PNNL-27530

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May 2018

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U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Summary

Atmospheric dispersion models were described and evaluated by Flaherty et al. (2017)[1] in the context of capabilities and gaps for Hanford tank farms needs. Dispersion models for real-time response and worker safety and emergency response applications for the mid-field (20 to 1,000 m) and far-field (beyond 1,000 m) distance bins (as defined by Washington River Protection Solutions [WRPS], the tank farm operator) were not available for use by WRPS. Based on the use of the Air Pollutant Graphical Environmental Modeling System (APGEMS; Glantz et al. 2002)[2] software at the Hanford Emergency Operations Center, and the ranking of the model presented by Flaherty et al. (2017), WRPS management selected the APGEMS model to fill a gap in the atmospheric modeling toolbox for the Hanford tank farms for portions of both the mid-field and far-field distance bins.

The APGEMS software was customized for the requirements of the Hanford tank farms, and this version of the software is called APGEMS-TF. Both models employ a Gaussian puff dispersion formulation to describe the concentration distribution resulting from an emission point. It uses data from the Hanford Meteorological Network to develop a three-dimensional wind field. Additional data sources, including in-farm meteorological stations, may be incorporated to improve wind estimates near the tank farms. Puff models simulate the release as a series of puffs, which are tracked on a temporally and spatially varying meteorological grid. The dispersion of each puff is computed based on a Gaussian puff width that varies as a function of atmospheric stability. Concentrations on the grid are determined by summing the individual contributions from each puff. Note that, for all Gaussian dispersion models, including APGEMS-TF, output within 100 m of a source may have large errors, and should only be used qualitatively (Flaherty et al. 2017).

The primary differences between APGEMS and APGEMS-TF are in the source terms and outputs. APGEMS was developed to support radiological emissions and consequence assessment, so emission rates and model output are expressed in radiological and dose units. APGEMS-TF, on the other hand, has been configured to support chemical vapor concerns in and around the Hanford tank farms. As a result, emission rates are expressed in grams per second. Model output is expressed in grams per cubic meter, with options to view the output in volumetric concentration units (e.g., parts per million by volume) as well as as a fraction of the 8-hour Occupational Exposure Limit.

The ability to treat multiple simultaneous emission points is another outcome of APGEMS-TF. In broad terms, multiple emission points within a single APGEMS-TF run are treated by superposition, which is a standard practice in dispersion modeling, including in U.S. Environmental Protection Agency regulatory models (Arya 1999).[3] Plumes from individual emission points are computed, mapped to a common grid, and combined.

Emission locations for the 200 East Area A Corridor and associated emission rate estimates for a selection of chemicals of potential concern are prepopulated within the APGEMS-TF software for ease of model setup. Test cases that use these locations and emissions are presented to demonstrate the plume output from both a single emission point as well as multiple emission points. These test cases demonstrate the

[1] Flaherty JE, BG Fritz, JP Rishel, J Bao, EI Mart, and JA Fort. 2017. *Atmospheric Dispersion Modeling Tools for Hanford Tank Farms Applications*. PNNL-25654, Rev 1, Pacific Northwest National Laboratory, Richland, Washington.

[2] Glantz CS, KJ Allwine, MA Pelton, and KJ Pattison. 2002. *User's Guide for the Air Pollutant Graphical Environmental Modeling System (APGEMS)*. PNNL-14043, Pacific Northwest National Laboratory, Richland, Washington.

[3] Arya SP. 1999. *Air Pollution Meteorology and Dispersion*. Oxford University Press. New York, New York.

capabilities and limitations of the APGEMS-TF version 1.0 model. The model is an appropriate tool for modeling chemical emissions within and around the tank farms, although the current version exhibits unrealistically large plumes within the nearest several kilometers of the sources when multiple emission points are modeled, which is a result of the relatively coarse grid employed to combine the multiple emission results. This model result will be resolved with the development of APGEMS version 1.1, to be released within fiscal year 2018.

Acknowledgments

This effort was performed under PNNL Project 69891, funded by Washington River Protection Solutions under the project management of George Weeks.

We acknowledge the contributions of our PNNL project manager, Tom Brouns, as well as our project controls specialists Jeanette Doty and Melanie Chiaradia. Lisa Middleton and Russell Swannack also provided quality assurance support. Brad Fritz served as a peer reviewer for this report, and Susan Ennor provided formatting and editorial support.

Acronyms and Abbreviations

AOP	Abnormal Operating Procedure
APGEMS	Air Pollutant Graphical Environmental Modeling System
APGEMS-TF	Air Pollutant Graphical Environmental Modeling System-Tank Farms
CAM	Consequence Assessment Modeling
COPC	chemical of potential concern
DOE	U.S. Department of Energy
EOC	Emergency Operations Center
HMN	Hanford Meteorological Network
HMS	Hanford Meteorological Station
min	minute(s)
OEL	Occupational Exposure Limit
PGEMS	Pacific Gas and Electric Modeling System
PNNL	Pacific Northwest National Laboratory
ppb	parts per billion (1E9), by volume
ppm	parts per million (1E6), by volume
ppq	parts per quadrillion (1E12), by volume
QA	quality assurance
QRA	quantitative risk assessment
SCAPA	Subcommittee on Consequence Assessment and Protective Actions
SODAR	Sonic Detection And Ranging
SQAP	Software Quality Assurance Plan
SWIHDS	Site Wide Industrial Hygiene Database Systems
TVIS	Tank Vapor Information Sheet
UTM	Universal Transverse Mercator
VCZ	Vapor Control Zone
VRZ	Vapor Reduction Zone
WRPS	Washington River Protection Solutions

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1.0 Introduction

Atmospheric dispersion models were described and evaluated by Flaherty et al. (2017) in the context of capabilities and gaps for Hanford tank farms needs. Dispersion models for real-time response and worker safety and emergency response applications for the mid-field (20 to 1,000 m) and far-field (beyond 1,000 m) distance bins (as defined by Washington River Protection Solutions [WRPS], the tank farm operator) were not available for use by WRPS. (By standard atmospheric dispersion model descriptions, these distances are all considered near-field.) As a result, the Air Pollutant Graphical Environmental Modeling System (APGEMS; Glantz et al. 2002) model was selected by WRPS management to fill a gap in the atmospheric modeling toolbox for the Hanford tank farms for portions of both the mid-field and far-field distance bins.

Pacific Northwest National Laboratory's (PNNL) development of the APGEMS model began in the 1980s, and has been furthered under this project to address specific requirements for the tank farms. The APGEMS model, in its original form, is a radiological emissions model that considers the exposure levels associated with an emission of a mixture of radiological chemicals from a single emission point. For WRPS use in the tank farms, the model has been restructured to treat individual chemical emissions from one or more emission points. The revised model has been designated as APGEMS for Tank Farms, or APGEMS-TF. Other changes incorporated in APGEMS-TF include a prepopulated list of emission positions within the 200 East Area of the Hanford Site, along with chemical emission rate estimates for those positions (see Section 2 for additional details).

APGEMS model development began in 1986 as the Pacific Gas and Electric Modeling System (PGEMS) to support routine air-quality assessments and emergency response needs of the Pacific Gas and Electric's (PG&E's) Diablo Canyon nuclear plant near San Luis Obispo, California. PGEMS 1.0 was evaluated in comparison to tracer experiments conducted near the power plant, and model improvements were implemented in PGEMS 1.1. In 1992, PG&E upgraded their emergency response program, and contracted PNNL to incorporate upgrades to the PGEMS model, which included the ability to accommodate multiple radionuclides, variable receptor configuration, and grid nesting. This resulted in PGEMS 2.0 (Allwine and Bian 1995).

The current APGEMS software is included in the U.S. Department of Energy (DOE) Subcommittee on Consequence Assessment and Protective Actions (SCAPA) Consequence Assessment Modeling (CAM) Toolbox[1] (https://sp.eota.energy.gov/EM/SitePages/SCAPA-CAM-APGEMS.aspx), which means it complies with SCAPA's published software quality assurance requirements. These quality assurance requirements are not as rigorous as the DOE requirements for safety software, but represent a graded approach for software products that are not classified as safety software. The APGEMS software is currently used at the Hanford Emergency Operations Center (EOC) as a near-real-time response tool in evaluating atmospheric dispersion and dose assessment from accidental radiological releases on the Hanford Site.

Based on the use of the APGEMS software at the Hanford EOC and recommendations from PNNL (Flaherty et al. 2017), WRPS contracted PNNL to develop APGEMS-TF. Additional details concerning APGEMS-TF model attributes are discussed in Section 2.0, while case studies using the model are described in Section 3.0. Section 4.0 provides a summary of installation requirements and user

[1] The Subcommittee on Consequence Assessment and Protective Actions is to be restructured, and will be consolidated under a newly established Subcommittee on Technical Analysis and Response Support (STARS). The web link provided will change in the future.

information. Section 5.0 provides an overview of the model development efforts described in the report, and describes future model development under consideration.

2.0 Model Overview

The APGEMS-TF model employs a Gaussian puff dispersion formulation to describe the concentration distribution resulting from one or more emission points. A three-dimensional diagnostic wind field is computed using mass-conserving interpolation of surface and upper-air wind speed and wind direction measurements. The Hanford Meteorological Network (HMN; Hoitink et al. 2005) collects meteorological data from across the Hanford Site, which provides the spatial coverage necessary for the diagnostic wind field model to represent the Hanford Site. Additional data sources, including in-farm meteorological stations, may be incorporated to improve wind estimates near the tank farms. Puff models simulate the release as a series of puffs, which are tracked on a temporally and spatially varying meteorological grid. The dispersion of each puff is computed based on a Gaussian puff width that varies as a function of atmospheric stability. Concentrations on the grid are determined by summing the individual contributions from each puff. Note that, for all Gaussian dispersion models, including APGEMS-TF, output within 100 m of a source may have large errors, and should only be used qualitatively (Flaherty et al. 2017).

The primary differences between APGEMS and APGEMS-TF are in the source terms and outputs. APGEMS was developed to support radiological emissions and consequence assessment, so emission rates are expressed in curies per second (Ci/s) and model output is expressed in curies per cubic meter (Ci/m^3). Dose impacts are computed based on the radiological emission rates for each emission point. APGEMS-TF, on the other hand, has been configured to support chemical vapor concerns in and around the Hanford tank farms. As a result, emission rates are expressed in grams per second (g/s), and each chemical is treated independently. Model output is expressed in grams per cubic meter (g/m^3), with options to view the output in volumetric concentration units (e.g., parts per million by volume; ppm) as well as as a fraction of the 8-hour Occupational Exposure Limit (OEL).

In addition, multiple simultaneous emissions points are available within APGEMS-TF. In broad terms, multiple emission points within a single APGEMS-TF run are treated by superposition, which is a standard practice in dispersion modeling, including in U.S. Environmental Protection Agency regulatory models (Arya 1999). Plumes from individual emission points are computed, mapped to a common grid, and combined.

This modeling approach minimizes run-time by computing a unit release from each location and scaling the output according to the emission rate for each chemical from that emission point. The current formulation of APGEMS-TF assumes that each of the chemicals emitted in the tank farms are in trace gas quantities, so no density effects (e.g., pooling) are expected. Additionally, chemical reactions between chemical species or between a chemical species and the environment (e.g., photolysis) are not treated by the model.

Features that remain the same between APGEMS and APGEMS-TF include the basic structure for retrieving near-real-time meteorological data, the geographic information system layers to view the Hanford Site, the wind field model, the puff model, and model time steps. The model also computes effective stack height from either buoyancy (i.e., emissions warmer than the environment) or momentum (i.e., emission vertical velocity). In addition, plume reflection on the ground and at the top of the mixing layer is assumed. Puff diffusion coefficients are based on historical diffusion data that have an inherent averaging time of 15 to 30 minutes, which guides the 15-minute meteorological time step used in APGEMS-TF.

The subsections below focus on the major model elements that were modified as part of APGEMS-TF development. Descriptions of elements that are unchanged from APGEMS can be found in the user's guide by Glantz et al. (2002).

2.1 Meteorological Input

Meteorological data are needed to provide input for the diagnostic wind model, which creates the gridded wind field. Meteorological data from the HMN are available, although coordination with Mission Support Alliance, the Hanford contractor that operates the network, is necessary to gain access to these data.

