2.0 The Corpus Christi Trajectory Analysis Tool

To assist in the analysis of the potential impacts of emissions from Corpus Christi ship channel industries on pollutant concentrations measured by the Project, UT Austin developed during the summer of 2005 an interactive web-based application, referred to as the "Corpus Christi Trajectory Analysis Tool" or simply "Trajectory Tool". The Trajectory Tool (http://www.utexas.edu/research/ceer/ccaqp/trajectory_tool.htm) is observationally based and can be used to provide an estimate of the paths of air pollution releases over short (0 – 10 miles) distances. The Trajectory Tool features accuracy, timeliness, and simplicity and has operated continuously since 2005 with only minor interruptions for software upgrades and maintenance. The application has been integral to the air quality activities of the Project, including "quick-look" access in support of routine data reviews, studies of climatological pollutant (e.g., TNMHC, benzene, 1,3-butadiene) transport trends (e.g., annual, seasonal, time-of-day), and evaluations of near real-time air quality events potentially associated with upset (i.e., non-routine) emissions (e.g., SO_2, TNMHC, benzene, and 1,3-butadiene, among others) from nearby industrial sources. The Trajectory Tool was also an essential component of the UT Austin Corpus Christi automated email alert system.

2.1 Background

An evaluation of potentially important emissions from nearby local sources to a given individual monitoring location often begins with an analysis of measured pollutant concentrations and co-located meteorological observations. For example, hourly sampling data can be used to generate a pollution wind rose to quantify the frequency of occurrence of concentrations grouped by specific conditions of wind speed and wind direction within the analysis time frame of interest (e.g., annual). The wind rose, which indicates the wind directions and/or speeds most frequently associated with relatively high pollutant concentrations, can inform investigations to identify and evaluate emissions sources in the upwind geographic regions to the monitoring location that might have contributed to measured concentrations. However, the meteorological observations from a single monitoring (point) location cannot capture the impact of spatial variations in environmental conditions, such as wind direction, that could have affected transport pathways from emissions sources to the monitoring location. This is of particular concern in coastal areas such as Corpus Christi that are commonly affected by diurnally-driven local-scale atmospheric circulation features such as the land/sea breeze.

While the utilization of local wind direction or daily meteorological conditions measured at a single ground monitoring location is useful towards analysis of pollution events and has been successfully employed in support of Project analyses for Corpus Christi, the role of both local and long range transport are typically investigated via trajectory or dispersion analyses (e.g., Stein et al., 2015). Air parcel trajectory models are commonly used to characterize the atmospheric transport pathways for airborne gases and aerosols in support of air quality studies (e.g., Fleming et al., 2012 and Stein et al., 2015 and references therein). Reviews of various aspects of trajectory models, including computational details, model accuracy, and applications, have been provided by Stohl (1998), Fleming et al. (2012), and Stein et al. (2015), among others. Briefly, interpolated, measured or simulated meteorological fields are used to project backwards or forwards in time the most probable paths of infinitesimally small particles of air that at the

starting time are located at the receptor (e.g., monitoring) location (Squizzato and Masiol, 2015). The results from an individual trajectory or collection of trajectories can indicate potential downwind impact areas (for forward trajectories) and upwind emissions source regions (for backward trajectories). The frequency and type of short-term pollution events can be tracked back to their source and seasonal and long-term trends can be studied and compared to seasonal and long-term air mass transport patterns.

Atmospheric flow that determines trajectory paths can be viewed in two potential fields of reference: Eulerian or Lagrangian (e.g., Stein et al., 2015). Eulerian models use a fixed reference (i.e., coordinate system) so that air flows through points fixed in space; in Lagrangian models, a moving frame of reference follows an individual air parcel through space and time typically using the average atmospheric motion. The most common air mass trajectory models for studying the transport of air pollutants are Lagrangian-based (Saunders et al., 2013). The pathline of the target air parcel, represented as an infinitesimally small particle, is plotted at regular time intervals using an input wind speed and wind direction dataset that can be spatially two-dimensional (horizontal, i.e. east-west and north-south winds only) or three-dimensional (horizontal and vertical motions). In reality, an air parcel is subject to convective and mechanical mixing processes that can cause horizontal and vertical dispersion of the target air mass. Models have been developed to handle vertical and small-scale mixing processes stochastically and via parameterizations by grouping multiple single particle (advection) components of motion within a Lagrangian framework (e.g., Stohl, et al., 2002; 2005; Draxler et al., 2014). As noted by Freitag et al. (2014), multiple trajectories may also be calculated by slightly varying initial starting conditions in space and time to investigate the impact of wind-induced deformation processes on the target air mass parcel (e.g., Merrill et al., 1985; Cape et al., 2000).

In long range transport, various exchange and mixing processes (e.g. deposition and advection), physical losses and chemistry in addition to emissions may have important contributions at a given receptor location (Fleming et al., 2012). One of the most widely applied air trajectory model is the Hybrid Single–Particle Langrangian Integrated Trajectory model (HYSPLIT), which is often used for long–range transport studies (Draxler et al., 2014; Stein et al., 2015). The three-dimensional meteorological data fields typically employed by HYSPLIT are characterized by a one-hour averaging period and a horizontal spatial scale of 50-100 km (http://ready.arl.noaa.gov/READYcmet.php) so are well-suited to investigating transport on a regional scale. Short-term transport, such as within an urban area in response to a localized pollution event (e.g., an accidental ground-level emissions release at an industrial facility), can be highly sensitive to nearby emissions sources and may be best represented by trajectories calculated using the near-surface wind field as measured by a ground monitoring network. One widely-applied Lagrangian particle dispersion model is FLEXPART (Stohl et al., 1995). FLEXPART calculates the trajectories of tracer particles using a mean wind modified by parameterizations representing mixing processes associated with turbulence and convective transport. The FLEXPART model has been used extensively in support of air quality applications (e.g., Fleming et al., 2012 and references therein).

