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Use of Air Quality Dispersion Models to Reconstruct Site Exposure Profiles



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June 2018

**Final Report
for June 2016 to February 2018**

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14. ABSTRACT Air quality dispersion modeling can be used to estimate both past and future localized exposures to occupational pollutants based on emission sources and meteorological conditions. There are several air quality dispersion models available, each with capabilities that are specialized for particular air quality situations. To demonstrate which models are appropriate for different applications, a suite of air quality models and geographical data analysis software was reviewed, including AERMOD, CALPUFF, HYSPLIT, QUIC, and ArcGIS. A similar simulation was run with all models except CALPUFF, which was not run due to weather data availability limitations. All models produced similar air pollutant dispersion patterns when given similar emission sources and meteorological input. However, QUIC produced substantially larger concentrations near emission sources than the other models reviewed. This is most likely due to a combination of QUIC overpredicting concentrations and the other models underpredicting concentrations. Comparison of each model's unique features and capabilities indicates that QUIC is the most relevant for short-term exposure applications where the exposure map for time steps less than 1 hour is desired, while AERMOD is more appropriate for estimating long-term exposures where the exposure map for time steps greater than 1 hour up to several years is desired. HYSPLIT is appropriate for a preliminary assessment of a current air quality situation (e.g., smoke from a forest fire). Uses of ArcGIS for the creation of surface geometry and for analysis of observed air quality were also discussed. Based on the information reviewed in this report, air quality dispersion modeling has been shown to be a useful tool to estimate past exposures and predict future exposures to support Air Force infrastructure decisions, epidemiological investigations, and the Air Force Total Exposure Health Initiative.					
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1.0 EXECUTIVE SUMMARY

Air quality dispersion models employ mathematical formulas to characterize the dispersion of pollutants based on emission sources and meteorological conditions. They are useful tools for both estimating past exposures and predicting future exposures based on the positioning of emission sources. Estimating past exposures is important because it can be used to support epidemiological studies designed to determine associations between exposures and health outcomes. One specific example is characterizing the effect of burn pits at deployed locations on the health of exposed populations. Predicting future exposures is important for making decisions regarding the positioning of emission sources and their effect on exposures. Once specific example is supporting decisions on how to position fleets of advanced aircraft on the flight line at an Air Force base to mitigate the potential for exhaust re-entrainment and exposure to maintainers, aircrew, and other personnel.

There are several air quality dispersion models available, each with capabilities that are specialized for particular air quality situations. The following four air quality dispersion models were reviewed:

1. AERMOD: The AMS-EPA Regulatory Model – a collaborative effort by the American Meteorological Society and the Environmental Protection Agency, adopted as the Environmental Protection Agency’s preferred regulatory model in 2005.
2. CALPUFF: The California PUFF model – developed in 1990 by Sigma Research Corporation for the California Air Resources Board.
3. HYSPLIT: The Hybrid Single Particle Lagrangian Integrated Trajectory model – a collaborative effort developed by the National Oceanic and Atmospheric Administration and Australia’s Bureau of Meteorology.
4. QUIC: The Quick Urban and Industrial Complex model – developed in the early 2000s in a collaborative effort between Los Alamos National Laboratory and the University of Utah.

ArcGIS, a geographic information system developed by the Environmental Systems Research Institute, was also reviewed as a tool useful for analysis of observed air quality conditions using inverse distance weighted techniques, geographic data analysis, geostatistical calculations, image analysis, building and terrain dataset development, and general cartography.

The flight line at Luke Air Force Base was used as a model site for generating comparative air quality dispersion models to demonstrate the usefulness for estimating the potential for jet exhaust re-entrainment and exposure to maintainers, aircrew, and other personnel on the flight line. Site profiles were constructed using each of the air quality dispersion models (with the exception of CALPUFF, for reasons discussed in section 2.1.2). The F-35 produces a greater risk than the F-16 for heat and chemical exposure to individuals on the flight line, as it produces about 1.6 times more thrust. However, the F-16 was chosen for these proof-of-concept model tests based on the availability of data for fuel consumption, which is a required model input.

Comparison of each model’s unique features and capabilities indicates that QUIC is the most relevant for the flight line exposure application, while AERMOD is more appropriate for estimating long-term exposures to support epidemiological studies linking exposure profiles to health outcomes. HYSPLIT is appropriate for preliminary assessment of a current air quality

situation (e.g., smoke from a forest fire) or for research on rural locations. However, it should not be used for in-depth research on urban areas due to its reliance on meteorological data files to supply surface terrain/geometry data.

2.0 SOFTWARE DESCRIPTIONS AND DATA SOURCES

2.1 Air Quality Dispersion Models

2.1.1 AERMOD. AERMOD (AMS-EPA Regulatory Model), adopted as the Environmental Protecting Agency's (EPA) preferred regulatory model in 2005 [1], is a steady-state dispersion model designed for calculating concentrations of EPA criteria pollutants over regulatory time periods within a model domain up to 50 km × 50 km [2]. It is a Lagrangian model, meaning that it treats the motions of the atmosphere as wavefunctions. The timestep is fixed at 1 hour. AERMOD produces output in both graphical and tabular formats; the tabular format is specialized for use in EPA reports. AERMOD output shows the time-average and/or peak concentration that occurred at a specific location during a given period of time. Criteria pollutants include carbon monoxide, nitrogen dioxide, particulate matter (PM) less than or equal to 10 µm in diameter (PM₁₀), PM less than or equal to 2.5 µm in diameter (PM_{2.5}), ozone, lead, and sulfur dioxide [3]. The available time-stepping intervals are based on the regulatory time periods indicated in the EPA National Ambient Air Quality Standards, which are regulations governing outdoor air quality and the conditions under which a municipality is in violation of the Clean Air Act [3]. The regulatory time periods include 1 hour, 2 hours, 3 hours, 4 hours, 6 hours, 8 hours, 12 hours, 24 hours, 1 week, 1 month, and 1 year. Longer simulation times (>1 year) are also possible to satisfy long-term regulatory situations such as EPA New Source Permitting, which is a legal regulatory process all potential major sources of criteria pollutants must go through prior to breaking ground on construction.

AERMOD's predictions have been validated by the EPA [4]. To validate AERMOD output, the EPA used quantile-quantile plots, in which observations and model output are ranked by percentile and plotted against each other to compare measured pollutant concentrations with modeled pollutant concentrations at the point of measurement. The findings of this study were that AERMOD output can be trusted to fall within a factor of 2 [between one-half and double] of the concentration observed in the field. A model prediction within a factor of 2 of observed measurements is the commonly accepted standard for acceptable performance for a regulatory air quality model [5].

The AERMOD software package purchased for this system was BREEZE AERMOD by Trinity Consultants (Dallas, TX). It includes the AERMAP terrain/land-use-land-cover processor, the AERMET meteorological data processor, and the AERMOD pollutant dispersion model in a single geographic information system (GIS) style graphical user interface (GUI) through which emission sources and buildings can be drawn in the model domain. Emission sources can be modeled as point sources, areas, or volumes. Measurement locations can be modeled as unique receptors, i.e., log-modeled pollutant concentrations at one point only, or gridded receptors, i.e., log concentrations for multiple points simultaneously. Emissions sources, receptors, and building properties can also be defined through software wizards and *in situ* spreadsheets. Detailed information on the operation of the BREEZE AERMOD software package can be found in the BREEZE AERMOD Practical Air Dispersion Modeling Workshop

textbook/workbook [6]. A detailed description of AERMOD's development and mathematical formulas can be found in EPA technical report EPA-454/R-03-004 [7].

2.1.2 CALPUFF. CALPUFF (California PUFF) is a non-steady-state puff dispersion model designed for the simulation of pollutant dispersion over areas from tens to hundreds of kilometers [8]. It is typically used for regulatory modeling, as a companion to AERMOD. Similar to AERMOD, it is a Lagrangian model. The timestep is manually variable with a maximum timestep of 1 hour [9]. CALPUFF is unique from AERMOD in that output can be written to time series and gridded data files, making it a true plume dispersion model. Further, CALPUFF's investigative scope is wider than AERMOD's, as CALPUFF includes a library containing chemical parameters for a wide variety of chemical species including all EPA criteria pollutants in addition to specific volatile organic compounds [10] and radioactive species [11]. CALPUFF also has the ability to model chemical reactions that occur in the atmosphere through its atmospheric chemistry options [12]. It is also possible for the user to input custom pollutants using chemical parameters. A disadvantage of CALPUFF is that it requires meteorological input data to be in a unique format [13], making high-quality data extremely difficult to obtain unless purchased from an air quality modeling consultancy.

The CALPUFF software package purchased for this system was CALPUFF-View by Lakes Environmental Software (Waterloo, Ontario, Canada). It includes the CALMET meteorological processor, the CALPUFF pollutant dispersion model, and the CALPOST data post-processor. Like BREEZE AERMOD, this software package is operated from a GIS-style GUI, through which emission sources, receptors (unique or gridded), and buildings can be drawn in the model domain. Terrain, emission source, receptor, and building properties can also be defined in a like manner to BREEZE AERMOD *via* software wizards and *in situ* spreadsheets. Due to the poor quality of freely available data and the cost of commercially available data, no output will be available from CALPUFF until such a time as it is required. Detailed information on CALPUFF can be found in the model formulation and user's guide for the CALPUFF dispersion model [13].

