in GFDL's global high-resolution chemistry-climate model (AM3).

- Occur when stratospheric air is transported deep into levels of the atmosphere typically associated with the troposphere.
- Can be caused by a variety of meteorological features including:
  - Tropopause folds
  - Cut-off lows at upper levels
  - Fronts and high-pressure systems at the surface
  - Areas with large vertical shear and strong meridional thermal gradients

Characterized by:

  - Areas with high Potential Vorticity
  - Commonly occur in the western states (higher altitude)
  - During the springtime
  - *Typically dry air masses*
  - *Coincides with high total ozone column*

Stratospheric O_3 transported downward in an intrusion is sufficient to create a sharp increase in O_3 concentrations measured at ground level air quality monitoring sites

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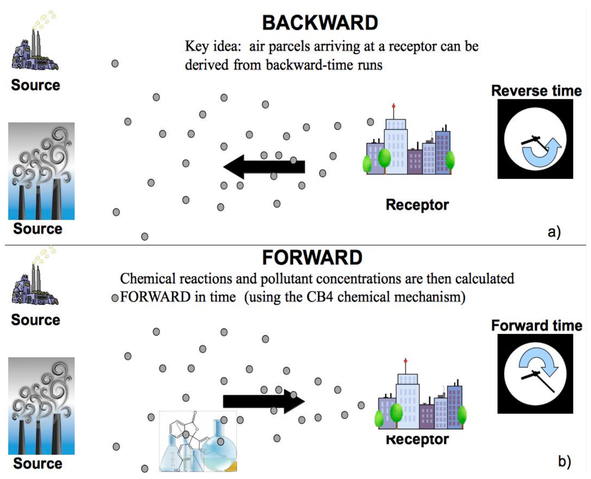
AIR QUALITY RESEARCH PROGRAM

The opinions and results shown here only reflect that of the authors, not of TCEQ or AQRP

Components of the *Exceptional Events Screening Tool*

STILT-ASP



Stochastic Time-Inverted Lagrangian Transport model

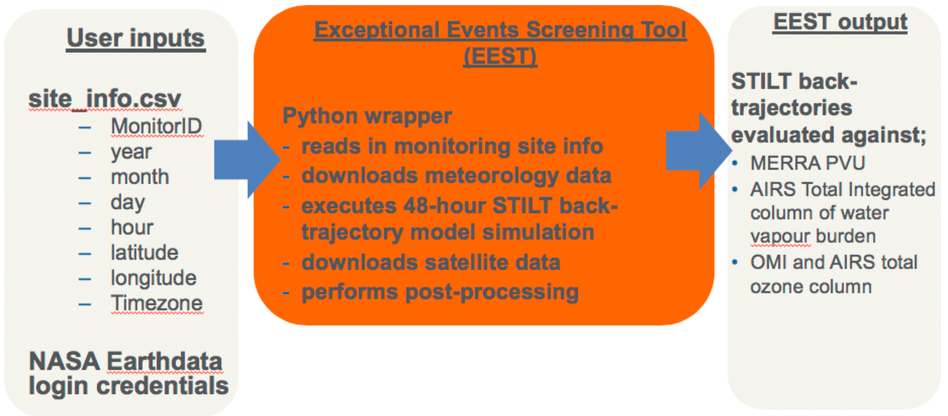
- Additional modifications that improve mass-conservation
- Allow the use of customized WRF meteorological fields (Nehrkorn et al., 2010)
- Extensively used at AER in inverse modeling studies to improve emission estimates for greenhouse gases (Henderson et al., 2015)

The Aerosol Simulation Program

- Models the formation of O_3 and SOA in plumes.
- Gas-phase chemistry
  - ≤C_4 gases follow MCM v3.2
  - Other organic gases follow RACM2 Inorganic aerosol thermodynamics
- OA thermodynamics using the VBS (Robinson et al., 2007)
- S/IVOC oxidation following Ahmadov et al. (2012)
- Evolution of aerosol size distribution and optical properties
- Can be run as a subroutine within 3D Eulerian and Lagrangian transport models

We have coupled STILT with ASP to better account for the impacts of long-range transport of emissions on CO, O_3, aerosols and other pollutants on the boundary conditions

Schematic



Data

Modern Era Retrospective-analysis for Research and Application (MERRA and MERRA2)