2.2 Approach

Because Lagrangian particle dispersion models are more complex to run and can require substantial computing resources, the calculation of single air parcel trajectories to estimate

atmospheric transport pathways has proven remarkably robust and continues to be widely used in air quality analysis applications. In support of the Project, the calculation of single Lagrangian particle back-trajectories representing upwind paths within about a 5-mile radius of the individual monitoring location have proved highly useful in the analysis and identification of potentially important industrial emissions sources. The general form of the trajectory advection equation used by the Trajectory Tool is similar to that employed by other practical trajectory models (Stohl et al., 2002) as provided below:

$$Dx_i = W_i * Dt$$

Where Dx is the position increment during each time step (Dt) resulting from the 5-minute average (non-turbulent) wind (W); the index (denoted by the subscript "i") for the Trajectory Tool runs from 1 to 2 to account for the east-west (U) and north-south (V) components of the horizontal wind.

The trajectory calculation employed by the Trajectory Tool assumes that the sampled air mass moves with the area-averaged winds as measured by the Corpus Christi network of surface monitoring stations. All available 5-minute observations of wind speed and wind direction collected at the seven Project and five TCEQ monitoring locations are used for the back-trajectory calculations. Ideally, the back-trajectories would be based on continuous observations of wind speed and direction at all locations throughout the entire Corpus Christi area. In reality, observations of wind speed and wind direction are only available from a limited number of monitoring stations so that winds at locations away from the monitors must be estimated using the available observations. An interpolation algorithm is used to provide these estimates.

The interpolation algorithm used by the Trajectory Tool more heavily weights wind data from nearby monitoring stations. The trajectory calculation algorithm begins by computing the distance between the starting location and each individual monitoring station. A weighting factor for each monitor is calculated as the inverse distance squared multiplied by the square root of the distance to the nearest neighbor. A minimum value for the inverse distance is currently set to three kilometers. The distance to the nearest neighbor for a given monitor is the distance to the closest monitor, and is included in the calculation so that data collected at isolated monitoring stations are more heavily weighted compared to monitors located in clusters.

The average 5-minute wind speed and direction obtained from the interpolation is then used to advect the hypothetical parcel backward or forward in time over a 5-minute period. The hypothetical air parcel is assumed to move along a linear path at the average wind speed and direction of its starting location. A new average wind speed and direction is then interpolated at the new back-trajectory location using all available wind data for the next 5-minute period. The calculation procedure is repeated until the trajectory is complete for the requested duration.

2.3 Uncertainties

Trajectories are dependent on the accuracy and representativeness of the input wind fields for the relevant flow patterns for the trajectory type of interest; thus, inaccuracies associated with the input wind dataset are often the largest source of positional errors (Stohl, 1998). Additionally, two potentially important effects neglected in particle air mass trajectory models, such as the

Trajectory Tool, are: (1) the path of an infinitesimally small particle is tracked by the calculated trajectory whereas trace gas measurements are samples of finite air volumes, and (2) the impact of vertical dispersion associated with turbulent mixing and convection is not considered. As discussed by Polissar et al. (1999), other sources of errors in trajectory calculations include the interpolation of sparse meteorological data to the actual trajectory positions, numerical computation inaccuracies, observational errors, sub-grid scale phenomenon, and the impacts of atmospheric processes such as evaporation and condensation.

A review of the types and uses for back trajectories, including the associated errors and uncertainties, has been provided by Stohl (1998). Total trajectory position errors, resulting from all of the previously described sources together, are difficult to determine and are in some cases inconclusive (Polissar et al., 1999; Stohl, 1998). Owing to errors and assumptions in the wind fields used to calculate trajectories, the uncertainty of trajectories increases with time along the path. A review of publications on trajectory reliability found that errors are on the order of 15–20% of the total distance travelled after a few days (Stohl, 1998). However, trajectory deviations up to 100% are possible if the input wind datasets are not sufficient to resolve the predominant atmospheric flow patterns (e.g., Stohl et al., 2002).

For surface back-trajectories generated by the Trajectory Tool, the density of monitors throughout the greater Corpus Christi area has substantial spatial variation; the Ship Channel region has the highest density with sparse coverage elsewhere. As such, the calculated trajectories are based on a relatively small dataset that may not capture important spatial and temporal variability in winds at locations away from the available monitoring locations. In addition, the surface back-trajectories assume that a given parcel moves with surface winds as measured by the network of monitoring stations throughout the trajectory period, and does not account for any vertical movement of air parcels. The vertical movement of air can have a substantial impact on the transport of emissions from a stationary source, particularly if vertical motions move the air parcel into a layer of the atmosphere characterized by a different wind speed and wind direction compared to that measured at the surface.

As illustrated in the example case studies shown in Section 2.6, page 2-11, it has been the experience of UT Austin that short-term back-trajectories generated by the Trajectory Tool have proven remarkably useful in the investigation of potential impacts on measured concentrations associated with nearby (often industrial) emissions sources. In general, an individual back-trajectory may potentially be associated with large uncertainty dependent primarily upon the variations in atmospheric conditions that impact advection and dispersion along the trajectory path as well as the release height of the emissions of interest. Overall, however, trajectory patterns that emerged when analyzing repeated types of air pollution events have provided a good indication of transport patterns due to the prevailing near-surface wind flow regimes.

2.4 Overview of Design and Implementation

The creation of the Trajectory Tool required a number of activities, including: 1) automation of the retrieval and processing of wind measurements in near real-time; 2) development of computational and visualization tools, and; 3) creation of the interactive website to allow public access to user-generated trajectories.