2.1.3 HYSPLIT. HYSPLIT (Hybrid Single Particle Lagrangian Integrated Trajectory) is a hybrid non-steady-state puff/particle plume dispersion model, meaning it simultaneously combines both puff and particle approaches to modeling an emission plume. Both approaches utilize a Lagrangian treatment of the atmosphere. The timestep automatically varies between 1 minute and 1 hour during a simulation [14]. This model was originally designed to serve as a rapidly deployable online regional pollutant dispersion model to provide short-term air quality simulations of between 1 hour and a few days in length for emergency services and to be capable of back-calculating trajectories to determine whether observed air contaminants have a local or remote source [15]. The ideal geographic domain is on the order of 10 km – 50 km [8], although it has been used to model pollutant dispersion across the entire planet. One useful feature of HYSPLIT is that model output can not only be extracted to data files but can also be written to ArcGIS (section 2.2.1) or Google Earth formats to allow for further graphical analysis. Neither BREEZE AERMOD nor CALPUFF-View is capable of writing output to ArcGIS, although CALPUFF-View can output to Google Earth. In keeping with this model's flexibility, all pollutants simulated using HYSPLIT must be user defined using chemical parameters. Chemical species can be either gaseous or particulate [16].

HYSPLIT is a freely available model produced by the National Oceanic and Atmospheric Administration (NOAA). It operates from a text-based GUI and automatically downloads both forecast and observed meteorological data with their associated terrain/surface data from the NOAA Atmospheric Resources Laboratory archive. It is able to simulate both emission plume trajectories and pollutant concentrations for multiple sources and chemical species (up to seven of each when defined in GUI, unlimited when defined from an external file) simultaneously. Mathematical details of the HYSPLIT model can be found in NOAA Technical Memorandum ERL ARL-230 [17].

2.1.4 QUIC. QUIC (Quick Urban and Industrial Complex) combines a simplified computational fluid dynamics engine (QUIC-URB) with a Lagrangian random-walk particle dispersion model (QUIC-PLUME) and a GIS interface. With a geographic grid on the order of 1 meter and a manually variable timestep where $0 \text{ seconds} < \text{timestep} < 10 \text{ seconds}$, QUIC is useful for the simulation of geographically small domains ($< 10 \text{ km}$) located in geometrically complex environments such as urban centers and industrial facilities. QUIC outputs gridded time series of particle locations and concentrations, thus making it a true plume model. Like HYSPLIT, all pollutants are user defined.

QUIC is a unique model produced by the Los Alamos National Laboratory in conjunction with the University of Utah as a fast-response chemical, biological, radiological, and nuclear attack simulator [18]. As such, it is a highly flexible model with a user-friendly interface. Unique features of QUIC include the ability to easily input (1) observed on-site meteorological data, (2) GIS-shapefile-formatted building data, and (3) moving point sources that can be set up to follow specific paths during the simulated time period [19]. Details of the mathematical processes used in QUIC can be found in the QUIC PLUME Theory Guide [20].

The models discussed above were summarized for comparison in Table 1.

2.2 Geographic Analysis

ArcGIS, which is produced by the Environmental Systems Research Institute, is the premier geospatial analysis tool currently available. It is useful for creating maps, visualizing geospatial data, analyzing geographic data statistically and spatially, analysis of imagery, as well as importation and extraction of air quality model input data. In relation to pollutant dispersion modeling, the primary application of ArcGIS is to generate the geometry containing structures and terrain that is imported into air dispersion models as surface data.

2.3 Data Sources

Terrain and weather data are two of the key required inputs to generate air dispersion models. Data sources not linked to directly by the models' user interfaces were cataloged for use, with the exception of CALPUFF-specific meteorological data (Table 2). Emissions source data are not included in Table 2, as they are typically gathered from literature or observations, as they were for this case.

Table 1. Comparison of Air Dispersion Models

Model	AERMOD	CALPUFF	HYSPLIT	QUIC
Typical Use	Regulatory	Regulatory	Emergency Response	Chemical, Biological, Radiological, & Nuclear Attack
Model Domain	<50 km	<1000 km	10 – 50 km	<10 km
Pollutants	EPA Criteria Pollutants	EPA Criteria Pollutants, Volatile Organic Compounds, Radioactive Species, User Defined	User-defined	User-defined
GIS-Style GUI	Yes	Yes	No	Yes
Developer	American Meteorological Society/EPA	Sigma Research Corp.	NOAA/Australia Bureau of Meteorology	Los Alamos National Laboratory/University of Utah
Steady-State	Yes	No	No	No
Custom Buildings/Terrain	Yes	Yes	No	Yes
Timestep (dt)	Fixed: dt = 1 h	Manually Variable ^a : dt < 1 h	Automatically Variable ^a : 1 min < dt < 1 h	Manually Variable ^a : 0 s < dt < 10 s
Puff/Particle ^b	Puff	Puff	Both	Particle

^aManually Variable: Prior to beginning the simulation, the user specifies the dt to be used for that model run; Automatically Variable: The model decides what dt to use in the differential equations governing the thermodynamic/fluid dynamic processes simulated. This decision is made while the model is running, without input from the user

^bPuff vs. Particle: Air parcels with a Gaussian (even) volumetric distribution of pollutant that are modeled as expanding with distance are called puffs. If an air parcel is not treated as expanding with distance, it is called a particle. HYSPLIT is considered a hybrid between the two approaches because when its parcels reach the size of the meteorological grid spacing, they split into multiple parcels, each containing a portion of the original parcel's pollutant contents.

Table 2. Terrain and Weather Data Sources

Type of Source	Source
States Providing AERMOD-Ready Meteorology Data	AL, AK, AR, CA, CT, FL, GA, IA, IN, KY, ME, MI, MN, MS, NC, ND, NH, NM, OH, SC, TX, UT, VA, WI
Unprocessed Meteorological Data for All States	EPA Support Center for Regulatory Atmospheric Modeling [21], Iowa State University Meteorological Terminal Aviation Routine (METAR) Archive [22]
Terrain Data	Multi-Resolution Land Characteristics Consortium [23]
Satellite Imagery and Aerial Photography	ArcGIS Online

In regard to meteorological data, it is important to note that virtually all public meteorological data are recorded at hourly intervals. There are a few datasets of higher frequency, but they are virtually always associated with a small local network of weather stations. Therefore, these data are of an extremely limited geographic scope. The weather stations associated with these networks are rarely located in urban areas and thus cannot provide data relevant to the circulation of the atmosphere in developed areas [24]. Furthermore, for the

purposes of microscale atmospheric modeling, the spacing of the weather stations in these networks is far too wide. For instance, the Oklahoma Mesonet – the most well known of these networks – has an average of one weather station for every 1508 km² [25]. For air pollution and pollutant dispersion studies, sensor networks with an area between 100 meters and 10 km are needed [25]. There are only five such networks providing data to the public in the United States: the Oklahoma City Micronet – Oklahoma City, OK; Quantum Weather – St. Louis, MO; CitySense – Cambridge, MA; Sensor Network Over Princeton – Princeton, NJ; and Woodlawn High School Network – Baltimore, MD [25]. This makes it necessary to observe weather conditions directly when creating a high-fidelity pollutant dispersion model. To best observe relevant weather conditions for input into such a model, it would be best to employ a mobile weather observation network similar in concept to that employed by the University of Oklahoma during the VORTEX Experiment [26], in which weather stations were mounted to automobiles that were then driven to locations of interest to observe small-scale meteorological phenomena including thunderstorms.

3.0 EXAMPLE DATA OUTPUT

Proof-of-concept domains were prepared in HYSPLIT, QUIC, and AERMOD for Luke Air Force Base (AFB) using 1200-1300 Arizona Standard Time on 10 June 2012 as the test period. This model duration was chosen due to the fact 1 hour is the shortest possible model timestep for AERMOD. The HYSPLIT model can be run for a duration anywhere from a few minutes to several days, and QUIC can only feasibly be run for a maximum model duration of a few hours at its highest quality.

The F-35 produces a greater risk than the F-16 for heat and chemical exposure to individuals on the flight line, as it produces about 1.6 times more thrust [27,28]. However, the F-16 was chosen for these proof-of-concept model tests based on the availability of data for fuel consumption, which is a required model input.

For the first set of examples, similar conditions were simulated using each of the models. Meteorological data for the models were assigned as follows: AERMOD – single observation for 1200 taken from AERMOD input data supplied by the Arizona Department of Environmental Quality (recorded at Sky Harbor International Airport); QUIC – single wind observation, 3-knot winds at 190° (1200 METAR); HYSPLIT – single hourly observation for 1200 taken from the North American Model 12-km weather forecast data – weather forecast model predictions for multiple grid points are included.

For the second set of examples, each model was run using model inputs more closely matched to the capabilities of each specific model. For the second QUIC and HYSPLIT model runs, Luke AFB METAR observations for 1155 (1200 observation) and 1255 (1300 observation) were used with the addition of observations interpolated every 10 minutes from 1210 – 1250. The 1200 METAR recorded 3-knot winds at 190° and the 1300 METAR recorded 8-knot winds at 130°. This interpolation was necessary because even though these models can be run for sub-1-hour timesteps, the corresponding meteorological data are rarely available in online databases.

All simulations were for PM_{2.5} with two independent point sources representing two F-16 jets operating at a fuel consumption rate comparable to that of cruising speed. One source was located at 33.532° N, -112.363° W, and the other was located at 33.538° N, -112.366° W. Each produced PM_{2.5} at a rate of 0.004 g/s for the entire duration of the model run. This production rate was calculated from information indicating aircraft turbine engines create approximately

0.011 g of particulates per kilogram fuel at idle [29] and from F-16 fuel consumption information gathered from primary sources [30] indicating a typical cruising fuel consumption of approximately 0.35 kg/s. For HYSPLIT, it was necessary to enter pollutant density as input data. A value of 1.5 g/cm^3 was obtained from Molenaar [31]. All model output is in g/m^3 .

3.1 AERMOD

A small and simple proof-of-concept model domain was created for Luke AFB in BREEZE AERMOD. Due to the large number of buildings and inefficient, AERMOD-specific, building creation process, only major buildings in the immediate vicinity of the sources were drawn. Terrain was derived from multi-resolution land characteristics data using ArcGIS and the AERMAP utility included with the BREEZE AERMOD package. The completed model domain can be visualized in the BREEZE AERMOD interface (Figure 1). Terrain is shown in green. Buildings are blue, and point sources are in cyan. The receptor grid is shown as a black grid overlaid on base imagery.