The HMN supplies five file types, four of which are required for APGEMS-TF to operate. These four file types are as follows:

1. Telemetry Data – contains the 15 min averaged wind direction, wind speed, temperature, precipitation, pressure, station elevation, station name, station latitude, and station longitude for each of the 30 near-surface meteorological stations deployed across and near the Hanford Site.
2. 200 ft Tower Data – contains the 15 min averaged wind direction, wind speed, and temperature at multiple heights from the three 200-ft towers located in the 100, 300, and 400 Areas, as well as the surface measurements of dew point, relative humidity, temperature, and delta-temperature (between the 200 ft and 30 ft levels) at the three 200 ft towers. Note that the delta-temperature is computed based on 5 sec values, so the difference listed among the two levels for the 15 min average may be a different value.
3. 400 ft Tower Data – contains the 15 min averaged wind direction, wind speed, and temperature at multiple heights from the 400 ft tower located at the Hanford Meteorological Station (HMS), as well as the solar radiation, dew point, and stability class for the site.
4. Observation Data – contains meteorologist observations and a summary of key instrument readings, including cloud ceiling height, visibility, atmospheric pressure corrected to sea level, dew point, wind direction, wind speed, station atmospheric pressure, dry bulb temperature, wet bulb temperature, relative humidity, sky cover, precipitation, solar radiation, and mixing depth.

The fifth file type is for sonic detection and ranging (SODAR) data, which are not available from the HMN. These files were created at a time when a SODAR was expected to be deployed, but such an instrument was never installed. Each file contains the 15 min average value for each of the variables measured. (One exception is precipitation data, for which the 15 min total value is given instead.) These data are processed at the HMS and posted on its server. The data are available to other users typically within 10 min of the end of the averaging period.

The meteorological input requirements of APGEMS and APGEMS-TF are similar, but APGEMS-TF allows users to incorporate additional meteorological measurement locations in the telemetry file. A file named metstations.xml contains each of the meteorological stations that are contained in the telemetry file. To add a new station to the telemetry file, a new met station must be added to the metstations.xml telemetry file; it must have a four-character station name, and the station location should be provided in State Plane coordinates in units of meters. When a station is listed in the metstations.xml file, that station must also be included in the telemetry file, or an error will occur in APGEMS-TF. If data are not available for a given time period, the variables should be populated with -999 (number format will depend on the variable in question).

2.2 Source Locations

Source location groups define one or more source locations for the simulation. Prepopulated source location groups contain prepopulated source locations from 200 East tank and stack emission locations, including the 242-A Evaporator Stack, AP Stack, AW Stack, AN Stack, AY/AZ Stack, and passive breather filter locations within the A, AX, and C Tank Farms. Figure 2.1 shows a portion of the 200 East

Area with the tank farm boundaries identified. This area contains the emission points that are prepopulated in APGEMS-TF. The 242-A Evaporator Stack, which is located near the A Tank Farm, is shown in Figure 2.2. The AP Stack, located near the eastern edge of the AP Tank Farm, is shown in Figure 2.3. The AW Stack, located in the southeastern corner of the AW Tank Farm, is shown in Figure 2.4. The AN Stack is shown in Figure 2.5. Finally, the AY/AZ Stack, which is located outside of the AY and AZ Tank Farms, is shown in Figure 2.6. The passive breather filter locations are not included in figures here, but are assumed to be near the center of each single-shell tank in the A, AX[1], and C Tank Farms.

Figure 2.1. Arrangement of Tank Farms in the "A Corridor" of the Hanford Site 200 East Area

[1] The AX farm was previously passively ventilated, but is now an actively ventilated tank farm. Source location and emission rate will need to be updated.

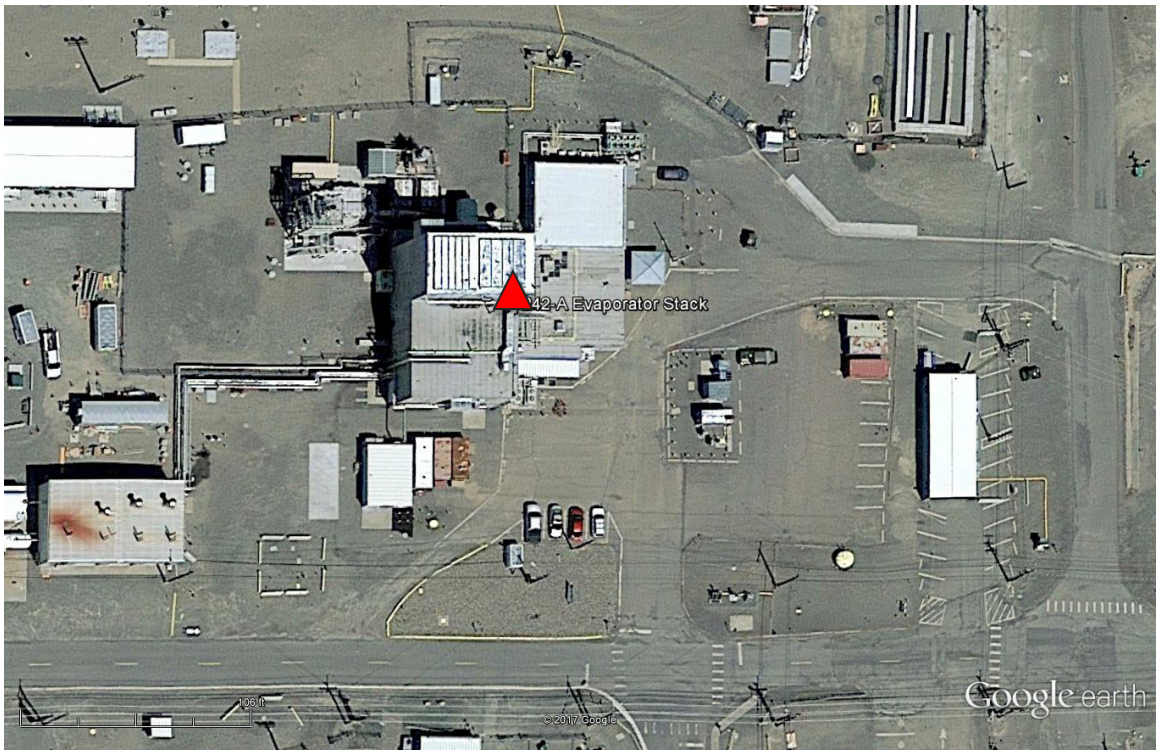

Figure 2.2. Location of the 242-A Evaporator Stack, Located South of the A Farm

Figure 2.3. Location of the AP Farm Stack, near the Eastern Fence of the AP Farm

Figure 2.4. Location of the AW Farm Stack, near the Eastern Fence of the AW Farm

Figure 2.5. Location of the AN Farm Stack, near the Center of the AW Farm

Figure 2.6. Location of the AY/AZ Farm Stack, West of the AZ Farm, on the 241-AZ-702 Building

Users can create a new location by creating a new source location group or adding the location to an existing source location group. The new source location may be one of the prepopulated locations or a unique, custom location. The custom location may be defined by selecting a point on a map or by providing a coordinate in the State Plane coordinate system.

Source location release parameters are predefined for the prepopulated source location groups, but may be modified by the user. Any new user-defined locations will require that these parameters be specified.

2.3 Emission Rates

Emission rates may be defined by the user by selecting a chemical and corresponding emission rate in units of g/s. The chemical database, composed of the current list of 61 chemicals of potential concern (COPCs; Way 2017), is included in Appendix A. Prepopulated source location groups contain prepopulated emission rates for selected chemicals. The prepopulated emission rates for each location are fairly conservative, such that users may be more likely to modify prepopulated rates downward to reflect current conditions, rather than increasing rates. The process used to develop the prepopulated emission rates for each of the prepopulated emission positions is outlined below.

The April 2017 Tank Vapor Information Sheet (TVIS) for each tank farm was consulted to assess the potential chemicals that may be emitted from the source(s) within that tank farm. The TVIS lists the COPCs that have been observed at concentrations greater than or equal to 10% of the OEL for the COPC. The main purpose of the TVIS is to inform tank farm workers of chemicals they may encounter within the tank farm; it does not provide a concentration or emission rate for the chemicals listed.

Next, the draft Respiratory Protection Protocol and Methodology Reports, also referred to as the Vapor Control Zone (VCZ) – Vapor Reduction Zone (VRZ) reports because they summarize the data and

modeling used to identify the dimensions of these zone, were consulted. The VCZ is the zone in which concentrations, based on the maximum observed source concentration, of one or more COPCs may be observed at concentrations greater than 50% of the OEL (based on the modeling described in the report). The VRZ, on the other hand, is the zone around a source in which concentrations, based on the maximum observed source concentration, of one or more COPCs may be elevated, but are not expected to exceed 50% of the OEL. These reports contain the maximum concentrations of COPCs that were observed in the previous decade within the Site Wide Industrial Hygiene Database Systems (SWIHDS), when those concentrations were at least 50% of the OEL for that COPC. The list of chemicals from the VCZ-VRZ reports was more specific about the exposure impacts of those chemicals, so, in general, the VCZ-VRZ reports were used to identify the potential chemicals in the mixture for each emission location.

Chemical concentrations from the SWIHDS headspace data, which were downloaded by a PNNL staff member in March and July 2017, were also included in our evaluation to assess appropriate emission rates. These data contain two years of headspace data, from late 2014 to late 2016, and their primary use has been for a separate PNNL project. Mahoney and Hoppe (2017) describe these data. Another data set consulted for emission rate estimates was a preliminary copy of the respirator cartridge sampling data. These data were last updated in November 2017 and contain data from approximately one dozen tank farms, taken primarily during the summer and fall of 2016 (e.g., Nune et al. 2016). Both of these data sources contained a limited number of the emissions sources that were considered for prepopulating the APGEMS-TF model.

A final resource for reviewing SWIHDS data, the Tank Farms – Data Access and Visualization Explorer (https://www.tankvaporsexplorer.com), was also consulted during our emission rate evaluation. This site provides a convenient way to view SWIHDS data from October 2008 through the present in categories of Headspace, Source, and Area. Headspace and Source data were considered as potential concentration measurements that could represent emission rates. The plots from this website (modified to primarily show the tank farms of interest) are included in Appendix B.

Other data sources included the quantitative risk assessment (QRA) analyses that were performed by Kenexis for WRPS (Kenexis 2017a, b, and c). At the time of this effort, the QRAs for the AP, AW, and A Tank Farms were available and additional QRA analyses for other tank farms were under way, but not yet available to the authors. The data sources described above did not include any information for the 242-A Evaporator. This source is unique in that the evaporator operates intermittently for periods that are described as “campaigns,” and the emission from the facility is, in large part, a function of the waste source that is being processed by the facility. Based on the suggestions of the WRPS Cognizant System Engineer for ventilation systems, the Connor (2005) report on emissions measurements from a March 2005 evaporator campaign was used as the basis for emission estimates included in APGEMS-TF. Air permits were also consulted, but these documents contained upper bounds of regulated chemicals, rather than emissions data based on measurements, and were therefore not included among the data sources used to develop the emission rates from tank farms point sources.

After consulting all of the available data, a single concentration value was selected to represent the emission point. This concentration was either the highest observed value when the data were continuous, or a second-highest or an approximation of the second-highest when it appeared that the highest concentration may be an isolated outlier. The concentration data were combined with the normal or estimated stack or passive breather filter flow rate to arrive at an emission rate in units of g/s for each chemical at each emission point. Details concerning the data distribution among these information sources, and the final emission rates for each emission position are available in Appendix B.

2.4 Model Output Viewer

After the "Run Simulation" button is selected from the menu, and the model run is completed, a new window with the model results is displayed. The output display is similar to the display from the APGEMS v3 software, but key differences exist within the APGEMS-TF software. There are three options for the contour units within APGEMS-TF. First, mass per unit volume concentrations with the default units of g/m^3 are displayed. In addition, the concentration contours can be represented in volumetric units of m^3/m^3. The corresponding ppm, parts per billion (ppb), and parts per quadrillion (ppq) levels are also indicated with this representation to provide users with a unit of measure that can be related to typical measurement concentrations or OELs. The final contour option is concentration contours as a fraction of the OEL. In this case, the mass or volume concentration (as appropriate) is divided by the OEL value of the chemical in question. Presenting the output in this way provides a convenient method for interpreting concentration regions in the context of worker exposure limits. In addition to the drop-down menu for the contour units, there is a drop-down menu from which to select the specific chemical for contouring. These display elements appear for both single-emission and multiple-emission simulations. All concentration contours produced by APGEMS-TF represent ground-level concentrations.

Note that, for model simulations that start in the past and proceed into the future, persistence of meteorological data is assumed, meaning that the meteorological conditions from the last time stamp that occurs in the past, for which data are available, will be assumed for future time stamps. The resulting contour lines, which assume persistence, are displayed with dashed lines rather than solid lines to signify the additional uncertainty associated with those results.

2.5 Model Output Files

Each model run produces a large number of output files. These include files that define the concentrations on the computational grid and the contour levels for the user interface plot. To evaluate a new installation of APGEMS-TF, test cases are included with the installation package. The files that are included for these test cases are *CNC files, which contain the concentration output on the output grid. These files are located in one of two file folders, depending on the number of emission points in the simulation.