- Potential Vorticity reanalysis based on GEOS-5 atmospheric data assimilation

Ozone Monitoring Instrument (OMI)

- Total Ozone Column (DU)

Atmospheric Infrared Sounder (AIRS)

- Total Integrated column of water vapor burden
- Total Ozone Column (DU)

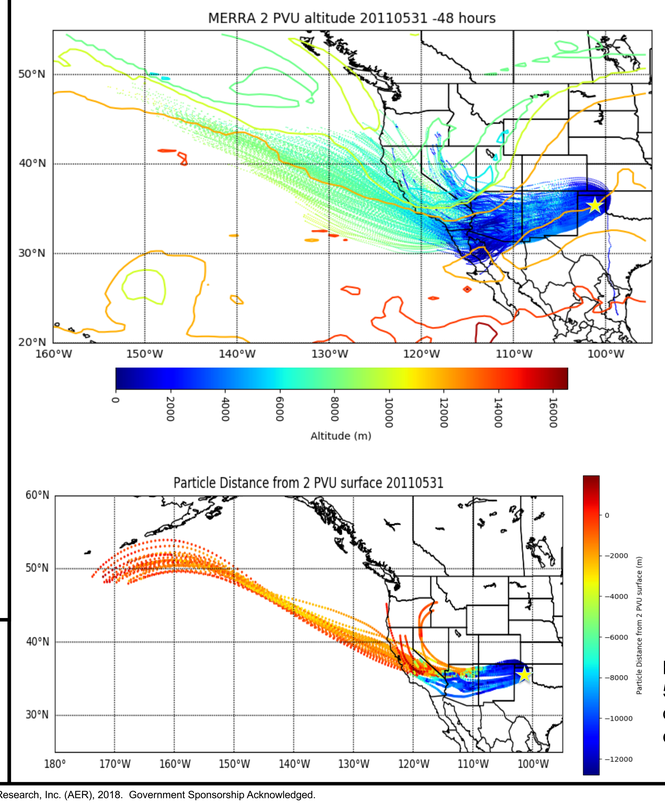
Containerizing Software using *Docker*

What is Docker?- a computer program that performs operating-system-level virtualization or "containerization"

- Containers in software engineering mitigate software development for the end user
- Require only the developers to gather and configure all of the dependencies necessary for a given model
- End-users only need to download the Docker client and then run a container locally
- Negates the need to install other dependencies, compile executables or handle any other model or system setup
- Gives end users the option of running a model (container) in almost any Linux, Windows, or Mac OS environment

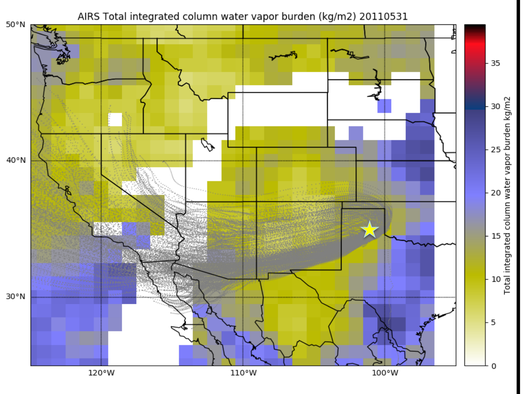
To gain access to the 'Exceptional Events Screening Tool' container, please email clonsdal@aer.com for instructions

Case Study



Top Left: STILT back trajectories for a 500-particle run initiated in Palo Duro, TX on May 31, 2011 plotted over the 2 PVU contoured by altitude. The color of the particle trajectories corresponds to their altitude and is plotted on the same color bar as the 2 PVU layer

Top right: STILT back trajectories for a 500-particle run initiated in Palo Duro, TX on May 31, 2011 plotted over Total Integrated column of water vapour burden (kg m^{-2}) from the AIRS dataset



Bottom Left: STILT 48-hr back trajectories that have crossed the 2 PVU surface, colored by their distance from the 2 PVU surface (m) at the time and location of that trajectory. Initiating at Palo Duro, Texas monitor site

Bottom Right: STILT back trajectories for a 500-particle run initiated in Palo Duro, TX on May 31, 2011 plotted over total ozone column (DU) from the OMI dataset