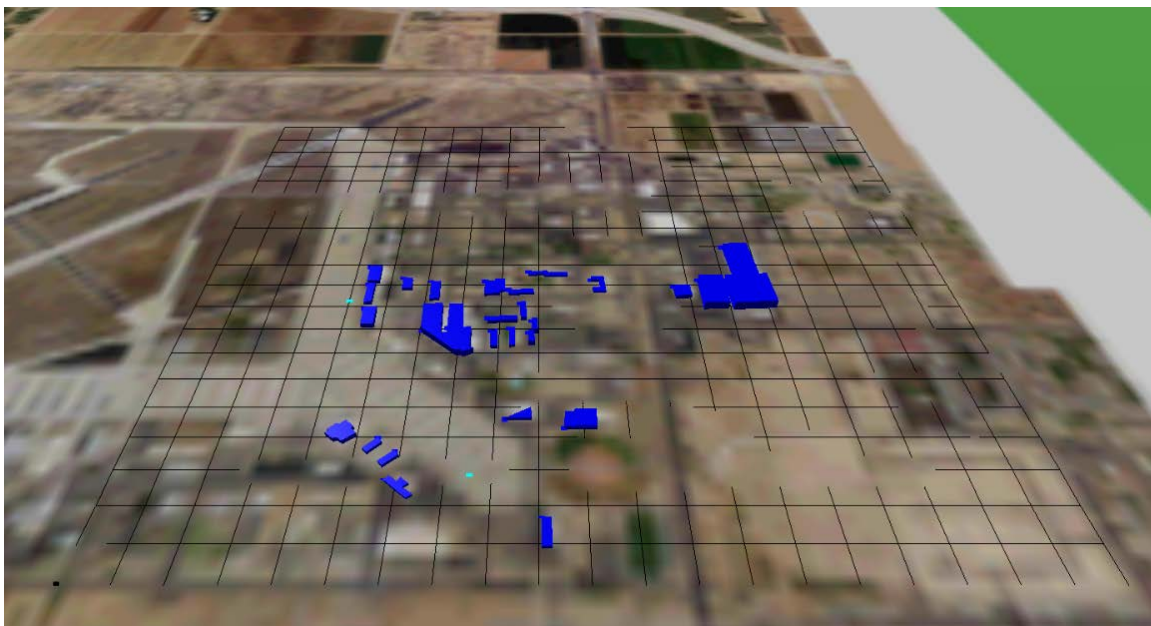


Figure 1. AERMOD domain.

AERMOD results show the hourly average concentration at each point on the receptor grid for the hour from 1200 to 1300 on 10 June 2012 (Figures 2 and 3). Results show this simulation resulting in very low concentrations – contours are for values between 5.08×10^{-5} and $0.407 \mu\text{g/m}^3$ (Figure 3). The concentrations at points A and B in Figure 3 are both on the order of $0.10 \mu\text{g/m}^3$. A maximum of $0.937 \mu\text{g/m}^3$, as denoted by the white x, was observed just to the northeast of the northern point source, just off the ramp and within the most built-up portion of the model domain (Figure 3). Pollutant dispersion follows from southwest to northeast, roughly in accordance with the 1200 METAR observation. It is of note that maxima are not located at the sources, but near buildings. A potential reason for this is the weak winds downwind of buildings allow pollutants to accumulate with time. These images were generated with the BREEZE 3D Analyst software, which came bundled with AERMOD as a separate program. Using 3D Analyst, it is possible to output AERMOD results to ArcGIS for further analysis.

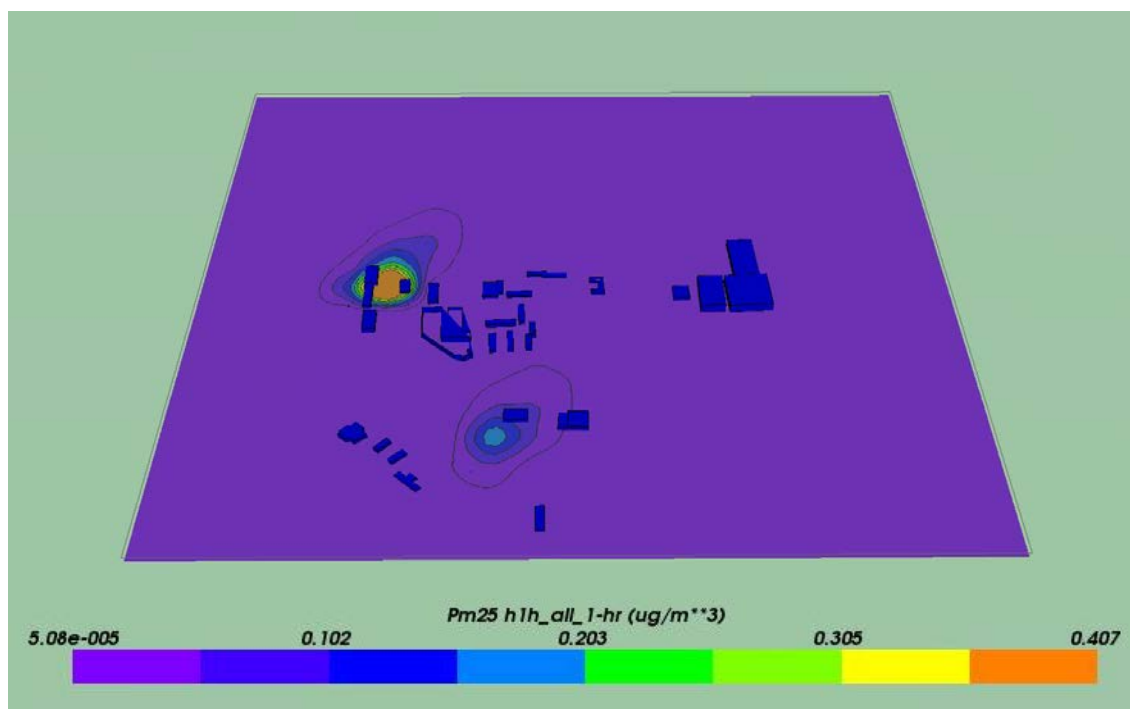


Figure 2. AERMOD hourly average: 1200-1300, 10 June 2012 (3D visualized).

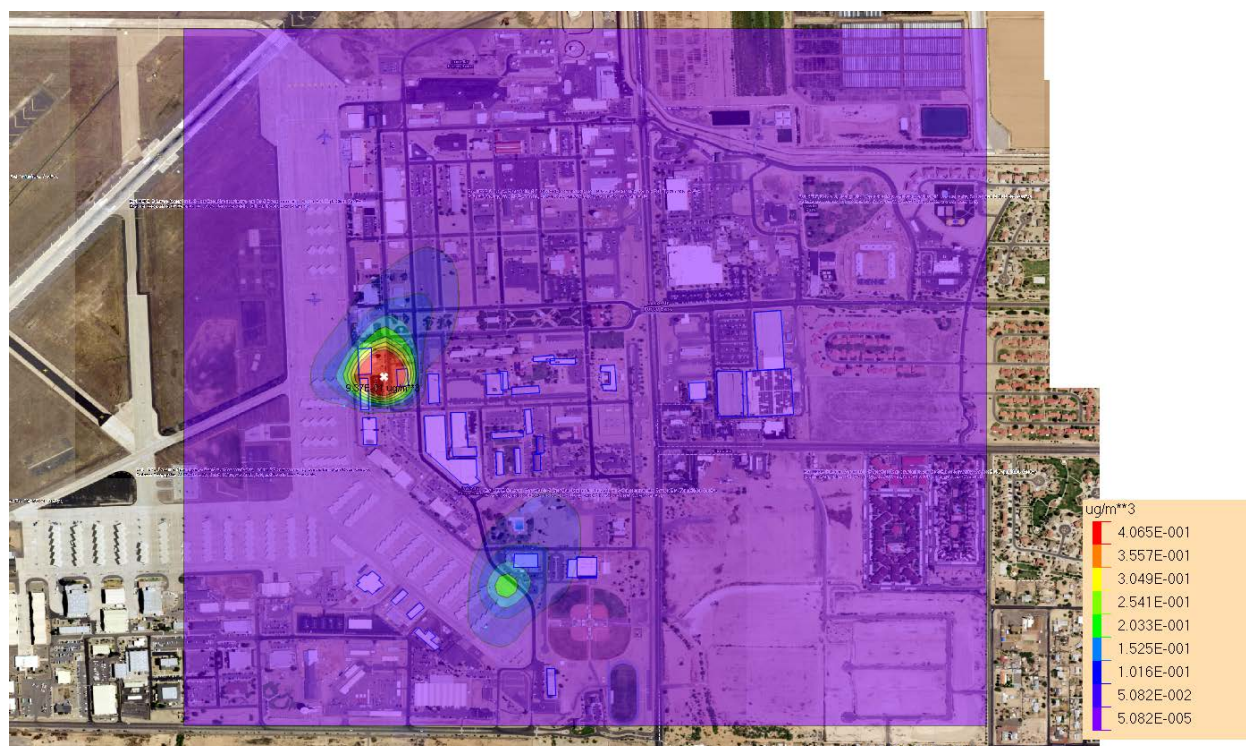


Figure 3. AERMOD hourly average: 1200-1300, 10 June 2012 (2D visualized).

As AERMOD is designed for longer simulations, a situation requiring a longer simulation time provides a better example of AERMOD's capabilities. To demonstrate the longer model duration capabilities of AERMOD, a full 24-hour run was completed, where the emission sources were present for the duration of the 24-hour period. The full 24-hour run shows that the peak hourly average PM_{2.5} concentration found during the 24-hour simulation was 3.07 µg/m³. The location of this maximum is to the southeast of the southern source, near the baseball diamonds, denoted by the white x in Figure 4. The locations of these maxima are provided in Universal Transverse Mercator coordinates under the Universal Transverse Mercator column of the report. Reports summarizing these data are generated automatically by the model and contain data for the entire model domain (Figure 5).