The Trajectory Tool utilized the available 5-minute observations of wind speed and wind direction (sampling height at approximately 10 meters above ground level) collected at the seven Project and five TCEQ monitoring locations previously shown in Figure 1-1, page 1-4. The 5-minute average wind speed and wind direction observations collected by the Corpus Christi monitoring network are electronically transferred to TCEQ's Leading Environmental Analysis and Data System (LEADS) on a routine near real-time basis. UT Austin established a private user account with TCEQ in order to obtain direct access to the web-based retrieval application that provided access to LEADS. An Internet spider program, referred to as the WebGet Internet File Retriever, was developed that generates the webpage interface input information to automate the retrieval of the 5-minute wind observations from LEADS. Based on the experience of UT Austin, the wind measurements from any given monitoring station were typically available from LEADS within 0.5-1.5 hours from the time of collection. Thus, the WebGet Internet File Retriever was initiated on an every 15-minutes schedule using Microsoft Windows Scheduler to provide continuous updates to the Trajectory Tool database archive of wind observations.

The results from the WebGet Internet File Retriever consisted of ASCII text files that contained various header, data quality, and footer information provided by the LEADS system in addition to the wind speed and wind direction observations required by the Trajectory Tool. Various Microsoft DOS and Visual Basic scripts were written to extract and process only the 5-minute wind observations for import into a Microsoft Access Database application. A series of Microsoft Access Database programs (consisting of multiple macros and queries) were written to perform routine quality assurance checks, correct for missing data records, insure record uniqueness grouped by monitoring location, and to reformat the 5-minute wind measurement data for input to the Trajectory Tool data archive. The results from the Microsoft Access Database application were exported into the Microsoft SQL database archive that provided all wind observations used as input to the Trajectory Tool.

The Trajectory Tool interactive web-based application was developed using HyperText Markup Language (HTML), Cold Fusion MarkUp Language (CFML), and Macromedia Flash software. The core software that ran the Trajectory Tool used Flash MX 2004 Professional and Flash ActionScripts. The main Flash routine consisted of a series of ActionScripts called in sequence of ten programming frames. The ActionScripts perform the primary tasks of the trajectory application, including retrieval of user input through the publicly accessible web-based interface, query and retrieval of wind observations from the database archive, calculation of the trajectory positions for each 5-minute time interval, and generation and display of the output trajectory over a geographic map of the Corpus Christi area. The core trajectory software module uses the Cold Fusion Server to retrieve the necessary wind speed and wind direction data from the Microsoft SQL database archive.

The user interface of the Trajectory Tool is shown in Section 2.5. The starting location for a user-generated trajectory could be specified by entering the latitude and longitude in the labeled text boxes or automatically loaded by clicking anywhere on the default home page or pre-defined zoomed thumbnail maps of the Corpus Christi area. The starting date, time, and trajectory duration were selected through the use of drop-down menus. The user also specified a forward or backward option before clicking the "submit" button to create and display the trajectory results.

After the user had submitted the required information, the Trajectory Tool core software retrieved the available 5-minute observations of wind speed and wind direction collected at the Corpus Christi network of ground monitoring stations corresponding to the trajectory calculation time period from the Microsoft SQL database. Valid data from a least nine monitoring stations (~75% of available monitors) were required to calculate the average wind speed and wind direction for each 5-minute time interval in the user-requested trajectory. If fewer than nine monitors are available, the trajectory was truncated and no interpolation across data gaps was performed.

For each 5-minute time interval, a trajectory position was calculated using the interpolation and advection scheme described in Section 2.2, page 2-2, of this report. Each trajectory position was then plotted as a circular green position label representing the estimated locations of an infinitesimally small (particle) air parcel at 5-minute intervals assuming the air parcel moved with the area-averaged winds as measured by the Corpus Christi network. The circular green position labels were connected by linear line segments to more easily visualize the estimated transport path. The diameters of the trajectory position labels were set to grow linearly at a rate of one mile per hour to provide a visual reminder of the uncertainty in the trajectory position as a function of time.