For simulations with a single emission point, the CNC files associated with the simulation are located in the APGEMSTF\TdmOut folder. The file-naming convention is

RunNNN_MM_DD_YY_HH_mm_Chem_TF*.CNC,

where NNN is the sequential number for the given run-time, and MM, DD, YY, HH, mm identify the month, day, year, hour, and minute for which the simulation was performed. (This is based on the computer clock time at the time of simulation run, rather than the release start time within the simulation.) Each chemical (Chem) included in the single emission point simulation is stored in a separate CNC file. As discussed in Section 2.4, the concentration output is presented in one of three units; these concentrations are stored in separate files for each of the concentration units. For files that end in TF.cnc, the volumetric concentrations, in units of m^3/m^3 are contained in the file. The mass concentration (g/m^3) is stored in a file that ends in *tf.orig.conc (original refers to the fact that the original output for APGEMS is in mass units, and conversions are applied to arrive at the other two units). Finally, the fraction of OEL is stored in a file that ends in *tf.oel.cnc.

For simulations with a single emission point, the CNC file contains two header lines, followed by a line that contains the month, day, year, hour, and minute of the simulation output, and a block of data

containing the grid node number, UTM easting, UTM northing, and concentration. This format, in which a date/time row is followed by block of data, is repeated for each time step included in the simulation. To evaluate the installation of the software, the CNC file resulting from the simulation performed with the new installation may be compared with the file provided within the test case folder. Small differences in the concentration values may exist due to system and compiler differences, but the results should be nearly identical.

For simulations that have multiple emission points, the CNC files associated with the simulation are located in the APGEMSTF\TdmOut\AggrCNC\TFRun_* folder. For each simulation, a separate folder is created with the date/time associated with the simulation start time. Within that folder, CNC files with the following naming convention are included: Aggr_Chem_MM_DD_YYYY_HH-MM-SS_AM*.cnc. Each chemical (Chem) included in simulations with multiple emission points is stored in a separate CNC file. However, unlike the single emissions case, MM, DD, YYYY is followed by HH-MM-SS_AM (or PM), and the month, day, year, hour, minute, second identify the time within the simulation. Each output time is saved in a separate file, rather than being stitched together as was done in the single emission case.

For simulations that have multiple emission points, the three different concentration outputs are stored in three separate files, similar to the single emission point convention. Files that end in *AM (or PM).cnc contain volumetric concentrations in units of m^3/m^3. The mass concentration (g/m^3) is stored in a file that ends in *AM (or PM).ORIG.cnc, and the fraction of OEL is stored in a file that ends in *AM (or PM).OELcnc.

The CNC file for multiple emission points is similar to the CNC file that is produced for a single emission point. There are two header lines, followed by a line that contains the month, day, year, hour, and minute of the simulation output, and a block of data containing the grid node number, UTM easting, UTM northing, and concentration.

2.6 APGEMS-TF Model Ranking

Flaherty et al (2017) included a model ranking that provided a sense of the strengths and weaknesses of specific models for specific model applications. The APGEMS model was included in the ranking for real-time modeling and worker safety and emergency planning applications. Appendix D contains tables comparing the APGEMS and APGEMS-TF model ranking for these two application areas. Because the core of the model was not changed, and the only quantifiable change made, relative to the model attributes included within the ranking table, is the addition of a multiple source capability, the final score for the APGEMS-TF model is only one point greater than that of the original APGEMS model. This illustrates the point that the model ranking approach can identify overall strengths and weaknesses of the models considered, but specific modeling goals should be examined carefully when selecting specific models for use.

3.0 Quality Assurance

The APGEMS-TF Software Quality Assurance Plan (SQAP; Swannack 2017) outlines the quality measures taken to develop, test, and deliver the APGEMS-TF software to the client. The structure of the code is such that the legacy code of the wind field and puff models remain intact, while "wrapper" software is modified. A broad overview of the quality assurance (QA) activities that have been performed for APGEMS is described in this section, followed by the specific steps and regression test cases that have been performed for APGEMS-TF.

3.1 Legacy QA Activities

As stated in Section 1.0, the PGEMS model code was evaluated in comparison with field data near the Diablo Canyon nuclear power plant in California. Formal documentation of this evaluation and subsequent model updates are not available, but Thuillier (1992) provides some review of the PGEMS model near the Diablo Canyon plant. As part of the inclusion of the APGEMS model in the SCAPA CAM Toolbox, QA documentation concerning the APGEMS model itself has been compiled. These documents primarily concern the function and documentation of the model, rather than an assessment of the model algorithms.

Baseline tests have been performed to ensure the proper performance of basic model functions, such as reading terrain data and meteorological data correctly, accepting user specification of release location and properly using the location for the release, accepting user specification of source strength, etc. Model intercomparisons have also been performed with both HotSpot (Homann and Aluzzi 2013) and National Atmospheric Release Advisory Center (Sugiyama et al. 2015) health physics models.

3.2 APGEMS-TF QA Activities

The SQAP for APGEMS-TF uses a graded approach that follows the PNNL How Do I workflow called "Develop Software for Delivery," because this software is neither safety nor high-assurance software. The WRPS Software Review Board has reviewed the software, and has graded it "NA." The SQAP addresses the need for documentation and retention of records. For this work, a project share drive has been established to serve as a working folder and document repository. In addition, Jira, Confluence, and Stash electronic repositories have been established for this project to store software issues, project records, and source code, respectively. The SQAP also identifies software tests to be performed, which include regression tests, test cases, and acceptance testing. Regression tests are described further below, and test cases and acceptance testing are described in Section 4.0.

Regression tests were performed to ensure that the changes made to implement APGEMS-TF did not inadvertently affect the output of the dispersion model. These regression tests were performed by visually comparing output from a unit release computed with APGEMS-TF to the output from the First Responder Model computed with APGEMS v3. Although the output units differ, the contour lines represent the same relative concentration values. For each case, the AX/AY/AZ Tank Farm location (which is a prepopulated position within the APGEMS v3 software) was used to emit a unit release on selected dates. Three time periods were selected to cover a range of meteorological conditions:

- June 6, 2017, 8 AM to 12 PM – a moderate wind period in the summer
- November 16, 2017, 8 AM to 12 PM – a high-wind period in the autumn
- November 28, 2017, 8 AM to 12 PM – a low wind period in the autumn.

The November 28, 2017 date also has significance as a date on which an Abnormal Operating Procedure-015 (AOP-015) event was reported. Workers in the 271AW instrument building, located west of the AW Tank Farm and southeast of the corner of 4th Street and Buffalo Avenue, reported odors at around 9 AM. An empty, lead-lined sample storage box within the tent was attributed to be the potential source for this AOP-015 event; but modeling this date may be illustrative of the atmospheric conditions during this event.

3.2.1 June 6, 2017 Regression Test

Mid-morning on June 6, 2017, winds were typically around 5 mph, with gusts between 10 and 15 mph. The wind direction was between northeast and northwest during this time period. Relative humidities were fairly low, between 20 and 40% over the course of the day. Temperatures climbed steadily from about 6 AM until 6 PM, and the high temperature reached about 87°F. During the 8 AM to 12 PM regression test period, temperatures were between 70 and 80°F. Figure 3.1 presents a summary of the meteorological data from the nearby HMN 200 East station, which is located southwest of the C Tank Farm.

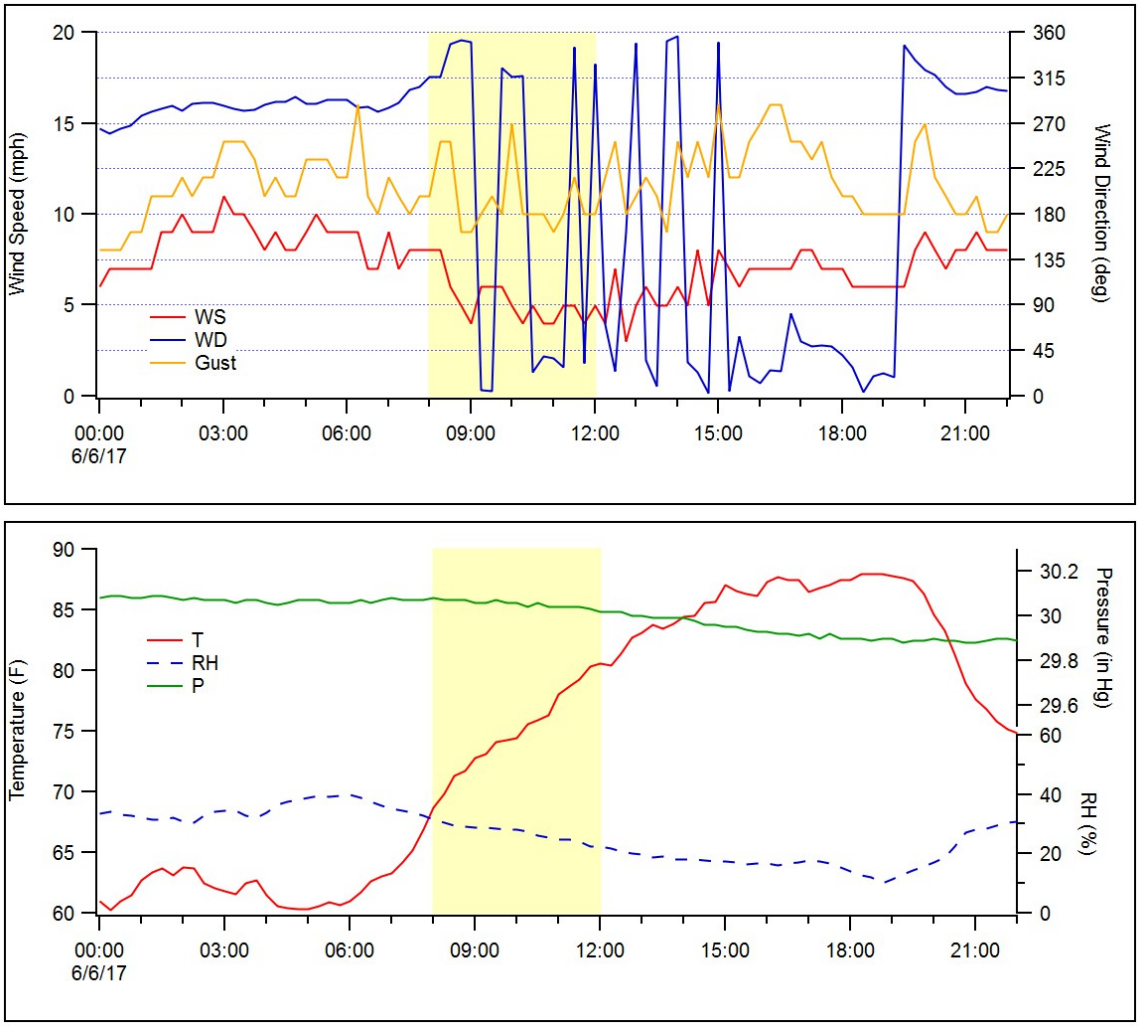

Figure 3.1. Meteorological Data from the HMN 200 East Station (#6) on June 6, 2017. The regression test comparison period is highlighted in yellow.

A regression test was conducted with both APGEMS v3 and APGEMS-TF for the 8 AM to 12 PM time period to ensure that the APGEMS-TF software produced comparable results. Figure 3.2 presents a side-by-side comparison of the plume contours for the 8:30 time period produced by APGEMS v3 (left panels) and APGEMS-TF (right panels). The upper panels in this figure show the overall plumes for both software versions; the plumes appears to have similar, if not identical, lengths and widths. The lower panels in this figure show more detail of the origin of the plume, and the surrounding 200 East Area. A minor difference between the contours is identified with a red arrow near the plume origin. This difference is attributable to differences in the compiler used in the two versions of the code, and does not affect any conclusions that may be drawn from the model output.