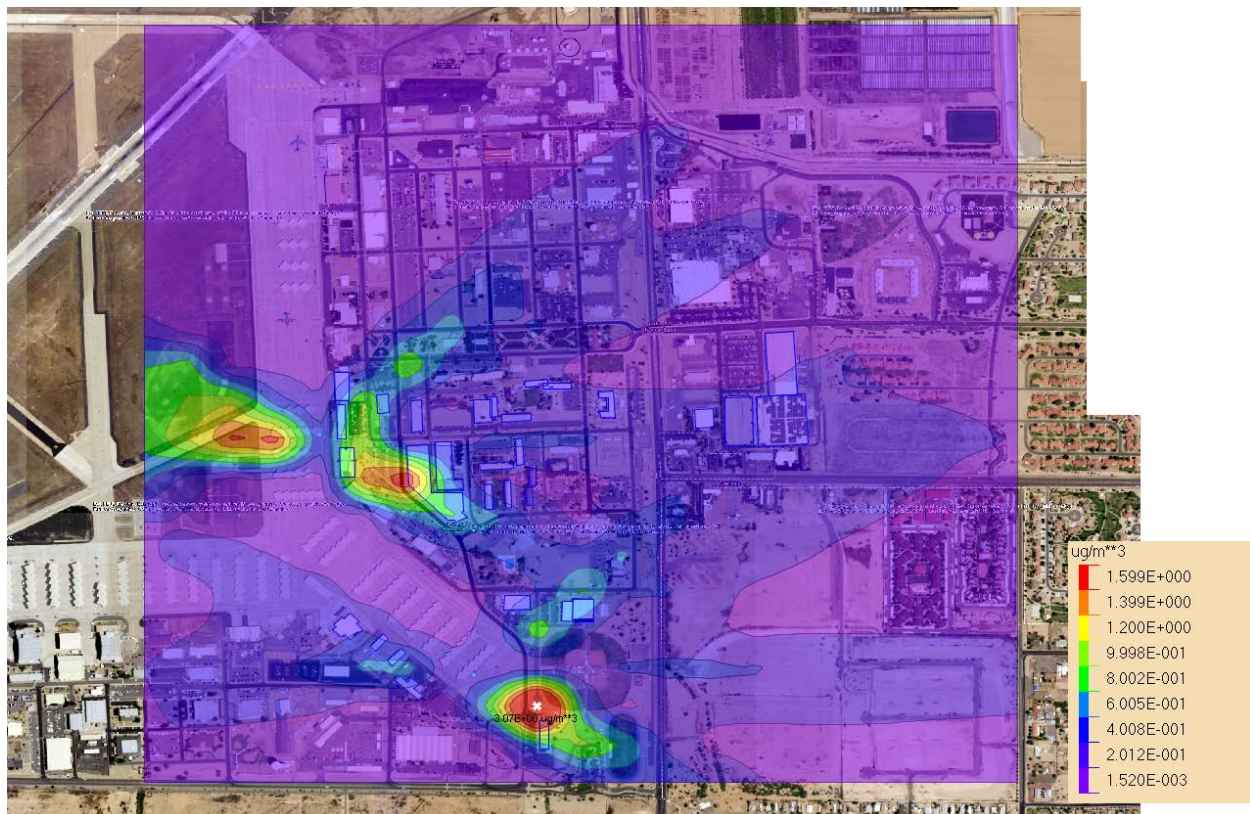


Figure 4. PM_{2.5} concentration, 24-hour maximum.

BREEZE AERMOD Model Results

Highest Results of Pollutant: PM25

Avg. Per.	Grp ID	High	Type	Val	Units	Date	UTM		Elev. (m)	Hill Ht. (m)	Flag Ht. (m)	Rec. Type	Grid ID
						YYMMDDHH	East (m)	North (m)					
1-HR	ALL	1ST	Avg. Conc.	3.07199	ug/m**3	12061021	373280.40	3711270.10	56.00	56.00	0.00	GC	AUQO3008
24-HR	ALL	1ST	Avg. Conc.	0.33020b	ug/m**3	12061024	372786.60	3711769.90	59.00	59.00	0.00	GC	AUQO3008
MONTH	ALL	1ST	Avg. Conc.	0.00000	ug/m**3	00000000	0.00	0.00	0.00	0.00	0.00		

Figure 5. AERMOD results summary report.

Based on the examples shown here, AERMOD works well for running longer term models lasting greater than 1 hour due to this being the smallest timestep available. AERMOD would excel in simulating constant or near-constant emissions from burn pits or smoldering aircraft crashes. In these cases, as the simulations would be long enough for pollutant exposure limits to come into effect, the display contours can be adjusted to show regulatory thresholds for the pollutant simulated. Health hazard exposures could then easily be calculated using ArcGIS based on personnel movements and a perimeter could be established at a distance where exposures are at a non-hazardous level.

3.2 HYSPLIT

The HYSPLIT domain was prepared to match the other models discussed here. One unique feature of HYSPLIT is that it derives its surface terrain and building data from the weather data files it uses as input. Therefore, there are no features in HYSPLIT for creation of terrain or buildings. For the first simulation, the observed weather conditions at the beginning of the hour were used as input for the entire full 1-hour simulation. The dispersion pattern was similar to that calculated by AERMOD, with similar concentrations produced and maxima in similar locations. Figure 6 shows plumes extending from either source to the northeast with concentrations between 1.0×10^{-9} and 1.0×10^{-6} g/m³ (1.0×10^{-3} to 1.0 µg/m³). The concentrations at points A and B in Figure 6 are both on the order of 0.10 µg/m³. It should be noted that despite the lack of ability to create buildings in the HYSPLIT interface, the model is “building-sensitive” at low model heights because it reads terrain data from meteorological input files. These files

contain a variety of terrain parameterizations, some at a fine enough scale that significant buildings can resolve as “terrain” features. Figure 6 shows this, as its data are at a height above ground level (AGL) of 2 meters and multiple buildings over 2 meters in height appear surrounded by the emission plumes.

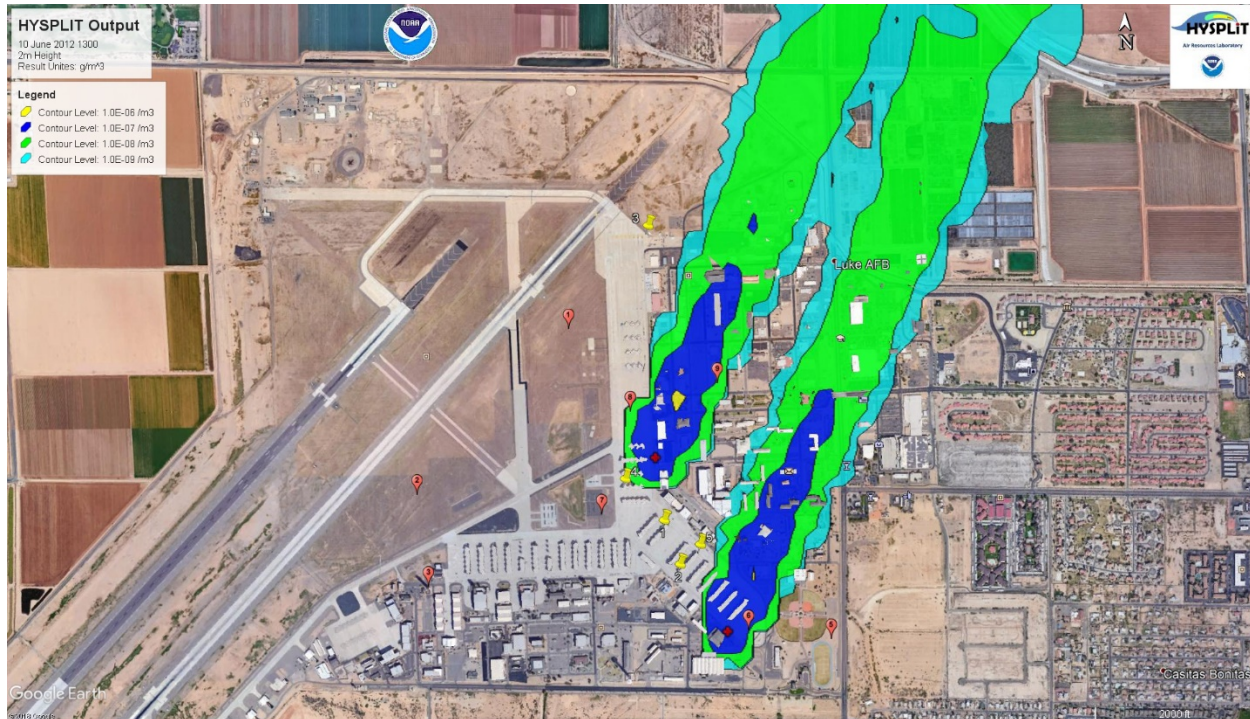


Figure 6. HYSPLIT results – 2-meter height AGL: 1200-1300, 10 June 2012.

A second HYSPLIT simulation was run with user-specified meteorological data reflecting the METAR data recorded at Luke AFB for the simulated times. Figure 7 shows that this simulation resulted in a fan-like pollutant dispersion pattern, produced as the winds rotated from 190° at 1200 to 130° at 1300. Maxima were on the order of 1 $\mu\text{g}/\text{m}^3$ and were located at the emission source. At point A, concentrations were on the order of 1 $\mu\text{g}/\text{m}^3$ and at point B concentrations were null. Here it is useful to include model output with values for each model grid cell, as shown in Figure 8, to later compare with QUIC output. Notice the large size of each grid cell.