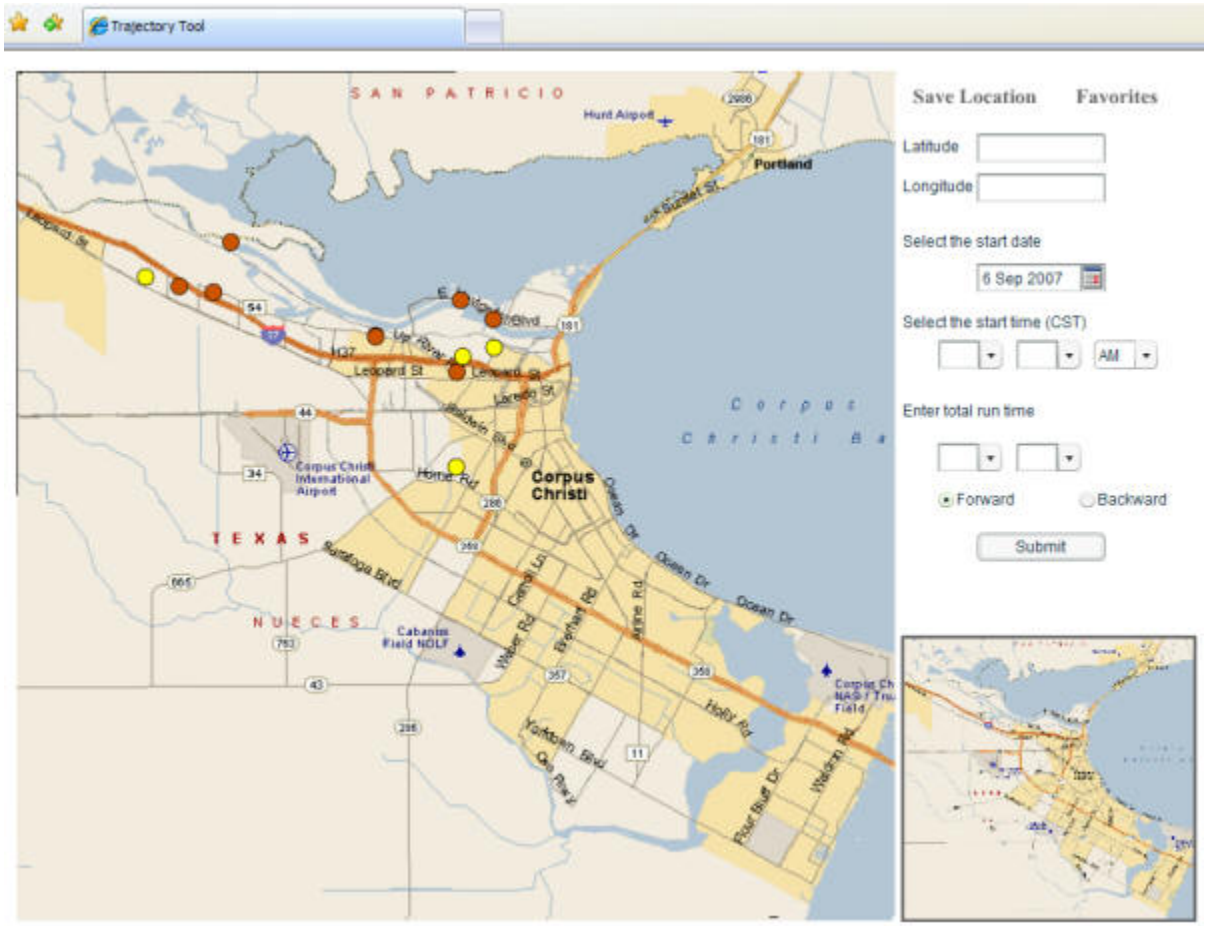
Although the trajectory application was built specifically for the Corpus Christi area, the program was designed so that it could be adapted to any geographic location. Because a variety of interpolation schemes could be used to estimate wind speed and wind direction for each time step, the interpolation scheme is contained entirely within one ActionScript file read as input by the core program. The information specific to a geographic location is provided as input data to the trajectory software. The input data requirements include monitoring information, static geographic maps and domain definitions, and 5-minute wind measurements. The monitoring specific information (e.g., latitude, longitude, monitoring site names) is specified in an XML file that can be modified using any ASCII text editor. The static geographic maps can be created using Microsoft MapPoint. The core program also requires that the domain coordinates for the main and inset (thumbnail) maps are defined in the first Macromedia Flash frame. Finally, the 5-minute wind speed and direction data must be stored in a database accessible by the trajectory tool software.

2.5 Trajectory Tool Tutorial

The operation of the Trajectory Tool was illustrated on the Project website (http://dept.ceer.utexas.edu/ceer/ccaqp/trajectory_tool_tutorial.htm) using a user tutorial. A summary of the original tutorial is provided below in order to demonstrate the access and operation of the interactive user interface. The Trajectory Tool was designed for a 1024 X 768 screen resolution to provide sufficient visual mapping detail and was subsequently tested by UT Austin using a variety of Internet Web Browsers (e.g., Internet Explorer, Mozilla Firefox, Safari).

Step 1. Loading the trajectory tool.
The trajectory application was accessed via the Project website (http://dept.ceer.utexas.edu/ceer/ccaqp/trajectory_tool.htm). A loading bar with a range of 0-

100% indicated when the application was ready for use. The image below displays the appearance of the default user input page when fully loaded.



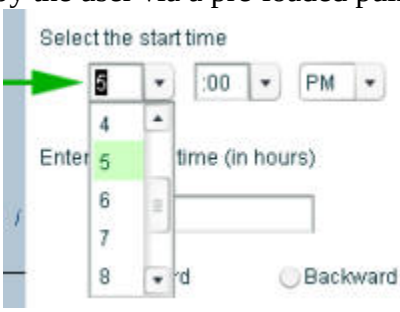
Step 2. Selecting the start location.
If known by the user, the initial latitude and longitude coordinates could be entered directly into the labeled input text boxes “Latitude” and “Longitude” provided in the upper right-hand corner of the user input page.

More commonly, a user would utilize the interactive graphic map of the Corpus Christi area to specify the starting location. As illustrated below, the user began by moving the mouse cursor over the map to select a shaded zoomed region within the geographic area of interest. Clicking on the appropriate shaded map allowed for two levels of zoom before a specific location was selected; the corresponding latitude and longitude would be automatically entered by the Trajectory Tool application into the “Latitude” and “Longitude” input boxes. In the example below, the middle shaded area was selected on the full resolution map followed by the selection of quadrant number “11” on the second zoomed-level map. The starting location was selected by an additional mouse click, or if the user made a mistake, a different location could be re-selected within the fully zoomed map or, alternatively, the “Zoom Out” button (which was located directly above the thumbnail map) provided for a reset of the Trajectory Tool mapping interface.

Step 3. Viewing the monitoring site labels.
Circular labels on the map indicated the locations of monitoring stations that collected the wind observations used to generate the trajectories; orange for Project and yellow for TCEQ. To identify each monitoring location, the user could position the mouse cursor over a station location and a pop-up label would appear showing the station name and CAMS number as shown in the example image below.

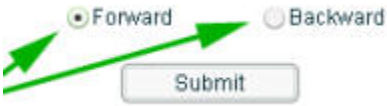
Step 4. Selecting the start date.
In order to minimize user error, dates were selected using a pre-loaded pull-down monthly calendar as illustrated below. Either the mouse or arrow keys could be used to scroll through the calendar to choose the day, month, and year of interest.

Step 5. Selecting the start time
The start time was also selected by the user via a pre-loaded pull-down menu.