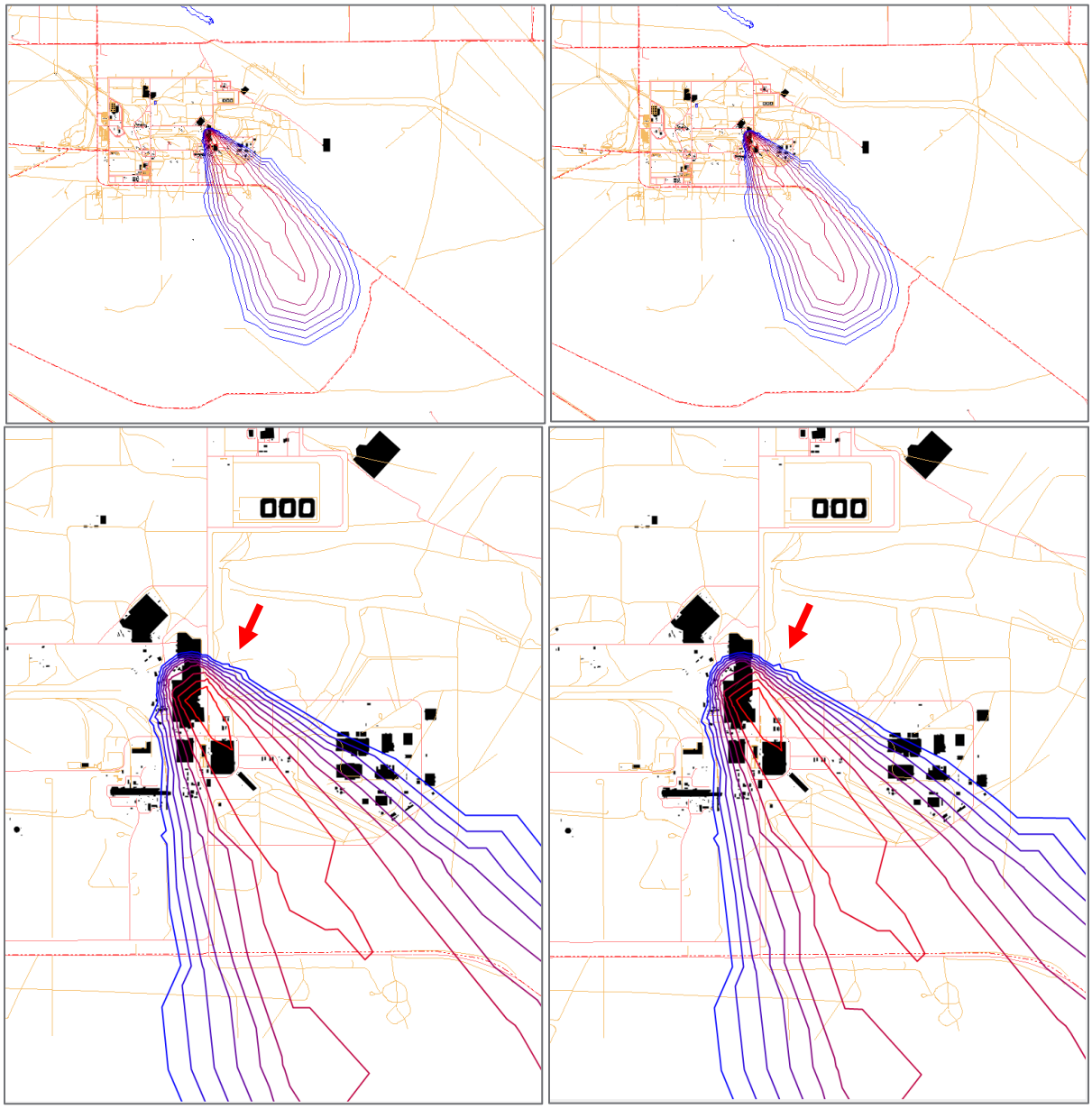

Figure 3.2. Comparison of APGEMS 3 (left panels) and APGEMS-TF (right panels) from a Unit Release on June 6, 2017 at 8:30 AM. Upper panels show the full plumes, while the lower panels show more detail around 200 East Area.

3.2.2 November 16, 2017 Regression Test

The mid-morning period on November 16, 2017 had winds that were climbing from under 5 mph to over 10 mph, with gusts that were about 7 mph greater than the 15 min averaged winds. The wind direction varied as well, featuring periods of winds from the north, northeast, west, northwest, and south. By noon, the wind direction was more stable out of the southwest. Relative humidities were fairly high on this autumn day, decreasing from about 90% in the morning to 40% in the afternoon. Temperatures climbed from about 40°F in the early morning to the mid-50s °F in the afternoon. During the 8 AM to 12 PM regression test period, temperatures were between 43 and 50°F. Figure 3.3 presents a summary of the meteorological data from the nearby HMN 200 East Station, which is located southwest of the C Tank Farm.

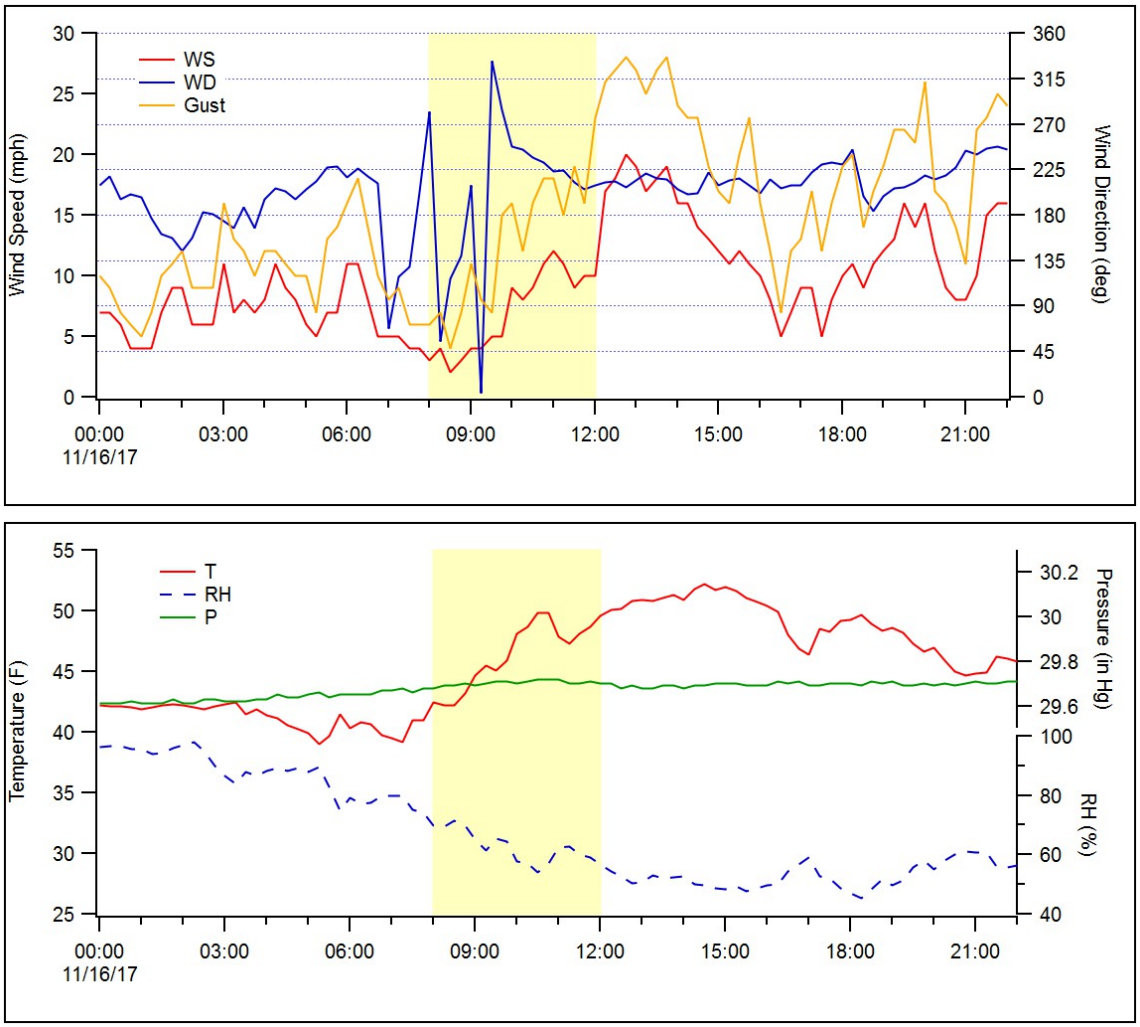

Figure 3.3. Meteorological Data from the HMN 200 East Station (#6) on November 16, 2017. The regression test comparison period is highlighted in yellow.

A regression test was conducted with both APGEMS v3 and APGEMS-TF for the 8 AM to 12 PM time period on November 16, 2017 to ensure that the APGEMS-TF software produced comparable results. Figure 3.4 presents a side-by-side comparison of the plume contours for the 8:30 AM time period produced by APGEMS v3 (left panels) and APGEMS-TF (right panels). The upper panels in this figure show the overall plumes, which appear to have similar, if not identical lengths, widths, and shapes for the

two software versions. Note that the plume for this day extends over a much larger geographical area than the plume modeled on June 6, 2017, due to the lower wind speed for this time stamp on November 16, 2017. The lower panels in this figure show more detail of the origin of the plume and the surrounding 200 East Area. Three minor differences between the contours are identified with red, green, and blue arrows near the plume origin. These differences are attributable to differences in the compiler used in the two versions of the code, and do not affect any conclusions that may be drawn from the model output.

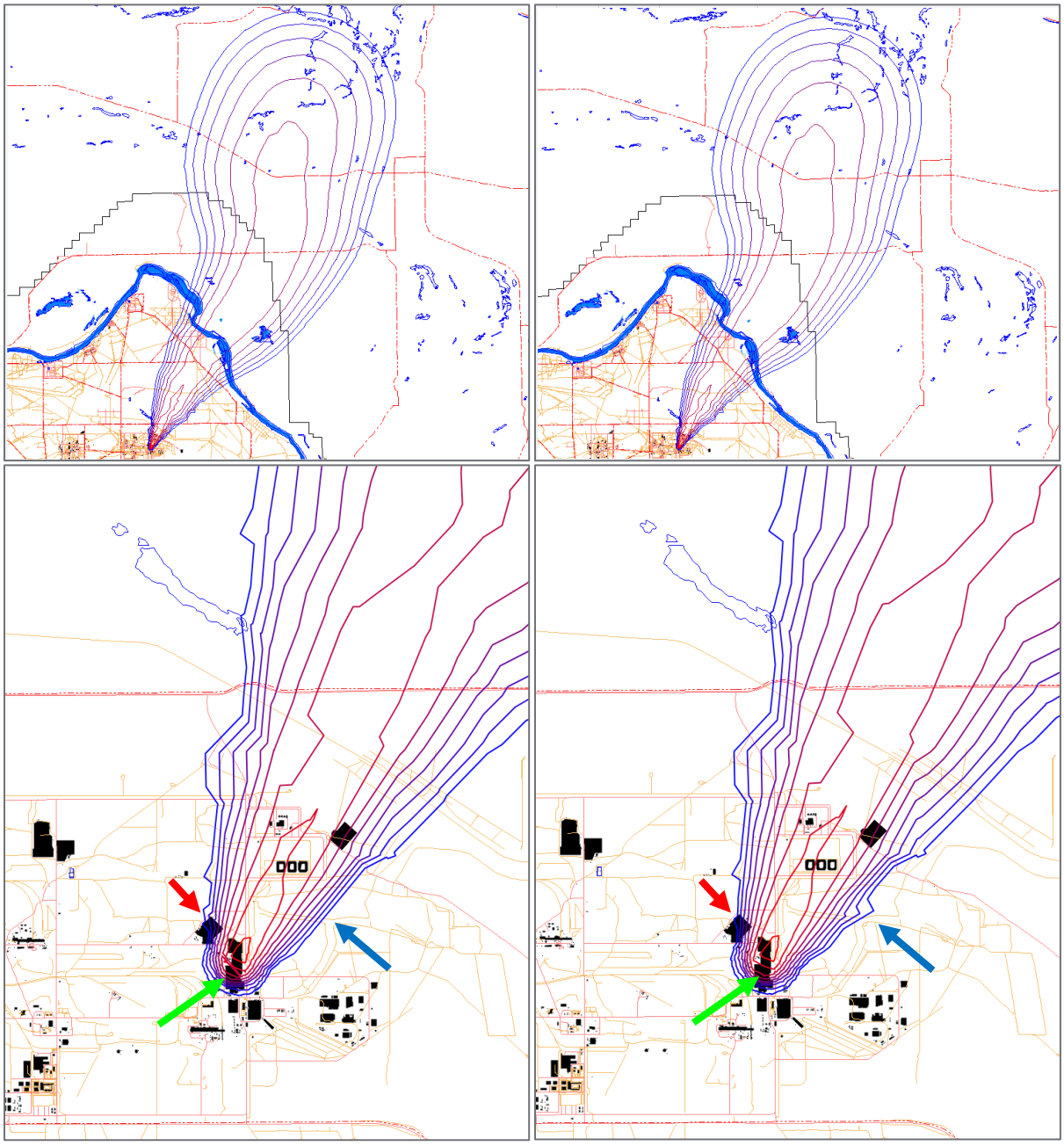

Figure 3.4. Comparison of APGEMS 3 (left panels) and APGEMS-TF (right panels) from a unit release on November 16, 2017 at 8:30 AM. Upper panels show the full plumes, while the lower panels show more detail around 200 East Area.