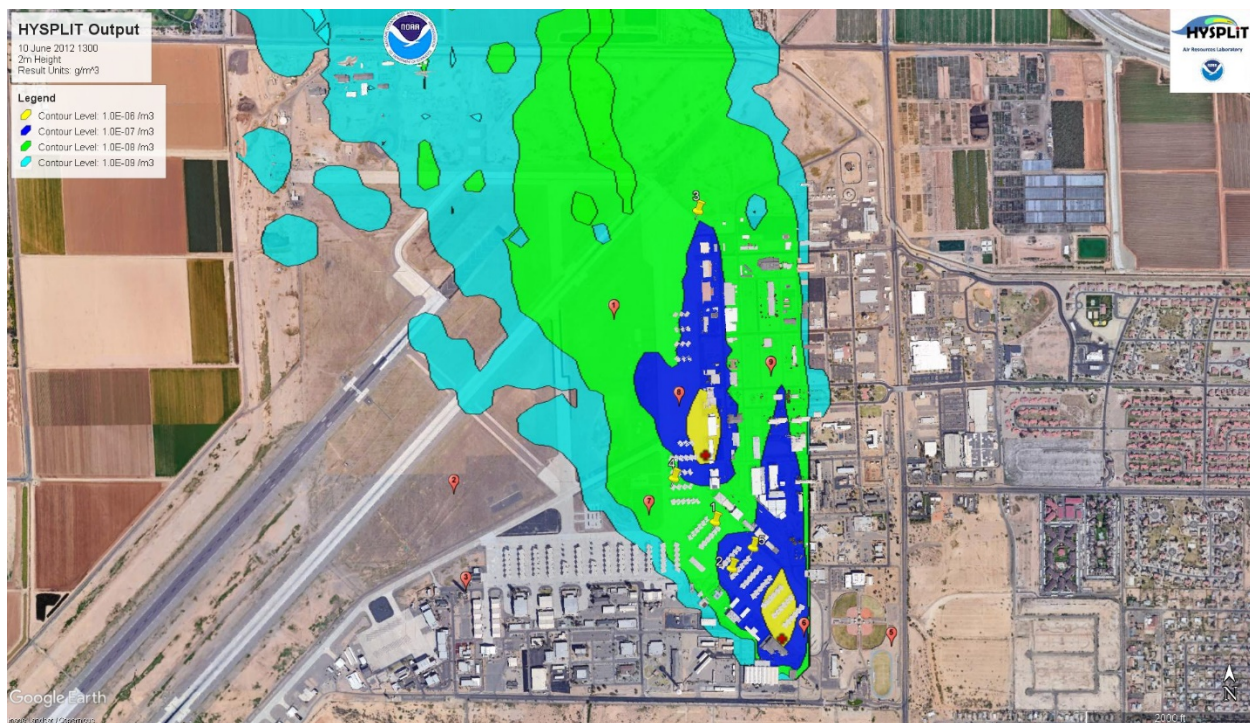


Figure 7. HYSPLIT results: 1200-1300, 10 June 2012, 1300, – 2-meter height AGL, with user-entered meteorological data.

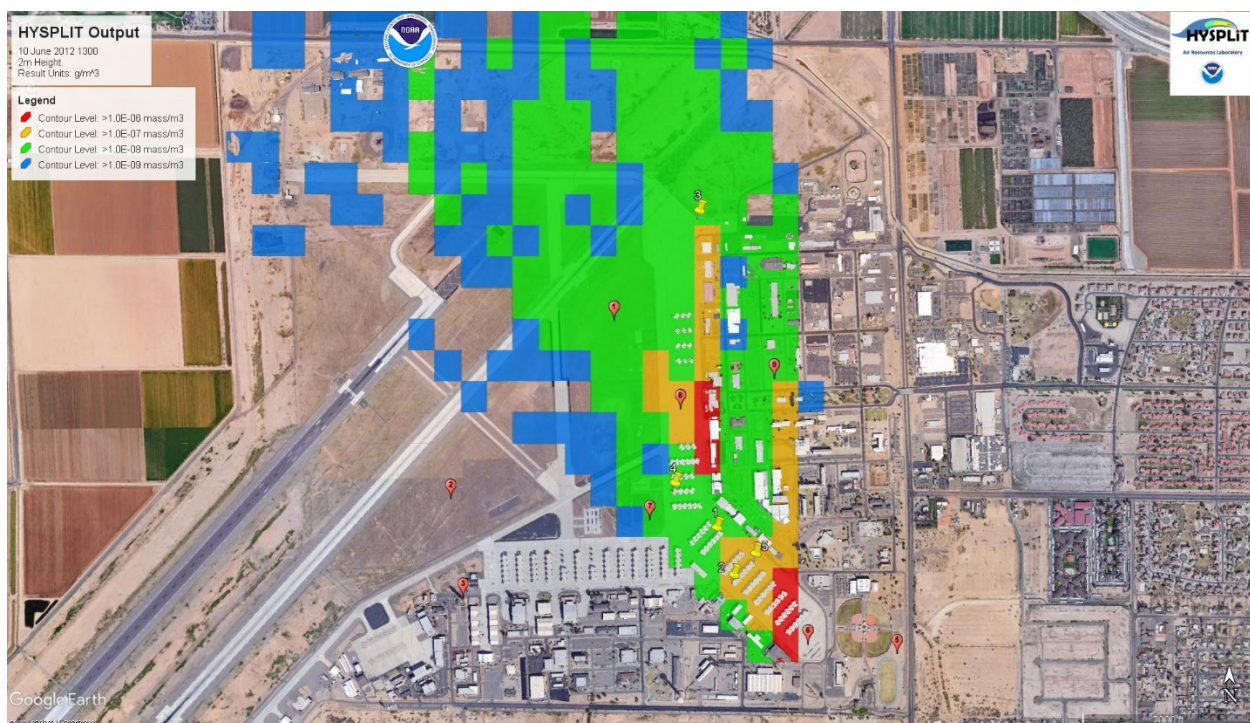


Figure 8. HYSPLIT model grid cell concentrations: 1200-1300, 10 June 2012, 2-meter height AGL.

3.3 QUIC

The QUIC domain was prepared by inputting a GIS shapefile containing building heights and locations, adding a surface height gradient reflecting the local terrain at Luke AFB. A model simulation was made with a single wind vector of 3 knots at 190°, reflecting the 1200 METAR. Figure 9 shows a portion of the wind velocity field calculated by QUIC for this simulation. It is apparent that the implementation of computational fluid dynamics methods and building height produce a distinct influence on local wind flow patterns.

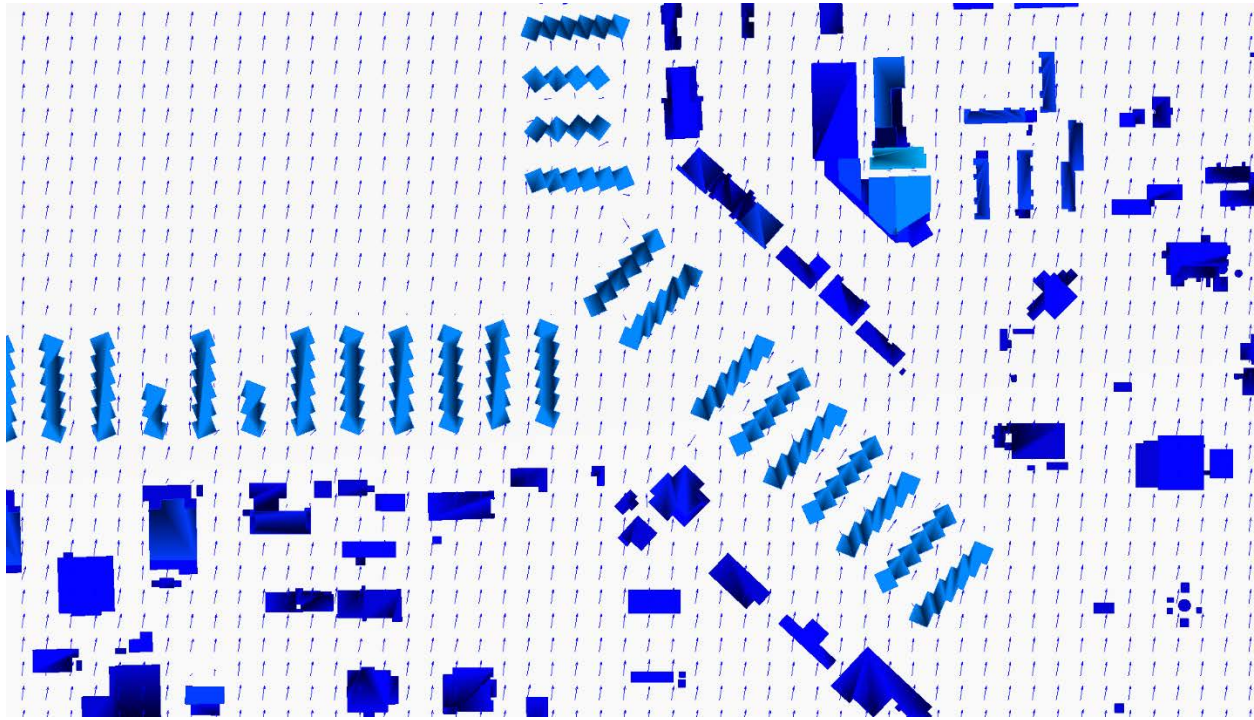


Figure 9. QUIC wind field for single wind vector simulation, 9-meter height.

Figure 10 shows that the pollutant dispersion pattern that was calculated when QUIC was run with a single wind vector representing the 1200 METAR observation was similar to that calculated by HYSPLIT, but that pollutant concentrations were higher. Concentrations at points A and B were on the order of $1 \mu\text{g}/\text{m}^3$. Data extracted to ArcGIS showed local maxima of $166 \mu\text{g}/\text{m}^3$ at the southern source and $149 \mu\text{g}/\text{m}^3$ at the northern source.