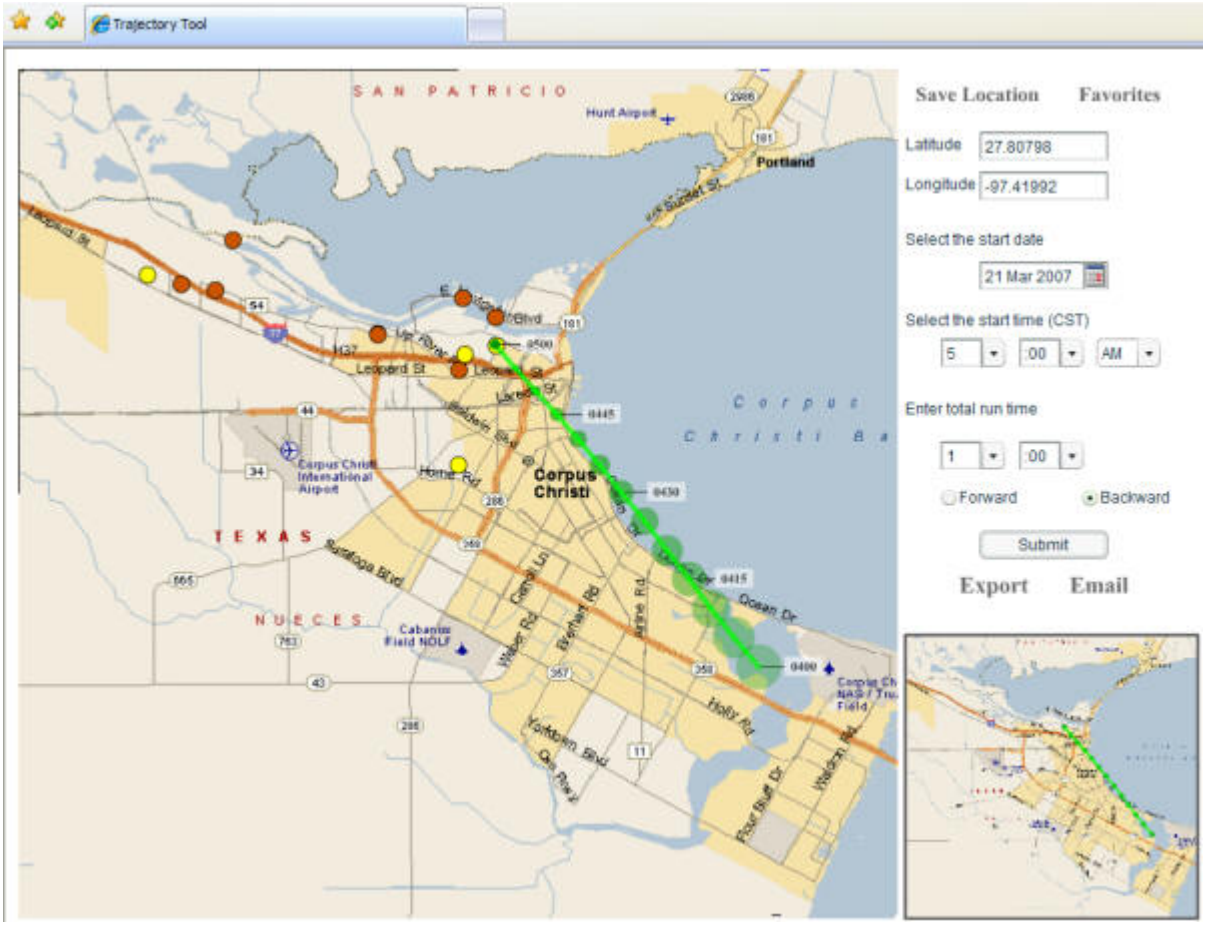


Step 6. Setting the trajectory run time.
The run time provided in the "Enter total run time" input box indicated the duration of time for the trajectory calculation. For example, a "backward" trajectory initiated at 5:00 p.m. with a run time of one-hour would end at 4:00 p.m. The resulting back-trajectory would consist of twelve individual 5-minute position locations.

Step 7. Selecting the trajectory type.
Either a forward or backward trajectory could be specified.



Step 8. Creating the trajectory.
After the user had provided input arguments for the following fields: **start location, start date, start time, run time, and trajectory type (i.e., forward or backward)**, a click of the "Submit" button would generate the trajectory. The resulting trajectory path would be plotted on the interactive map using circular green position labels to show the trajectory positions at 5-minute intervals. The trajectory positions were labeled at 15-minute intervals beginning at the start time. The diameters of the trajectory position labels were set to grow at a linear rate of one mile per hour in order to provide a visual estimate of the uncertainty in the trajectory position as a function of time.



If a greater geographic resolution was desired, the user could click on the two levels of zoomed maps to view the results. The trajectory would remain on all maps until the browser was refreshed or a new trajectory was submitted. Common to any web page, the trajectory map could be printed by selecting "file" then "print" in the browser menu.

Step 9. Other (Optional) Features

Save/Bookmarking a starting location using the “Save Location” button: A starting location could be bookmarked to save the latitude and longitude coordinates.

Favorites: The “Favorites” button could be used to recall previous starting locations.

Exporting the trajectory coordinates: UT Austin often used the “Export” button to generate a comma-delimited ASCII text file containing the latitude and longitude coordinates of the trajectory 5-minute positions. The exported position locations could then be used in other analysis software packages to display the trajectory path in support of, for example, complementary air quality analysis activities.

Emailing the trajectory: The “Email” button allowed a user to recreate the trajectory on another machine by generating a clickable link to the Trajectory Tool that had the appropriate inputs and

attributes. Both the “Email” and “Export” buttons appeared only after a trajectory was successfully generated.

2.6 Example Results

The Corpus Christi Trajectory Tool has been an essential component of the Project’s air quality analysis activities since its original development by UT Austin in the summer of 2005. Trajectories have been generated at one or more monitoring locations in support of short-term, recurring, or sporadic pollutant event investigations in addition to studies of longer-term trends. In order to demonstrate the utility of the Trajectory Tool, a select number of example case studies and historical analysis results are provided.