3.2.3 November 28, 2017 Regression Test

The morning of November 28, 2017 had winds that were typically between 2 and 5 mph. Gusts were not significantly higher on this day, and were typically on the order of 5 mph higher than the 15 min averaged winds. The wind direction varied on this day, although during the mid-morning period, winds were generally from the NW to N or NNE. Relative humidities were fairly high on this autumn day, ranging from about 90% in the morning and evening to about 70% around noon. Temperatures were also relatively flat over the course of the day, ranging from the mid-30s to mid-40s °F. Figure 3.5 presents a summary of the meteorological data from the nearby HMN 200 East Station, which is located southwest of the C Tank Farm.

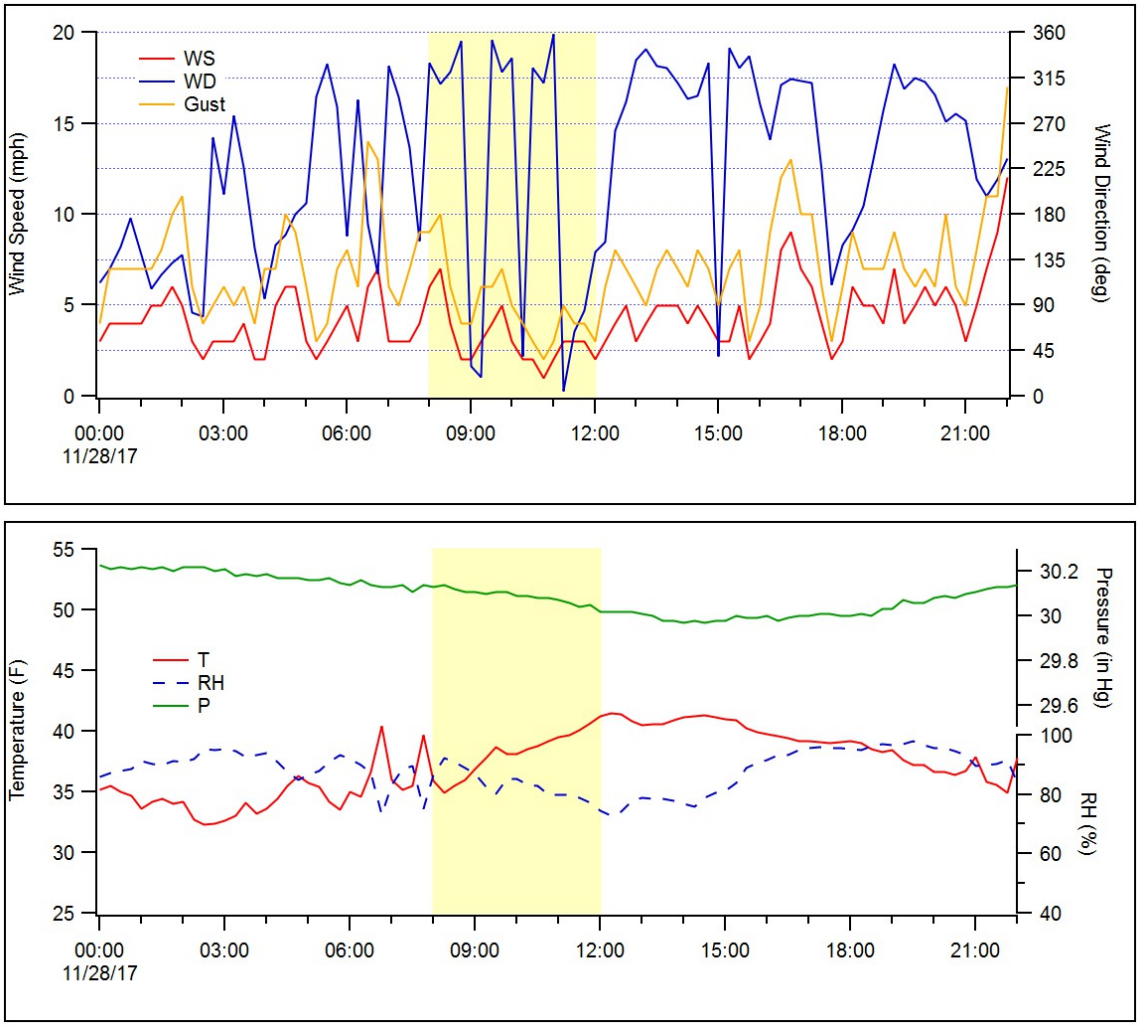

Figure 3.5. Meteorological Data from the HMN 200 East Station (#6) on November 28, 2017. The regression test comparison period is highlighted in yellow.

A regression test was conducted with both APGEMS v3 and APGEMS-TF for the 8 AM to 12 PM time period on November 28, 2017 to ensure that the APGEMS-TF software produced comparable results. Figure 3.6 presents a side-by-side comparison of the plume contours for the 8:30 AM time period produced by APGEMS v3 (left panels) and APGEMS-TF (right panels). The upper panels in this figure show the overall plumes, which appear to have similar, if not identical, lengths, widths, and shapes in both software versions. The size of the plume for this period is smaller than the plume modeled at the

same time on June 6, 2017, due to the lower wind speed observed during this period. The lower panels in this figure show more detail of the origin of the plume and the surrounding 200 East Area. Two minor differences between the contours are identified with a red arrow and a green arrow near the plume origin. These differences are attributable to differences in the compiler used in the two versions of the code, and do not affect any conclusions that may be drawn from the model output. The orientation of this plume appears to indicate that the source of the AOP-015 event on this date was likely to the NW of the AW tent, or perhaps local to the tent area.

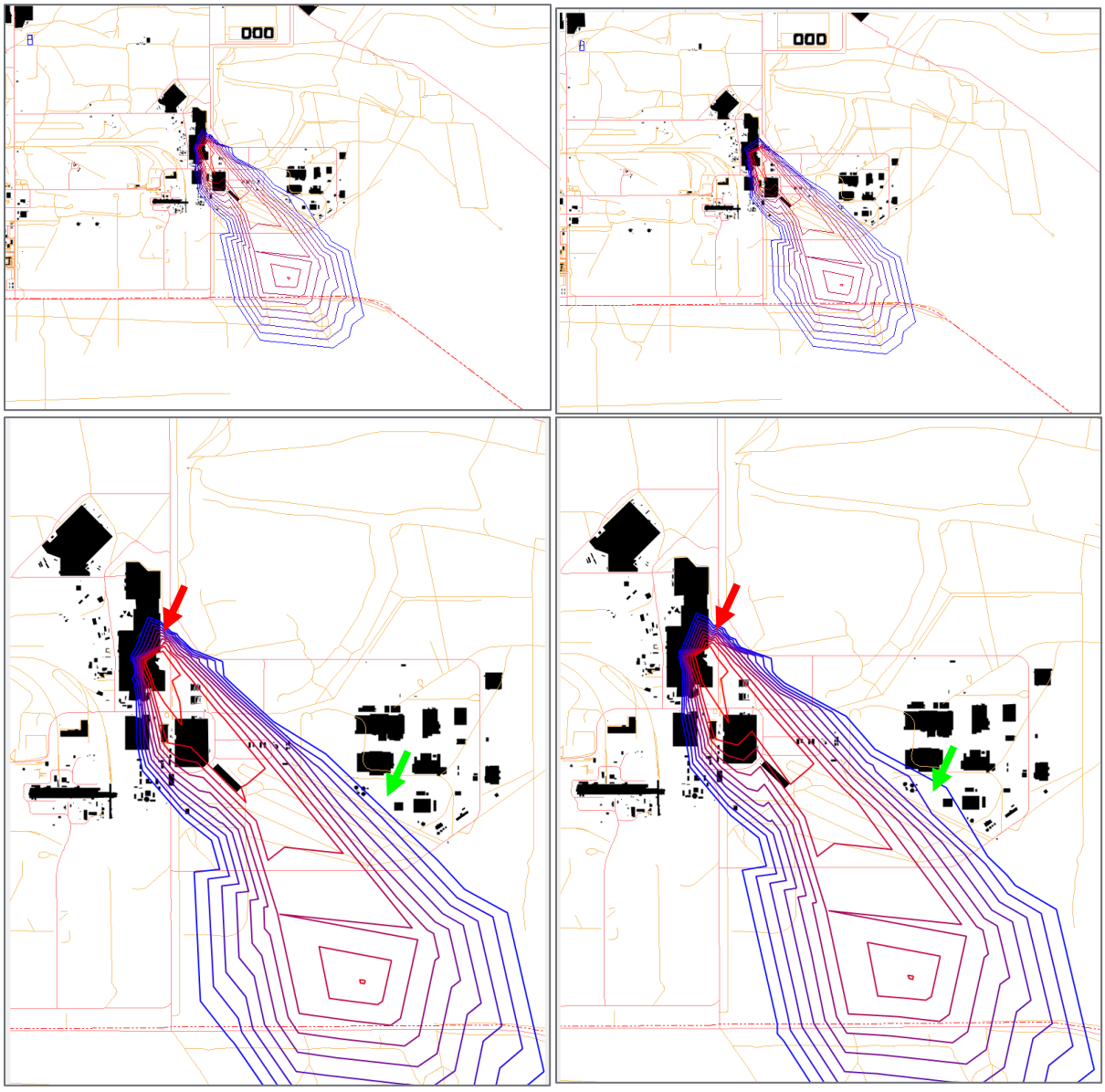

Figure 3.6. Comparison of APGEMS 3 (left panels) and APGEMS-TF (right panels) from a Unit Release on November 28, 2017 at 8:30 AM. Upper panels show the full plumes, while the lower panels show more detail around 200 East Area.

3.2.4 Regression Test Summary

The objective of regression testing was to verify that previously developed and tested software functions still perform correctly within APGEMS-TF. The test cases were identified to cover a range of meteorological conditions which, although not exhaustive, represent sufficient variety to identify potential software concerns. The results explicitly presented in the sections above were for only one of the model output time periods; the remaining time periods for each model run were assessed for each regression test case. Other time periods also contained minor differences in contour lines, which are attributable to differences in the compilers, which use different optimizations for floating point numbers. The conclusion drawn from the results of these tests is that the revision made to the software to accommodate the tank farms needs has not affected the original dispersion code.

3.2.5 Additional QA Activities

As described above, the regression tests were used to address the comparison of the plume model itself, but they do not address the changes made to the model that are distinct from the previous APGEMS version. To evaluate these changes, separate tests were performed, and test results are reported in documents contained in the project share folder on the PNNL network.

In general, the additional QA activities performed for the APGEMS-TF model cover the four topics listed below:

- concentration unit conversions
- aggregation of individual emissions into a single multiple emission output
- prepopulated information
- graphical user interface functions.

To evaluate the concentration unit conversions, the three output units (mass, volume, and OEL) from selected chemicals from a single emission case and a multiple emission case were compared to ensure that the appropriate conversion factors were applied in each case. The conversion from a unit release to a scaled release based on the emission rate was also confirmed. Aggregation of individual emissions into a single multiple emission output was examined using several approaches. First, the final output was assessed against the output from the individual emissions to evaluate how reasonable the final plume appeared to be. Subsequently, a mathematical evaluation of selected points from the output grid was conducted to ensure that the concentrations from each of the individual releases was combined in accordance with the algorithm.

Prepopulated information, such as the emission rates and the source release parameters, were computed from information summarized in a document file as well as in a spreadsheet file. Both the author of the files and an independent reviewer checked through these files to ensure that calculations were correct and that the data were transferred correctly into the XML files used by the model.

Graphical user interface functions were tested primarily as part of the performance of the case studies (described in Section 4.0). As part of each simulation, various model interface elements were exercised to ensure that these interface elements performed as expected. This testing included both the model setup and model output screens. One model limitation identified as part of this testing was that, when emission rates are newly defined, users must click on another emission rate cell to validate the entry. Otherwise, the final input value will be listed as zero for the simulation.

The regression tests, along with the additional software tests and reviews, have been performed in accordance with the SQAP for this project, and ensured that the APGEMS-TF model is functioning as designed.

4.0 Case Studies

WRPS identified two case studies to demonstrate the use of the APGEMS-TF model. These case studies demonstrate a single emission point at the 242-A Evaporator Stack as well as multiple, simultaneous emissions from the AP, AW, and AN Tank Farms. Specific dates, times, or modeling conditions were not specified in the Statement of Work, so modeling periods were selected based on dates on which AOP-015 events were reported, or, conversely, dates featuring meteorological conditions during which an AOP-015 event would be unlikely to occur based on dispersion conditions. These case studies also serve as test cases and acceptance test cases for QA purposes.