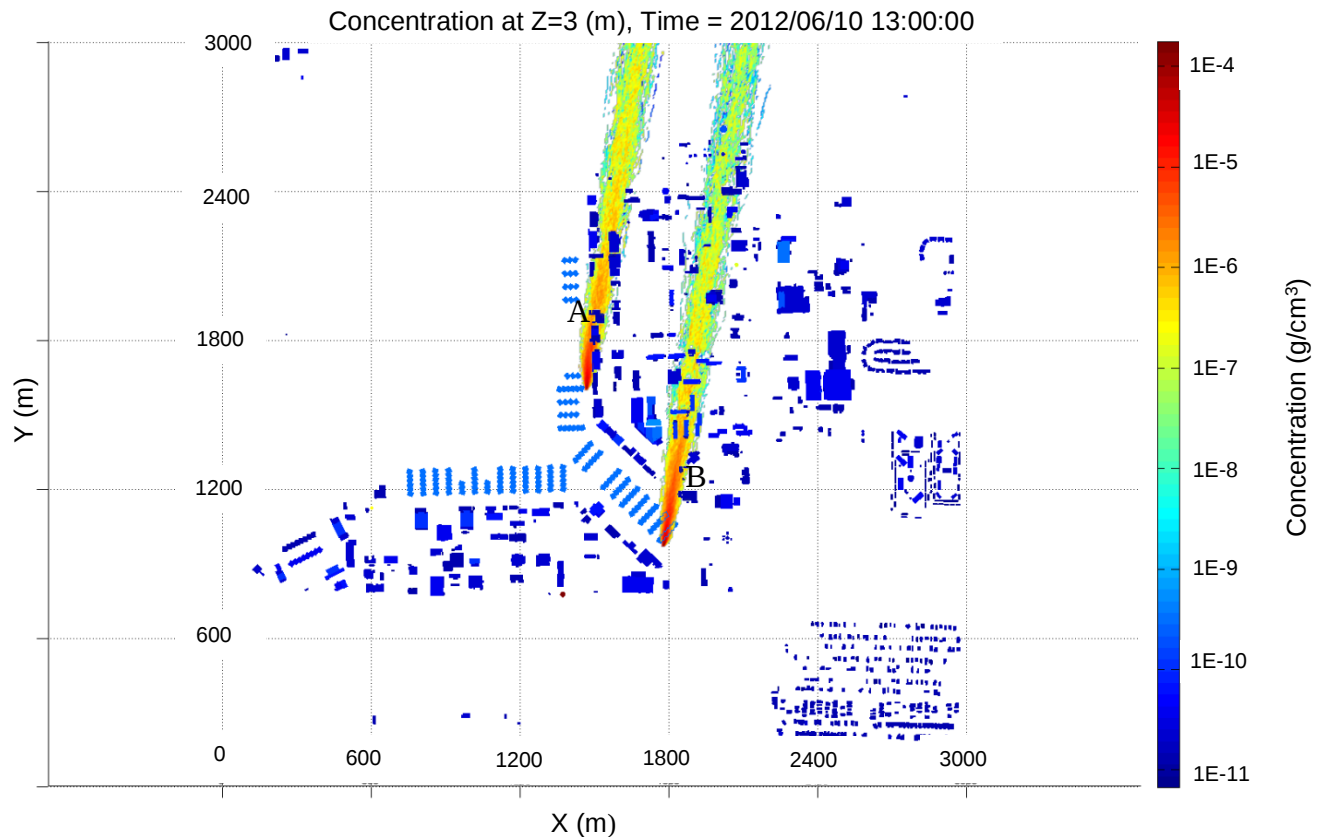


Figure 10. QUIC hourly average concentration – single wind vector; 1300, 10 June 2012.

Data extracted to ArcGIS showed peak concentrations of $85 \mu\text{g}/\text{m}^3$ for the southern source and $47 \mu\text{g}/\text{m}^3$ for the northern source. Both peaks were located at the emission source. QUIC is known to overpredict concentrations near the emission source and near ground level [32], while HYSPLIT [14] and AERMOD [4] are known to underpredict concentrations near the emission source. Additionally, when AERMOD performance was tested at different timescales, it was found that underprediction was inversely proportional to the timescale, where underprediction was greater for shorter model runs [33]. It was found that HYSPLIT is also known to underpredict concentrations during the summer months [34]. Given this information, it should not be surprising that QUIC produced higher concentration peaks than AERMOD and HYSPLIT. It should be noted that the issue of overprediction and underprediction appears to be confined to the area immediately surrounding the emission source. One possibility to be investigated further is that the finer model grid of QUIC may allow it to simulate concentrations near the emission source with greater fidelity.

A second QUIC simulation was run with user-specified meteorological data reflecting the METAR data recorded at Luke AFB for the simulated times. Figure 11 shows wind velocities generated by QUIC. It can be seen that the model calculates atmospheric motions on a very fine scale, allowing the influence of individual buildings to be seen even in a constant wind field. In the center of Figure 11, it can be seen that the buildings have affected the local wind flow to the extent that winds can become calm or even reversed from their primary direction depending on the location and the shape of the buildings present.

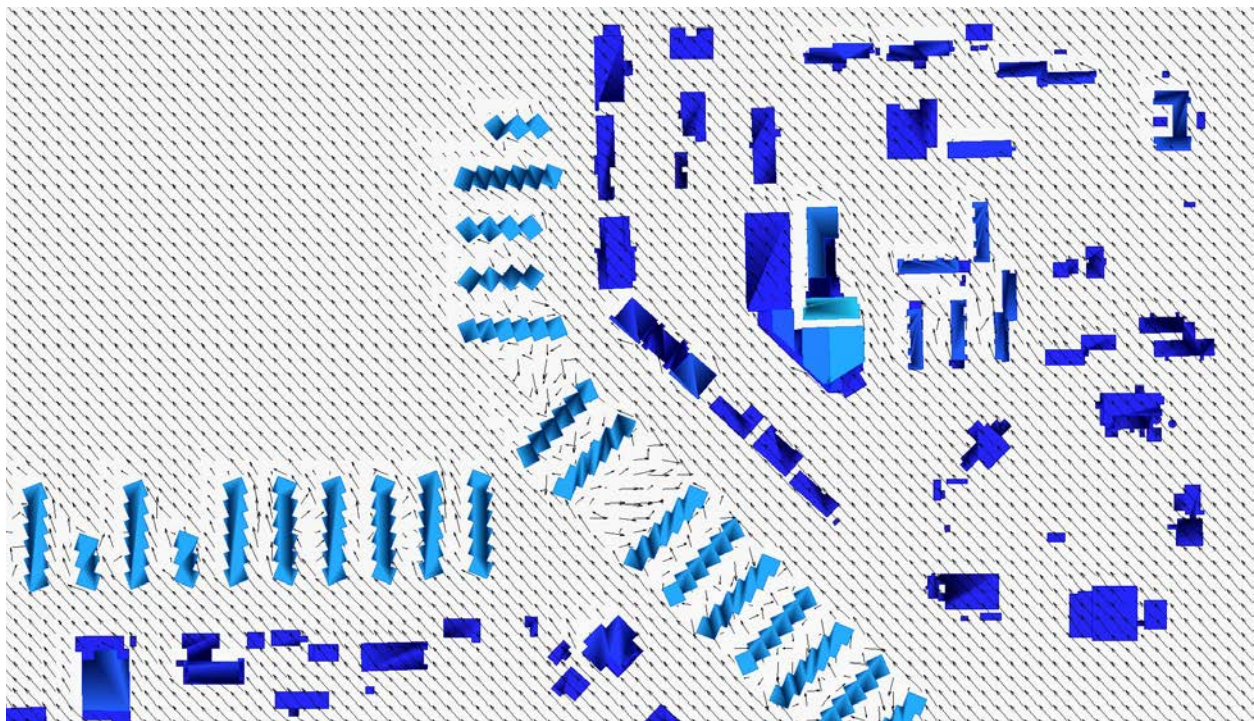


Figure 11. QUIC wind vector output; 1300, 10 June 2012, 9-meter AGL.

QUIC output is typically shown as particle locations at a particular point in time. This allows the movement of an emission plume to be shown with respect to time (Figure 12). Figure 12 shows emission plumes moving in a counterclockwise manner as the wind rotates from 190° at 1200 to 130° at 1300.

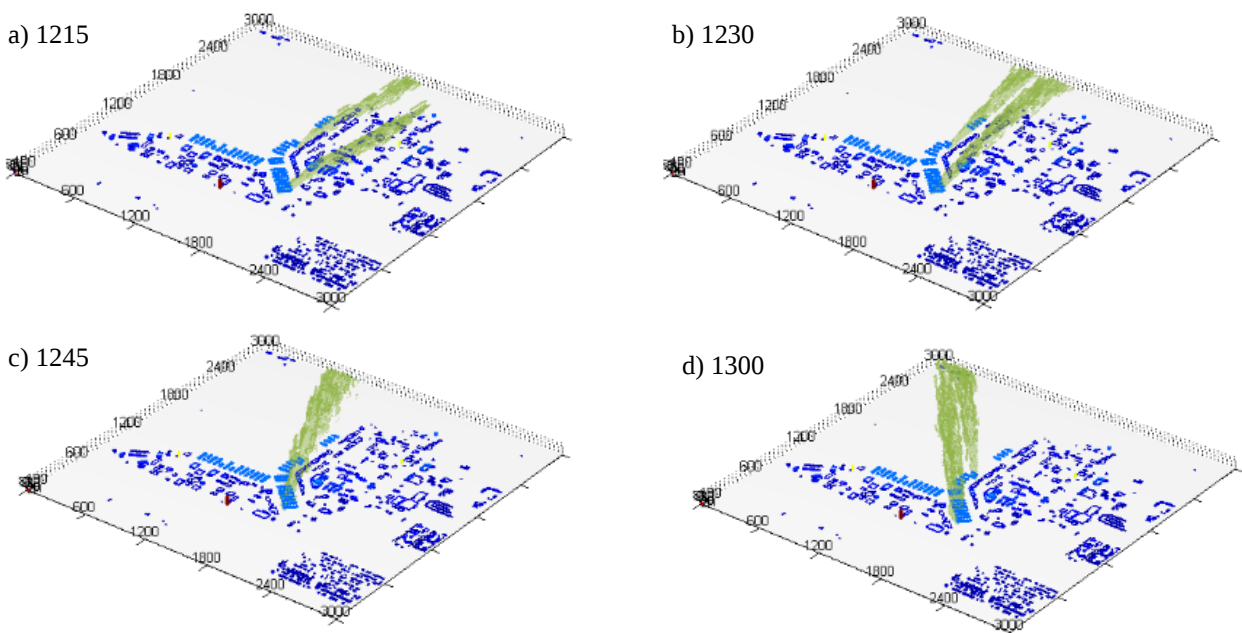


Figure 12. Emissions plumes at a) 1215, b) 1230, c) 1245, and d) 1300.