Example 1: Quick-look analysis in support of the Corpus Christi automated email alert system
The Trajectory Tool was an essential component of the UT Austin Corpus Christi automated email alert system. Figure 2-1, below, contains the text of an example email message generated by the alert system on April 3, 2012 indicating elevated sulfur dioxide (SO_2) concentrations had been measured at the J. I. Hailey monitoring station. If a recipient clicked on the first “Click Here” link, a URL to the Trajectory Tool was created that had the appropriate back-trajectory inputs and automatically opened in the recipient’s default Internet Browser. Figure 2-2, page 2-12, shows the resulting webpage result. The near real-time capability of the Trajectory Tool within the context of the automated email alert system was a well-received feature and routinely used by UT Austin and TCEQ throughout the duration of the Project.

Figure 2-1. Example of an automated email alert with a “Click Here” link to generate a back-trajectory.

The following alert has been received in the Corpus Christi Area:
emrs_medium_alert_48355003742401_20120403_1130.txt
SO2 MEDIUM trigger at site J.I. Hailey C630.
92.94 >= 75.00 ppbV
WD = 177 degrees
WS = 12.1 mph
time of trigger 11:30 (CST) 2012.04.03
17:30 (UTC) 2012.04.03
-97.43 | 27.81 | CITGO REFINING & CHEMICALS CO
To see the graphical output from the Corpus Christi Trajectory Tool of this alert click the following link:
Click Here
Click this link to go to the Alert Archive to view other alerts in the Corpus Christi area:
Click Here

Figure 2-2. A surface back-trajectory that was automatically generated and displayed in an Internet Browser after using the first "Click Here" link in the email message shown in Figure 2-1.

Example 2: Analyses of relatively high SO_2 concentrations at J.I. Hailey

The measurement of sulfur compounds (SO_2 and H_2S) has been an important component of the Project monitoring network since operations began in 2005. Some of the highest SO_2 concentrations throughout the program were measured at J.I. Hailey, with a maximum 5-minute SO_2 concentration of 444 ppbV observed on January 27, 2005. Prior to August 2010, the applicable National Ambient Air Quality Standard (NAAQS) for SO_2 included a 24-hour average primary standard at 140 ppbV, an annual average primary standard at 30 ppbV, and a three-hour, secondary public welfare standard of 500 ppbV; none of these concentration thresholds were exceeded at any Project monitoring location. However, EPA subsequently revised the SO_2 NAAQS to a one-hour standard of 75 ppbV, effective August 23, 2010. The statistically based one-hour standard is exceeded at a given monitoring location if the three-year average of the 99th percentile annual daily maximum one-hour average concentrations (referred to as the design value) exceeds 75 ppbV. Table 2-1, below, provides the one-hour SO_2 design values at each Corpus Christi monitoring location for years 2007 - 2015; the design values at J.I. Hailey for 2007-2012 were greater than 75 ppbV.

Table 2-1. One-hour SO_2 design values (ppbV) at Corpus Christi monitors for years 2007-2015.

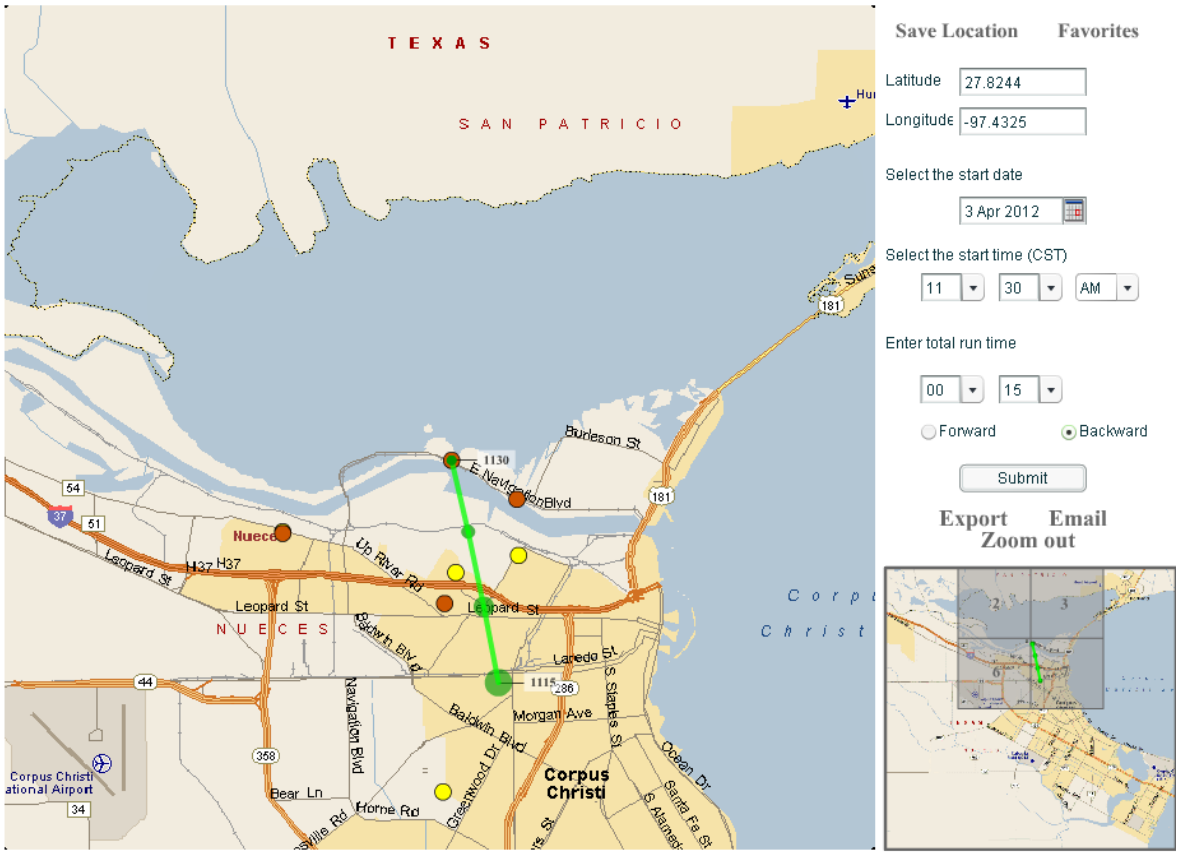
Years	West	Tuloso	Huisache	Port Grain	J.I. Hailey	Inner Harbor	FHR	Solar Estates	Dona Park
2005-2007	23.9	8.3	36.1	33.6	118.7	38.0	20.6	50.5	34.4
2006-2008	20.9	8.3	32.5	30.6	131.2	32.8	19.1	31.4	31.0
2007-2009	17.6	8.6	27.7	29.8	88.9	32.4	16.6	20.9	22.7
2008-2010	17.2	9.4	33.1	26.4	102.7	21.2	12.9	10.6	22.3
2009-2011	12.3	9.0	27.0	18.7	79.9	15.2	12.8	29.9	19.9
2010-2012	9.8	7.7	23.3	15.3	76.2	8.4	12.0	39.9	11.7
2011-2013	6.6	6.2	10.2	11.3	47.0		12.1	51.0	7.9
2012-2014	5.0	4.4	5.6	11.3	33.2		12.5	28.4	6.5
2013-2015	4.4	3.9	4.1	6.1	15.8		10.4	15.7	5.2