An additional group of case studies was proposed during the course of the project to investigate APGEMS-TF concentrations in comparison to data collected at a typically downwind location. Each case study set is described in subsections below.

4.1 242-A Evaporator

The 242-A Evaporator is a facility used to reduce the volume of tank waste by evaporating the liquid in the waste. This facility is not in constant operation; instead, periods of operation, called evaporator campaigns, occur one to four times per year. Each evaporator campaign may be as short as several hours and as long as several months. Limited data were available for the emissions at this facility; Conner (2005) was referenced to obtain emissions estimates, which included ammonia, mercury, and n-nitrosodimethylamine. In addition to emission rates, emission characteristics are input to the APGEMS-TF model. Source data that were specified are included in Table 4.1.

Table 4.1. Release Parameter Data for the 242-A Evaporator Stack

	242-A Evaporator Stack
Height of Release	33.7 m (110.5 ft)
Stack Exit Velocity	16.6 m/s
Stack Gas Exit Temperature	25°C
Stack Diameter	0.15 m (5.8 in.)

Two dates were selected for demonstration of the APGEMS-TF model using the 242-A Evaporator as the emissions source. November 16, 2017 was a high-wind-speed date, while June 13, 2017 had moderately high winds and an AOP-015 event in and around a building near the intersection of 4th Avenue and Buffalo Street. For each of the 242-A Evaporator cases, the simulation output was set to 30 minutes and the outer domain was set to 100 km.

4.1.1 November 16, 2017 Test Case

The meteorological conditions for this test period are described as part of the regression testing description in Section 3.2.2. A continuous, 4-hour emission that began at 8:00 AM was modeled from the 242-A Evaporator in the 200 East Area to demonstrate a single emission case using APGEMS-TF under relatively high-wind conditions. Related ammonia volumetric concentration contours and mercury concentration contours are presented in Figure 4.1 and Figure 4.2, respectively.

Figure 4.1 presents the progression of the ammonia plume with contours at three selected time periods. The highest concentration level for this case is 10 ppb. The influence of varying wind direction across the

domain is visible in the bend in the plume centerline in the 10:00 and 12:00 time periods. Plots near the source show the influence of the near-field wind direction as indicated by differences in the plume axis.

Figure 4.2 presents the mercury concentrations for the 8:30 time period with the three concentration representations. The volumetric contours are intended to be used for comparisons with measurements for most compounds. However, in the case of mercury, the concentration is more likely to be presented in mass/volume units. The OEL fraction is presented as a convenient way to identify the relationship between exposure limits and modeled concentrations. Overall, one can see that the contour shapes are similar between the different concentration representations, as expected.

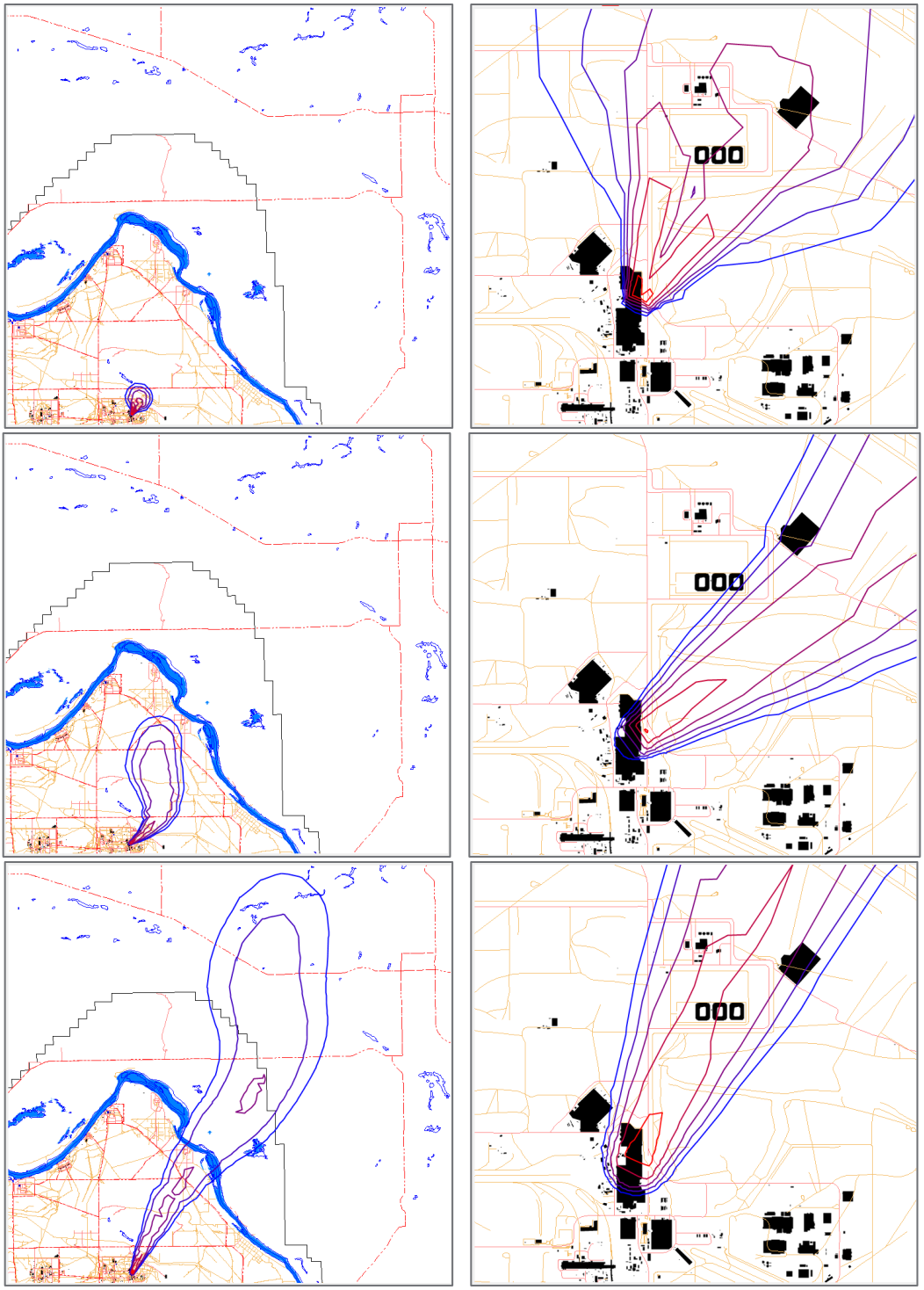

Figure 4.1. Ammonia Volumetric Concentration Contours at 8:30 (top panel), 10:00 (middle panel), and 12:00 (bottom panel) on November 16, 2017 from the 242-A Evaporator. Contour levels shown range from 100 ppq to 10 ppb. The overall plume view is shown in the left panels, while the area around 200 East Area is shown in the right panels.

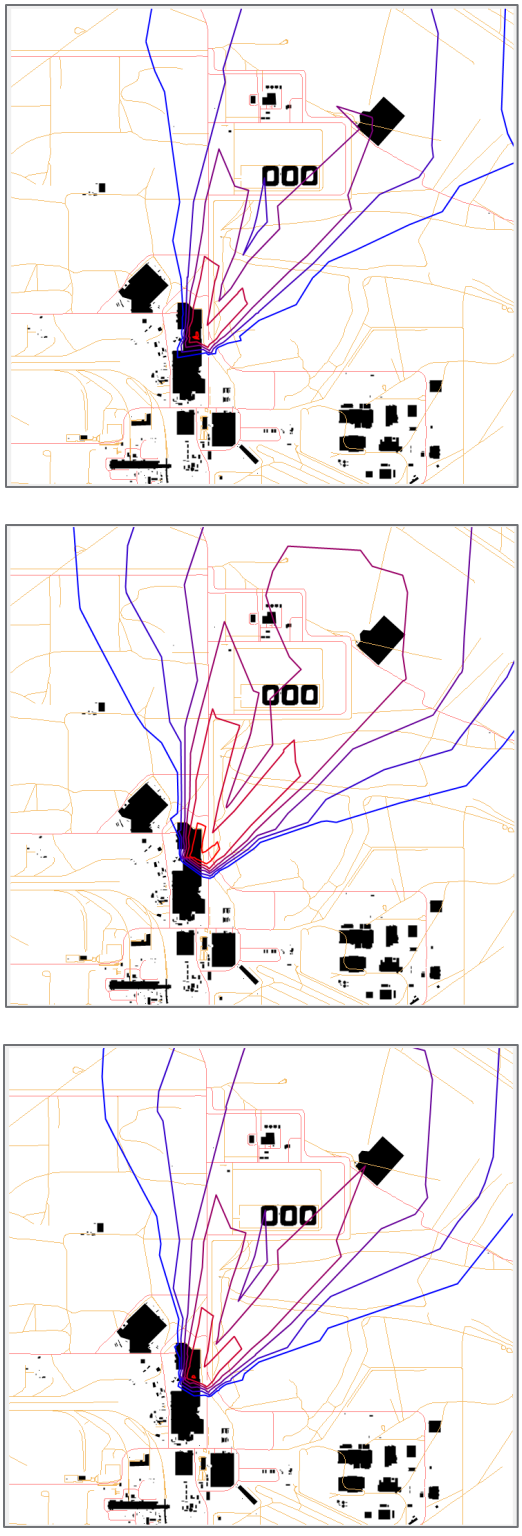

Figure 4.2. Mercury Concentration Contours at 8:30 AM on November 16, 2017 for Volumetric Units (top panel), OEL Fraction (middle panel), and Mass Units (bottom panel) from the 242-A Evaporator. Volumetric concentration contours shown range from 0.1 ppq to 1ppt, OEL fraction contours range from 1E-9 to 1E-4, and mass contours range from 1E-13 to 1E-8 g/m^3.

4.1.2 June 13, 2017 Test Case

The June 13, 2017 test case was not a regression case, but was a date on which an AOP-015 was reported near the intersection of 4th Street and Buffalo Avenue. The AOP-015 occurred in and around the 285-A Building at approximately 7:35 AM. Meteorological conditions for the test case period are presented in Figure 4.3. Winds were generally out of the west and west-northwest, and although winds were often on the order of 20 mph during the 4-hour test case period, the wind speed at the time of the AOP-015 event was 13 mph. Wind gusts as high as 35 mph were observed during the 4-hour test period. Barometric pressure was relatively flat, and temperatures increased from about 57°F to 67°F. Relative humidity remained relatively flat, decreasing from 43 to 27% in this time period.

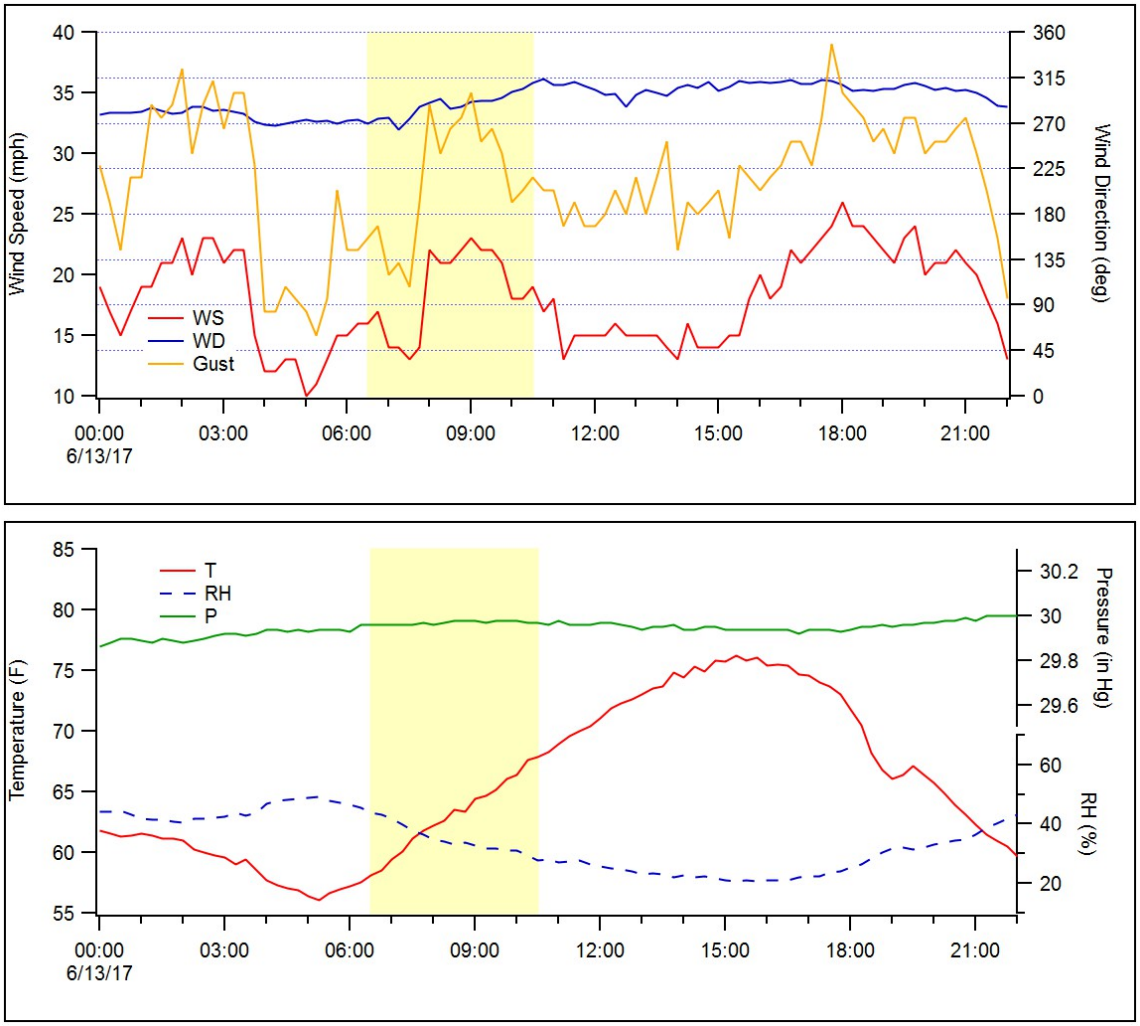

Figure 4.3. Meteorological Data from the HMN 200 East Station (#6) on June 13, 2017. The test case period is highlighted in yellow.