The hourly average can also be visualized (Figure 13). Note the similarity between the areas covered by the grid cells with the highest concentrations, as well as the similarity of concentration levels outside of these areas for the model generated using HYSPLIT using similar inputs (Figure 8).

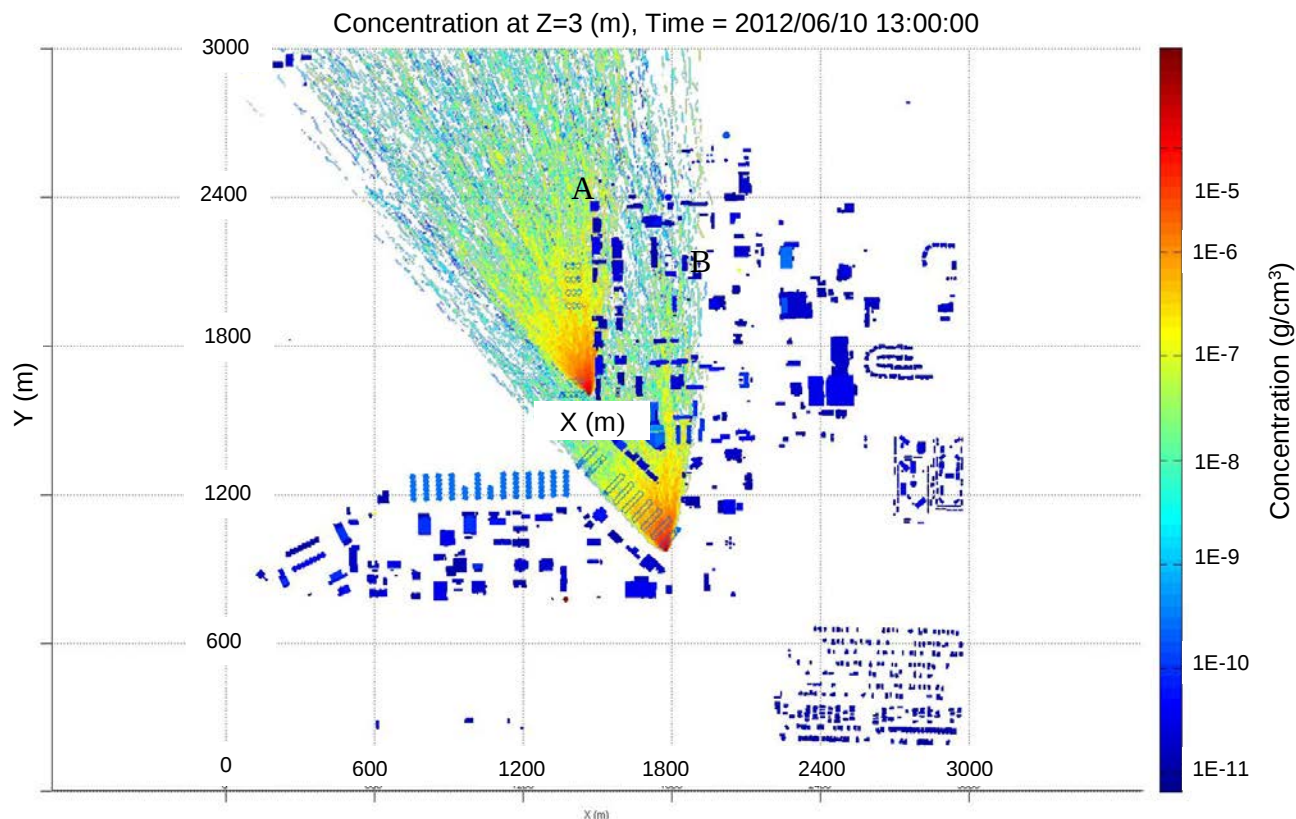


Figure 13. QUIC hourly average concentration; 1300, 10 June 2012.

3.4 ArcGIS

One application of ArcGIS is for the production of an inverse distance weighted dataset based on observed data representing ambient air quality. An example was generated using baseline air quality data at Luke AFB (Figure 14). The plot in Figure 14 shows the estimated distribution of nitric oxide (NO) based on actual data collected from four observation locations using a gas meter equipped with an electrochemical sensor for NO (MultiRAE, RAE Systems, San Jose, CA). The data were averaged over 1 hour.

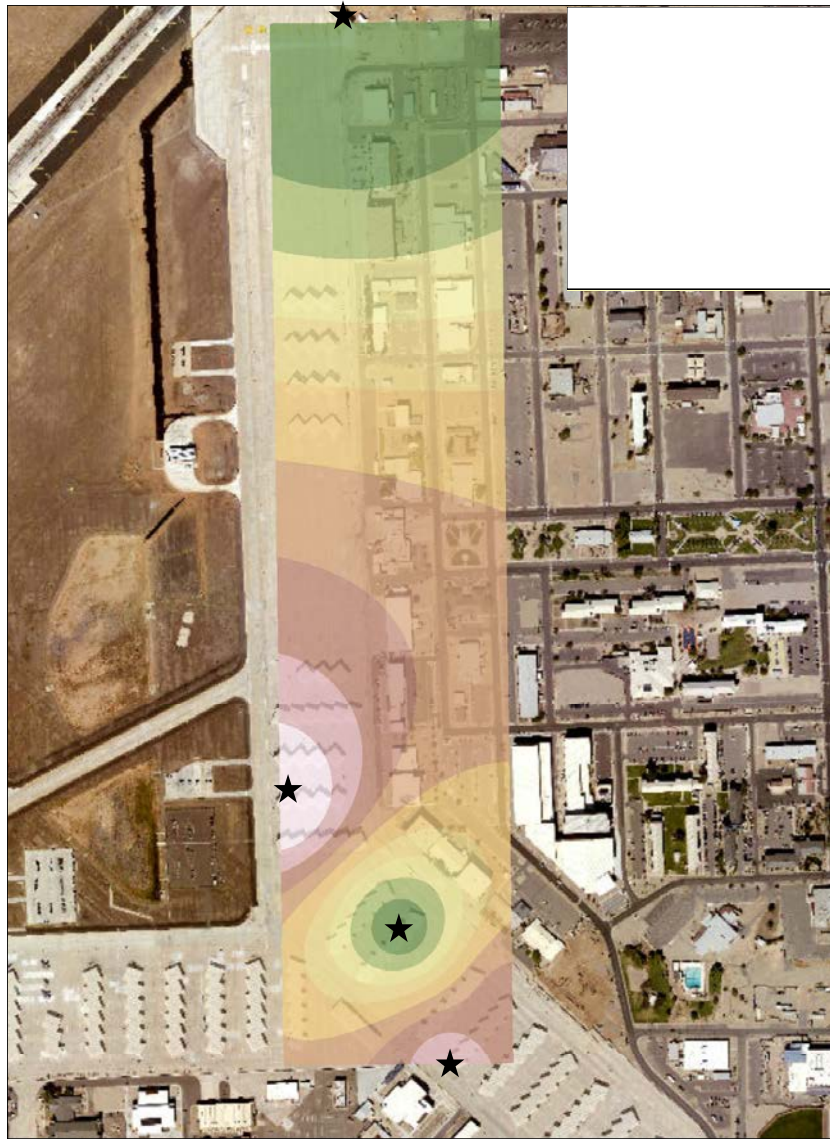


Figure 14. Example of inverse distance weighted air quality data for Luke AFB. The data collection points are labelled using black stars.

The data output shown in Figure 14 could be used to provide visualization for the distribution of air pollutants across a region and estimate exposures at locations between sensors. It could also be used to optimize the minimum number of sensors required to accurately record the distribution across an area. Future work will include the addition of measurement points to determine whether there is additional variation between the original locations. As a follow-on, model predictions could be made based on a smaller subset of data to determine whether a similar conclusion about pollutant dispersion could be made with fewer sensors and a smaller quantity of data.

4.0 CONCLUSIONS AND FUTURE RECOMMENDATIONS

It is apparent that the three models examined here are tailored to three unique purposes. AERMOD is well suited as a long-term exposure prediction model, with a minimum timestep of 1 hour, maximum run duration of up to 5 years, and time-averaged output. HYSPLIT provides a rough initial assessment of the local air quality situation for time periods from a few hours to a few days, and QUIC is a high-fidelity model for short time periods (<1 hour). Together, these three models provide a pollutant dispersion modeling suite suitable for most foreseeable situations.

Although not tested here, it is readily apparent from the technical specifications of CALPUFF that it is uniquely suited for detailed modeling of large domains and unusual pollutants [13]. Given its capabilities of modeling a large domain, an adjustable sub-1-hour timestep, and outputting data to time series and gridded data files, CALPUFF is also better suited to be used for research projects where the meteorological aspects of air quality are more heavily emphasized. Additionally, CALPUFF would be the model of choice when investigating chemical reactions occurring in the atmosphere due to its atmospheric chemistry parameterization options. However, these situations are relatively rare and the cost of CALPUFF-ready weather data is significant; therefore, it is recommended that CALPUFF be employed only when necessary to answer the unique research questions for which it is distinctly suited.