UT Austin engaged in an on-going pollutant event analyses that utilized the Corpus Christi alert system to identify potential emission sources contributing to high SO_2 concentrations at J.I. Hailey. The routine analysis included a periodic review of back-trajectories for those 5-minute sampling periods that had measured concentrations greater than 75 ppbV. Figure 2-3, page 2-14, presents an example trajectory at 11:30 CST on April 3, 2012, which had a monitored SO_2 concentration of 93 ppbV. The back-trajectory indicates low-level flow from the south; the immediate upwind region includes the adjacent Corpus Christi ship channel as well as industrial facilities across the channel to the south. This low-level flow pattern was common when relatively high SO_2 concentrations were measured at J.I. Hailey.

Investigations by UT Austin that focused on industrial sources along and to the south of the Ship Channel eventually found that emissions associated with diesel-fueled engines aboard ships and barges were the most likely culpable source. An on-going review of back-trajectory paths for high SO_2 concentration events identified a few specific docks in the immediate upwind region to J.I. Hailey. Complementary analysis of selected events confirmed that ships were often docked at one or more of the dock locations and the primary source of SO_2 emissions during these events was hypothesized to be associated with the burning of high-sulfur diesel fuel used by the dockside ships' auxiliary engines. Recent investigations by TCEQ verified that emissions from ships were a likely source of the relatively high SO_2 concentrations at J.I. Hailey (Sullivan et al., 2012).

Interestingly, over the latter half of 2012 and throughout 2013-2015, SO_2 concentrations at J.I. Hailey decreased dramatically relative to those observed during previous years. On March 26, 2010, the International Maritime Organization amended the International Convention for the Prevention of Pollution from ships within specific portions of U.S., Canadian, and French waters; these new regulations for sulfur content in diesel fuels for marine vessels went into effect on August 1, 2012 (https://www.epa.gov/sites/production/files/documents/finalfuelavailabilityguidance-0626.pdf). The new rules applied to all vessels navigating the Corpus Christi Ship Channel including the large ships typically docked in the upwind area when high SO_2 concentrations were monitored at J.I. Hailey. It appears likely that the new regulations led directly to the relatively low design value of 47 ppbV during 2013 at J.I. Hailey, and may have contributed to declines in measured SO_2 at other monitoring locations in Corpus Christi as well.

Figure 2-3. Fifteen-minute back-trajectory initiated from J.I. Hailey at 11:30 CST on April 3, 2012.



Alert ID: emrs_medium_alert_48355003742401_20120403_1130

SO2 MEDIUM trigger at site J.I. Hailey C630. Higher trigger level.
92.94 >= 75.00 ppbV
WD = 177 degrees
WS = 12.1 mph
time of trigger 11:30 (CST) 2012.04.03
17:30 (UTC) 2012.04.03

Example 3: Identification of a highly-emitting industrial source of 1,3-butadiene

From the onset of monitoring in March 2005 through 2012, relatively high (e.g., up to 143 ppbC) hourly concentrations of 1,3-butadiene were sometimes measured at the Solar Estates monitoring location when the near-surface wind directions in Corpus Christi were generally from the southwest. UT Austin performed a case study analysis for a high pollutant concentration event that occurred on the morning of September 27, 2009. The auto-GC instrument at Solar Estates monitored unusually high concentrations of 1,3-butadiene for multiple hours, with concentrations of 35 ppbC during the two one-hour periods beginning at 5:00 a.m. CST and 7:00 a.m. CST. In order to investigate potential upwind emission sources, back trajectories were generated by UT Austin using the Trajectory Tool initiated at the mid-point of each hourly 1,3-butadiene measurement for the 00:30 a.m. - 8:30 a.m. CST period. The back-trajectory locations were exported to an ASCII text file and the 5-minute locations were plotted over satellite imagery using Google Earth Pro as illustrated in Figure 2-4, page 2-15. The trajectory 5-minute position labels were color-coded based on the 1,3-butadiene hourly concentrations measured at Solar

Estates. The concentrations during the initial three hours were low and the back-trajectories (plotted in white) indicated generally southerly low-level wind flow towards Solar Estates. As shown in subsequent images, the concentrations increased during later hours as the back-trajectory paths became more southwesterly.