A continuous, 4-hour emission that began at 6:30 AM was modeled from the 242-A Evaporator in the 200 East Area to demonstrate another single emission case using APGEMS-TF. Figure 4.4 presents the ammonia contours from three selected time periods from the June 13, 2017 test case. The plume is primarily transported to the east in accordance with the westerly winds. The plume at 8:30 shows a difference in wind direction across the river with the plume axis shifting toward the northeast. Near the

source, the plume axis is largely unchanged between the three time periods that are presented. The highest contour concentration is 100 ppt.

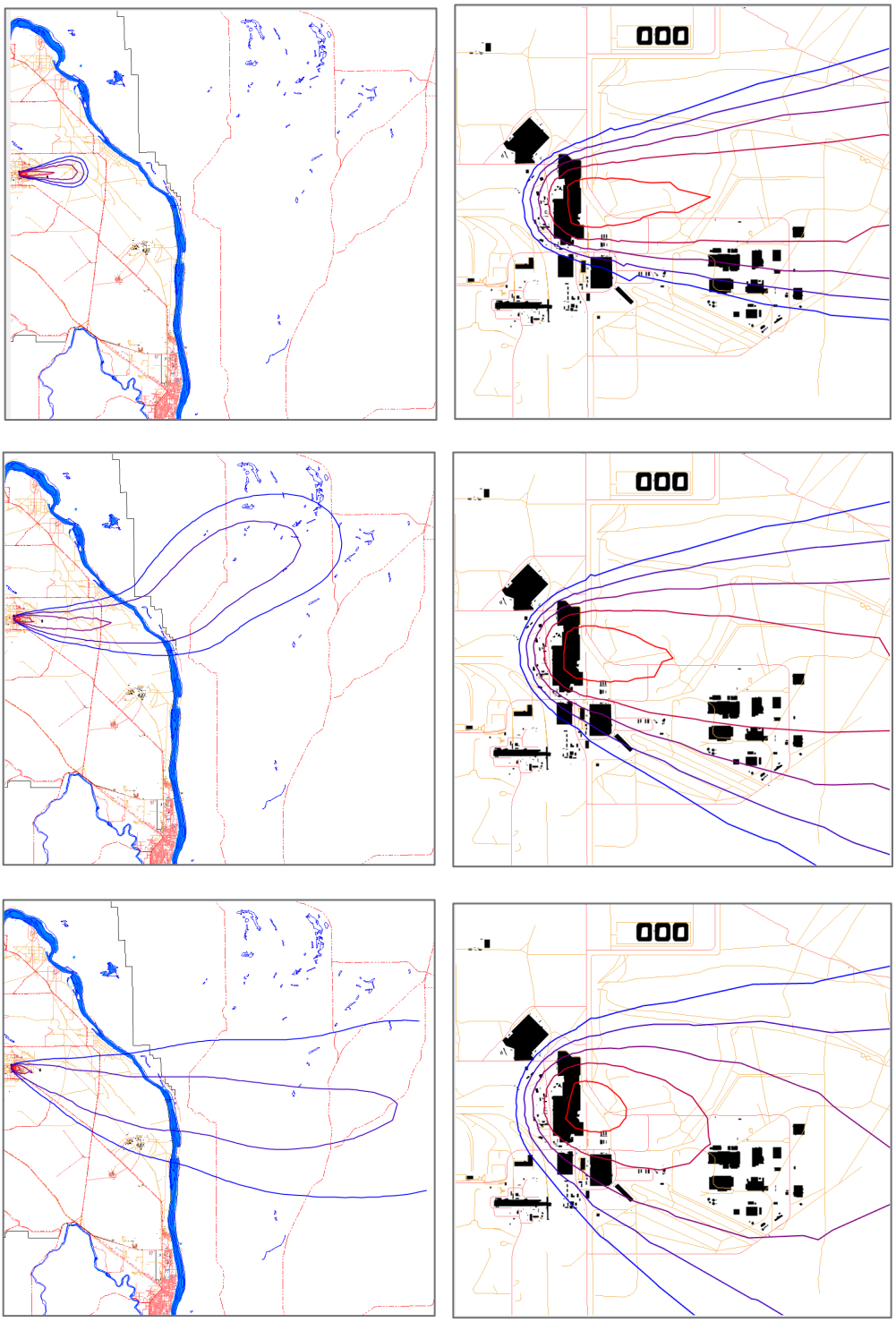

Figure 4.4. Ammonia Volumetric Concentration Contours at 7:00 (top panel), 8:30 (middle panel), and 10:30 (bottom panel) on June 13, 2017 from the 242-A Evaporator. Contour levels shown range from 10 ppq to 100 ppt. The overall plume view is shown in the left panels, while the area around 200 East Area is shown in the right panels.

Based on modeling results, it appears unlikely that a source near the 242-A Evaporator contributed to the AOP-015 event reported on this date. (The evaporator was not operating on this date, so the evaporator itself was not a potential source.) However, modeling does show that the evaporator does result in some upwind transport resulting in some low concentrations at the 285-A building. Figure 4.5 shows an aerial map with the 285-A building identified, along with the 242-A Evaporator location. The event investigation report identified the sanitary tanks, which were serviced earlier that day, as the potential source of odors noted on June 13, 2017. These tanks were located at several buildings northwest of the 285-A building, in the vicinity of the text identifying these locations in Figure 4.5. Based on wind conditions, this appears to be a reasonable source of the odors identified on this date.

Figure 4.5. 242-A Evaporator Location Relative to the 285-A Building, Where an AOP-015 Was Reported on June 13, 2017.

4.2 AP, AW, and AN Stacks

A major model modification made for APGEMS-TF was the capability to model multiple simultaneous emissions. To demonstrate this new capability, test cases with the AP, AW, and AN Stacks simultaneously emitting the estimated combination of chemical emissions for each source were conducted. Each of these stacks ventilates between 6 and 8 double-shell tanks from within the tank farm that they serve. Emission characteristics for each of the stacks were specified in the APGEMS-TF model as listed in Table 4.2. For each case, the output interval was set to 30 minutes and the outer domain was 100 km.

Table 4.2. Release Parameter Data for the AP, AW, and AN Stacks

	AP Stack	AW Stack	AN Stack
Height of Release	12.2 m (40 ft)	8.5 m (27.9 ft)	8.5 m (27.9 ft)
Stack Exit Velocity	15.8 m/s	10.7 m/s	19.6 m/s
Stack Gas Exit Temperature	25°C	25°C	25°C
Stack Diameter	0.25 m (10 in.)	0.25 m (10 in.)	0.25 m (10 in.)

4.2.1 November 28, 2017 Test Case

The meteorological conditions for this test period are described as part of the regression testing description in Section 3.2.3. A continuous, 4-hour emission starting at 8:00 AM was modeled from each of the AP, AW, and AN Stacks in the 200 East Area to demonstrate a multiple emission case using APGEMS-TF under relatively low wind conditions, during which an AOP-015 event was reported in a tent near the AW Tank Farm.

Figure 4.6 presents the ammonia volumetric concentration from three selected time periods from this test case to show the progression of the plume over the course of the 4-hour simulation. Note that the 8:30 AM plume is squared-off in shape as a result of the paucity of data points in the near-field that results from the 1 km uniform common grid used to combine the plumes from the individual release positions. As the plume grows in subsequent time steps, the contours become more rounded or smoothed. In comparison with the regression test performed from a ground-level test for the 8:30 AM time period (Figure 3.6), this test case plume is not as clearly oriented toward the southeast. However, the individual plumes (not shown) are oriented toward the southeast as was seen with the test case, so the boxy plume that results from the combination of the individual plumes and the obscurity of the true plume orientation are a result of the common grid. Based on this feature, it is advised, when continuous emissions are modeled, that the simulation be initiated an hour ahead of the time period of interest, when the plume size is likely to be larger and smoother, and the plume position is expected to be more valuable for users.

Figure 4.6 also indicates the range of concentrations that may be expected based on the combination of these three stack emissions. The highest concentration contour level from this figure is 1 ppb, meaning that the model does not predict concentrations as high as 10 ppb from the estimated emission rates for this meteorological condition.

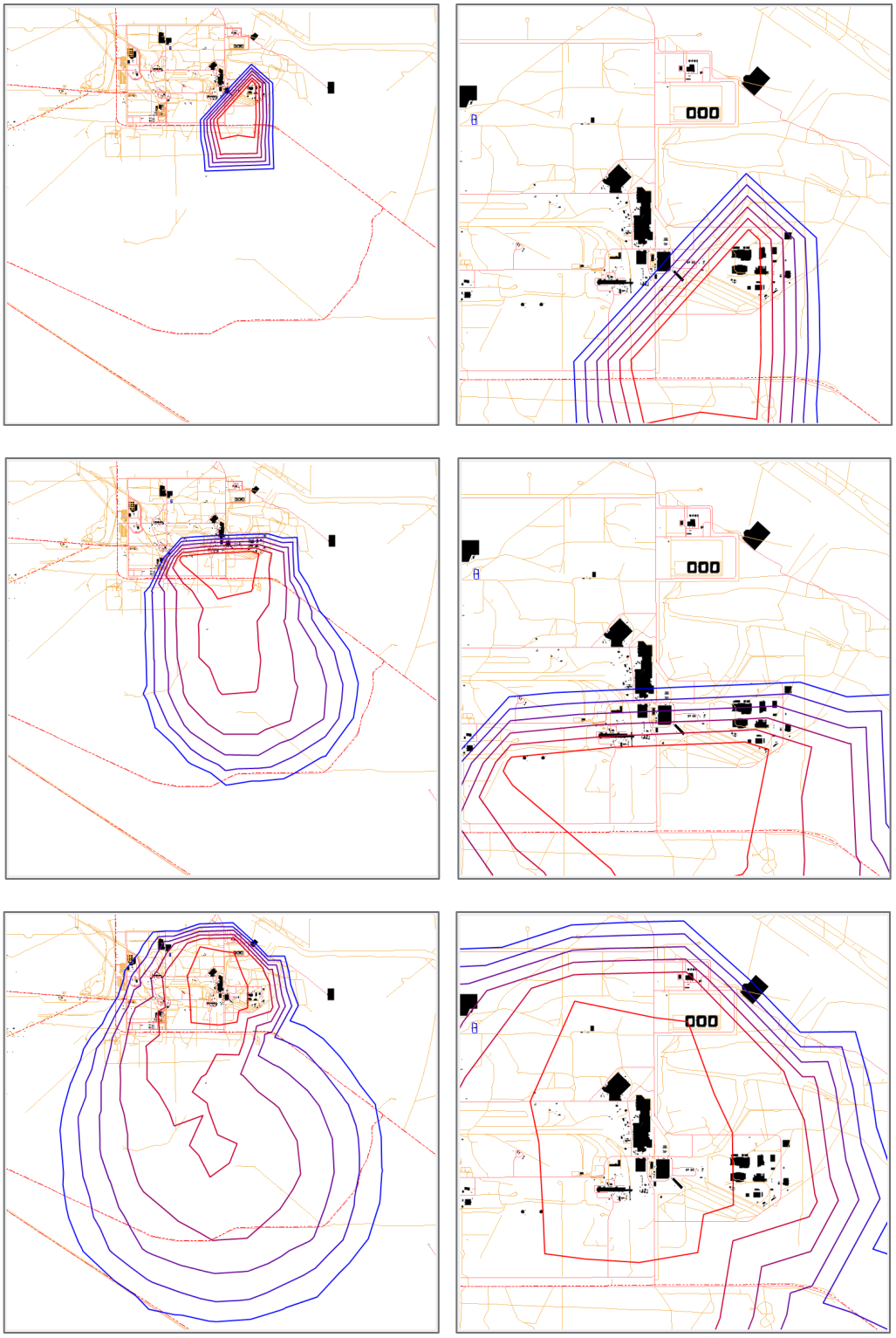

Figure 4.6. Ammonia Volumetric Concentration Contours at 8:30 (top panel), 10:00 (middle panel), and 12:00 (bottom panel) on November 28, 2017 from the AP, AW, and AN Stacks. Contour levels shown range from 100 ppq to 10 ppb. The overall plume view is shown in the left panels, while the area around 200 East Area is shown in the right panels.