With regard to all models discussed here, it is recommended that full advantage be taken of these capabilities to pre-evaluate environmental air quality-related projects in Force Health Protection research and in civil engineering/infrastructure development to streamline both research and decision-making processes. One application of this suite of models is as a means of providing environmental intelligence for future changes in U.S. Air Force infrastructure due to changes in fleet composition (new aircraft require different infrastructure arrangements than old aircraft). Another application pertains to the ongoing investigation into unexplained physiological events and possible connections with flight line operations and exhaust re-entrainment. Of the models compiled here, QUIC would be the most suitable for such investigations due to its fine geographic and temporal scales. For correlating long-term exposures at deployed locations to future health outcomes, AERMOD would be the model of choice due to its very long timescale and simple output. In the event of a sudden or unexpected air quality event, as HYSPLIT can back-calculate past wind trajectories in addition to future wind trajectories and pollutant dispersion, it can easily be used to determine both the source and future transport of the pollutant in question. In combination, these models provide a powerful tool for estimating air pollution exposures of personnel expected to work both very close to and further away from pollution sources.

5.0 REFERENCES

1. U.S. Environmental Protection Agency. Revision to the Guideline on Air Quality Models: adoption of a preferred general purpose (flat and complex terrain) dispersion model and other revisions. Washington (DC): National Archives and Records Administration; 2005. 70 FR 68217, 40 CFR 51.

2. Brode RW. AERMOD technical forum. EPA R/S/L Modelers Workshop; 2006 May 16; San Diego, CA. [Accessed 1 Feb 2018]. Available from https://www.cleanairinfo.com/regionalstatelocalmodelingworkshop/archive/2006/documents/Brode_AERMOD_TechnicalForum.pdf.
3. National primary and secondary ambient air quality standards. 40 CFR 50. 2016. [Accessed 1 Feb 2018]. Available from <https://www.gpo.gov/fdsys/granule/CFR-2016-title40-vol2/CFR-2016-title40-vol2-part50>.
4. Paine RJ, Lee RF, Brode R, Wilson RB, Cimorelli AJ, et al. Model evaluation results for AERMOD. Washington (DC): U.S. Environmental Protection Agency; 1998. [Accessed 1 Feb 2018]. Available from <https://www3.epa.gov/scram001/7thconf/aermod/evalrep.pdf>.
5. Chang JC, Hanna SR. Air quality model performance evaluation. Meteorol Atmos Phys. 2004; 87(1-3):167-196.
6. Trinity Consultants, Inc. Practical Air Dispersion Modeling Workshop; 2016 Jun 1-3; Denver, CO.
7. Cimorelli AJ, Perry SG, Venkatram A, Weil JC, Paine RJ, et al. AERMOD: description of model formulation. Research Triangle Park (NC): U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Emissions Modeling and Analysis Division; 2004. Report No. EPA-454/R-03-004. [Accessed 1 Feb 2018]. Available from https://www3.epa.gov/scram001/7thconf/aermod/aermod_mfd.pdf.
8. Oppenheimer V. Prototyping the use of dispersion models to predict ground concentrations during burning of deployed military waste [Thesis]. Wright-Patterson AFB (OH): Air Force Institute of Technology; 2012. AFIT/GEM/ENV/12-M16. [Accessed 1 Feb 2018]. Available from <http://www.dtic.mil/docs/citations/ADA558447>.
9. Scire J. Development, maintenance and evaluation of CALPUFF. Presentation at the 9th Conference on Air Quality Modeling; 2008 Oct 9-10; Research Triangle Park, NC. [Accessed 1 Feb 2018]. Available from https://www3.epa.gov/scram001/9thmodconf/scire_calpuff.pdf.
10. Karamchandani P, Chen SY, Seigneur C. CALPUFF chemistry upgrade. San Ramon (CA): Atmospheric and Environmental Research, Inc.; 2008. Document CP277-07-01.
11. An HY, Kang YH, Song SK, Kim YK. Comparison of CALPUFF and HYSPLIT models for atmospheric dispersion simulations of radioactive materials. J Korean Soc Atmos Environ. 2015; 31(6):573-584.
12. TRC Environmental Corporation. CALPUFF chemistry updates: user's instructions for API chemistry options. Lowell (MA): TRC Environmental Corporation; 2010.
13. Scire JS, Strimaitis DG, Yamartino RJ. A user's guide for the CALPUFF dispersion model (version 5). Concord (MA): Earth Tech, Inc.; 2000.
14. National Oceanic and Atmospheric Administration, Air Resources Laboratory. HYSPLIT basic tutorial contents. [n.d.]. [Accessed 1 Feb 2018]. Available from <https://ready.arl.noaa.gov/documents/Tutorial/html/>.
15. Fleming ZL, Monks PS, Manning AJ. Review: Untangling the influence of air-mass history in interpreting observed atmospheric composition. Atmos Res. 2012; 104-105:1-39.
16. Draxler RR. HYSPLIT_4 user's guide. Silver Spring (MD): National Oceanic and Atmospheric Administration; 1999. NOAA Technical Memorandum ERL ARL-230.
17. Draxler RR, Hess GD. Description of the HYSPLIT_4 modeling system. Silver Spring (MD): National Oceanic and Atmospheric Administration, Air Resources Laboratory; 1997. NOAA Technical Memorandum ERL ARL-224.

18. Brown M. QUIC (quick urban and industrial complex) dispersion modeling system. Los Alamos (NM): Los Alamos National Laboratory; 2002. LA-UR-02-2559. [Accessed 1 Feb 2018]. Available from http://www.lanl.gov/projects/quic/open_files/QUIC_factsheet.pdf.
19. Nelson M, Brown M. The QUIC start guide (v 6.01). Los Alamos (NM): Los Alamos National Laboratory; 2013. LA-UR-13-27291. [Accessed 1 Feb 2018]. Available from http://www.lanl.gov/projects/quic/open_files/QUICv6.01_StartGuide.pdf.
20. Williams MD, Brown MJ, Singh B, Boswell D. QUIC-PLUME theory guide. Los Alamos (NM): Los Alamos National Laboratory; 2004. LA-UR-04-0561.
21. U.S. Environmental Protection Agency. Air modeling – observational meteorological data. 2016. [Accessed 1 Feb 2018]. Available from <https://www.epa.gov/scram/air-modeling-observational-meteorological-data>.
22. Iowa State University. Iowa environmental mesonet. METAR archive. [n.d.]. [Accessed 1 Feb 2018]. Available from <https://mesonet.agron.iastate.edu/sites/locate.php>.
23. Multi-Resolution Land Characteristics Consortium. National land cover database (NLCD). 2018. Washington (DC): U.S. Department of the Interior, 2018. [Accessed 20 Apr 2018]. Available from <http://www.mrlc.gov>.
24. Basara JB, Illston BG, Fiebrich CA, Browder PD, Morgan CR, et al. The Oklahoma City micronet. Meteorol Appl. 2011; 18(3):252-261.
25. Muller CL, Chapman L, Grimmond CS, Young DT, Cai X. Sensors and the city: a review of urban meteorological networks. Int J Climatol. 2013; 33(7):1585-1600.
26. Straka JM, Rasmussen EN, Fredrickson SE. A mobile mesonet for finescale meteorological observations. J Atmos Ocean Technol. 1996; 13(5):921-936.
27. U.S. Air Force. F-35A Lightning II. 2014. [Accessed 10 Apr 2018]. Available from <http://www.af.mil/About-Us/Fact-Sheets/Display/Article/478441/f-35a-lightning-ii/>.
28. U.S. Air Force. F-16 Fighting Falcon. 2015. [Accessed 10 Apr 2018]. Available from <http://www.af.mil/About-Us/Fact-Sheets/Display/Article/104505/f-16-fighting-falcon/>.
29. Agrawal H, Sawant AA, Jansen K, Miller JW, Cocker DR III. Characterization of chemical and particulate emissions from aircraft engines. Atmos Environ (1994). 2008; 42(18):4380-4392.
30. F-16.net. Average fuel consumption. 2004. [Accessed 1 Feb 2018]. Available from <http://www.f-16.net/forum/viewtopic.php?t=1102>.
31. Molenaar JV. Theoretical analysis of PM_{2.5} mass measurements by nephelometry. Proceedings of the Specialty Conference on PM2000: Particulate Matter and Health; 2000 Jan 24-28; Charleston, SC. Paper 110.
32. Williams MD, Brown MJ, Boswell D, Singh B, Pardyjak E. Testing of the QUIC-PLUME model with wind-tunnel measurements for a high-rise building. Fifth Symposium on the Urban Environment; 2004 Aug 23-26; Vancouver (BC). Boston (MA): American Meteorological Society; 2004:810-820.
33. Zou B, Zhan FB, Wilson JG, Zeng Y. Performance of AERMOD at different time scales. Simul Model Pract Theory. 2010; 18(5):612-623.
34. Stajner I. Operational dispersion predictions at NOAA and development of aerosol capabilities for the next generation global prediction system (NGGPS). 19th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling; 2015 Jun 9-11; Fairfax, VA.

LIST OF ABBREVIATIONS AND ACRONYMS

AERMOD	AMS-EPA Regulatory Model
AFB	Air Force base
AGL	above ground level
CALPUFF	California PUFF
dt	timestep
EPA	Environmental Protection Agency
GIS	geographic information system
GUI	graphical user interface
HYSPLIT	Hybrid Single Particle Lagrangian Integrated Trajectory
METAR	Meteorological Terminal Aviation Routine
NO	nitric oxide
NOAA	National Oceanic and Atmospheric Administration
PM	particulate matter
QUIC	Quick Urban and Industrial Complex