Figure 2-4. Surface back-trajectories for September 27, 2009, initiated each hour 0:30 CST through 8:30 CST, are shown in this figure. The trajectories are color-coded by the 1,3-butadiene hourly concentrations at Solar Estates; white = 0 parts per billion-carbon (ppbC), yellow = 2 to 6 ppbC, red = 35 ppbC. The facility of interest is circled in green shown in the upper left image image.

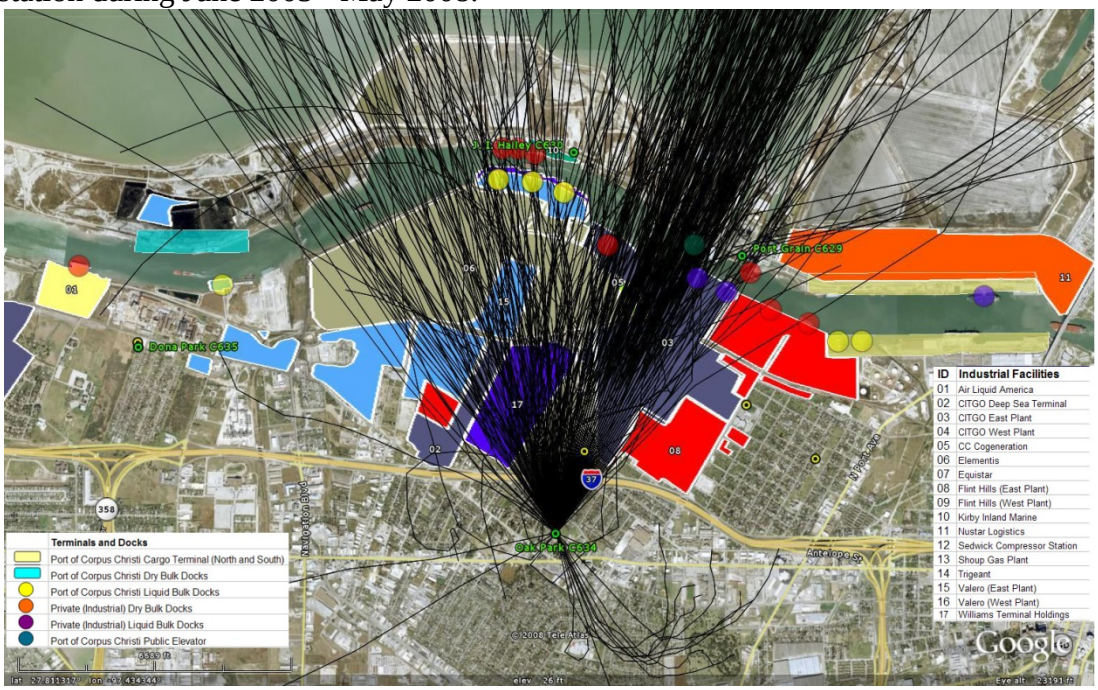
An analysis of the trajectory results identified an industrial facility, located approximately three miles to the southwest of Solar Estates, that was commonly along or near to the trajectory paths when relatively high concentrations were measured. The industrial facility was confirmed to be a known emitter of 1,3-butadiene and studies of additional events indicated that emissions from this facility were likely a primary contributor to the high 1,3-butadiene concentrations measured at the Solar Estates location. Subsequent operational modifications at the facility were associated with a cessation of 1,3-butadiene emissions that were correlated with a substantial reduction in measured 1,3-butadiene concentrations at Solar Estates.

Example 4: Analysis of potentially important geographic source regions of benzene emissions
A conceptual model was developed that describes the seasonality, day-of-week, and diurnal variability of concentrations of selected air toxic compounds measured at the Project ground monitoring locations (McGaughey et al., 2009). The conceptual model had a description of meteorological conditions most likely to lead to higher concentrations of air toxics, and included an analysis of local transport patterns to identify potentially important local industrial emissions source regions.

The conceptual model was developed in 2009 by UT Austin and used observational data collected during June 2005 – May 2008. A crucial component of the analysis at each of the seven Project monitoring stations was the generation of back-trajectories for relatively high concentrations of specific pollutant species. For example, in order to identify the potentially important geographic emissions source regions for benzene, high concentrations were defined as those hours with a concentration of 30 ppbC or greater at the Solar Estates or Oak Park monitoring stations. The Trajectory Tool was used to generate one-hour surface back-trajectories for all hours with high benzene concentrations; the back-trajectories were initialized at the half-hour (i.e., midpoint) of the one-hour averaging period.

Figure 2-5, page 2-17, presents the trajectory results for the Oak Park monitoring station. Although near-surface winds with a southerly component are very common in Corpus Christi, there is a notable absence of trajectories indicating southerly flow into Oak Park; this finding suggests a lack of important emissions sources to the south of Oak Park. In contrast, the back-trajectories are clearly consistent with important emissions sources generally located to the north-northwest through (especially) north-northeast of Oak Park. These nearby regions are highly industrialized and subsequent analyses confirmed numerous industrial sources of benzene emissions in the upwind areas indicated by the back-trajectory paths.

Figure 2-5. Surface back-trajectories generated by the Corpus Christi Trajectory Tool for all hours characterized by a benzene concentration of 30 ppbC or greater at the Oak Park monitoring station during June 2005 - May 2008.



2.7 Summary

Lagrangian based particle trajectory models are routinely used for studying the transport of air pollutants. In support of Project air quality analysis activities, UT Austin developed an interactive web-based Trajectory Tool that used near-surface wind observations to calculate forward or backward trajectories. The Trajectory Tool application was made available during the summer of 2005 and has been used extensively in support of both near real-time and historical air quality analyses. The current trajectory calculation algorithm uses an inverse distance squared weighting factor modified by the distance to the nearest neighbor to interpolate wind observations to any location. While this trajectory application was developed specifically for Corpus Christi, Texas, the trajectory analysis software could be modified for use in any geographic location by providing the necessary static geographic base maps, location-specific monitoring information, and database of wind observations.

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