4.2.2 June 13, 2017 Test Case

The meteorological conditions for this test period are described as part of the 242-A Evaporator test case description in Section 4.1.2. A continuous, 4-hour emission starting at 6:30 AM was modeled with each of the AP, AW, and AN Stacks in the 200 East Area as emissions sources to demonstrate a multiple emissions case using APGEMS-TF for another date on which an AOP-015 event was reported.

Figure 4.7 presents the ammonia volumetric concentration from three selected time periods from this test case to show the progression of the plume over the course of the 4-hour simulation. Note that the 7:00 AM plume is quite a bit larger for this case than for the first time step from the November 28, 2017 case due to the higher winds during this June case. As a result, the first time step plume is relatively smooth in appearance, rather than boxy. However, the 8:30 AM plume appears to have "staircase" shaped edges on the eastern third of the plume due to the combined effects of the concentration grid and contouring algorithm.

Finally, this case demonstrates the maximum plume size limitation from the common grid domain size. The 10:30 AM plume extended to the east and terminated abruptly at the edge of the concentration grid field. To resolve this, if concentrations at these distances are of interest, the outer domain size may be increased to enclose the total plume. (Note that, at this time, testing has shown that extending the outer domain to 200 km results in missing contours or oddly shaped contours, so it is recommended that users maintain the outer domain size at the default value of 100 km.)

A final note concerning the plume characteristic in the 200 East Area is that the highest two concentration contours (10 and 100 ppt) cover essentially the entirety of the 200 East Area. This demonstrates that the details concerning the individual plume contributions may be lost for multiple emissions cases, and that the combination of multiple emissions results in a broad plume with a relatively uniform concentration across the area. These results present 30-minute averaged concentrations, so instantaneous concentrations are expected to be higher in certain locations.

Based on modeling results, it appears that, with multiple emissions sources, upwind transport may result in low concentrations at the 285-A building. Figure 4.8 shows an aerial map with the 285-A building identified, along with the AN, AW, and AP Stack locations. As described in Section 4.1.2, the event investigation report identified the sanitary tanks, which were serviced earlier that day, as the potential source of odors noted on June 13, 2017. These tanks were located at several buildings northwest of the 285-A building, in the vicinity of the text identifying these locations in Figure 4.8. Based on wind conditions, this appears to be a reasonable source of the odors identified on this date.

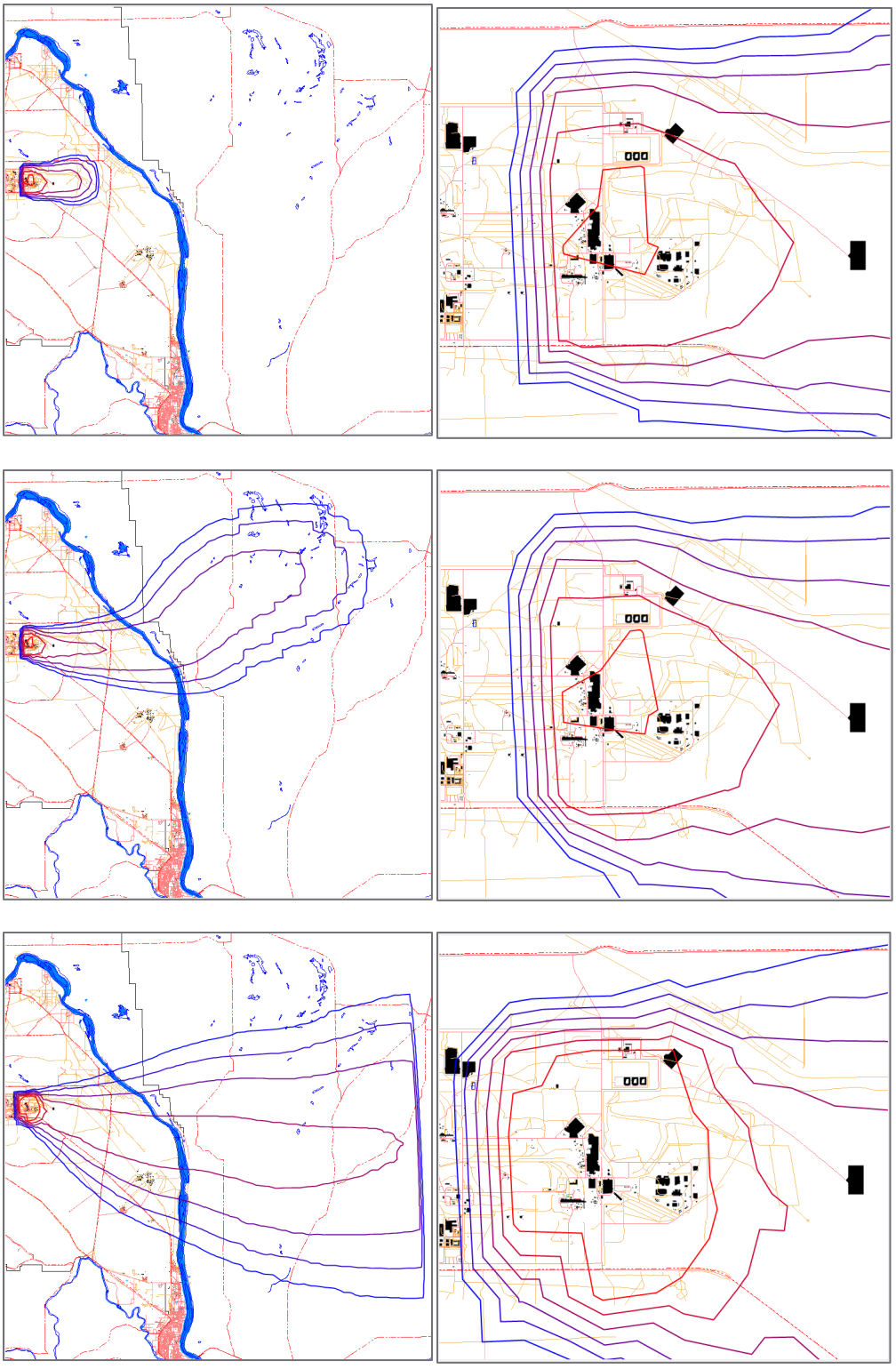

Figure 4.7. Ammonia Volumetric Concentration Contours at 7:00 (top panel), 8:30 (middle panel), and 10:30 (bottom panel) on June 13, 2017 from the AP, AW, and AN Stacks. Contour levels shown range from 1 ppq to 100 ppt. The overall plume view is shown in the left panels, while the area around 200 East Area is shown in the right panels.

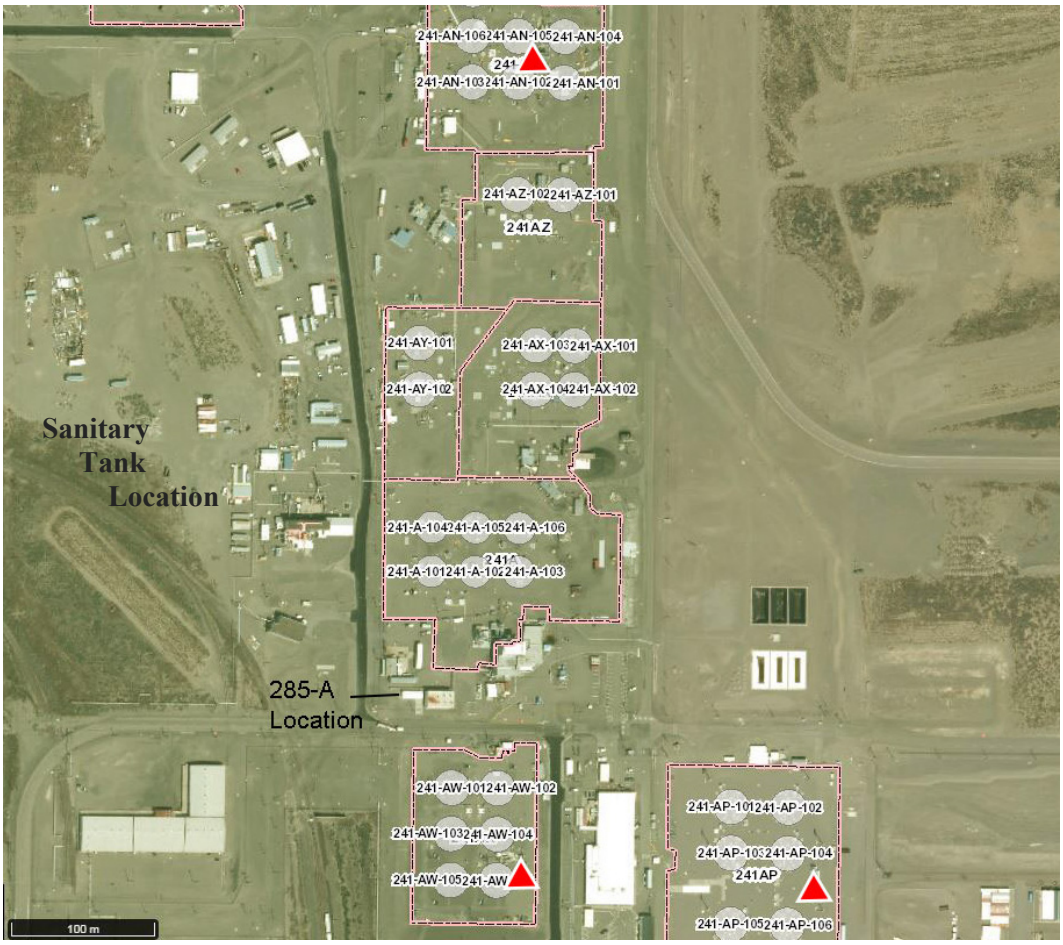

Figure 4.8. AN, AW, and AP Stack Locations Relative to the 285-A Building, Where an AOP-015 was Reported on June 13, 2017

4.3 242-A Evaporator, AP, AW, AN, AY/AZ Stacks

During the course of the project, WRPS proposed an additional set of case studies be conducted to investigate APGEMS-TF concentrations in comparison to data collected by the RJ Lee Picarro gas analyzer. For these cases, a sampling system was located at a position, unknown to the modeling team, that was typically downwind of the tank farms. The ammonia concentrations measured at this location, denoted as Site 4A, are listed in Table 4.3.

Table 4.3. Ammonia Measurements from the Picarro at Site 4A

Time and Date of Measurement	Ammonia Concentration at Site 4A
9:00 PM July 24, 2017	85 ppb
5:00 AM August 4, 2017	35 ppb
4:00 AM August 14, 2017	8 ppb
4:00 AM August 23, 2017	35 ppb

The approach taken in evaluating these data was to simultaneously model emissions from the stacks that are prepopulated within APGEMS-TF: the 242-A Evaporator, AP, AW, AN, and AY/AZ Stacks for each

of the periods listed in Table 4.3. To observe any impacts of meteorological variability, each period included a constant, continuous emission that began 1 hour before the time listed in the table, and continued through the subsequent hour after the listed time. The time stamp in Table 4.3 represents the start of the hour-long averaging period of the measurement at Site 4A.

Wind data from the nearby HMN Station 6 location for each of these dates are presented in Figure 4.9. A common trait among all four of the Picarro test periods is that the wind direction was primarily out of the west, indicating a likely measurement location to the east of the 200 East Area sources. The highest wind speed (approximately 10 mph) observed was on August 14, 2017; this indicates that the background-level concentrations measured on this date may be due to dilution. The subsequent sections will present plume estimates from each of these Picarro measurement dates. Note that the background ammonia concentration has not been removed from the measurements, so the models should be compared with concentrations that are 7 to 10 ppb lower than the measured value to account for the background concentration in this area.

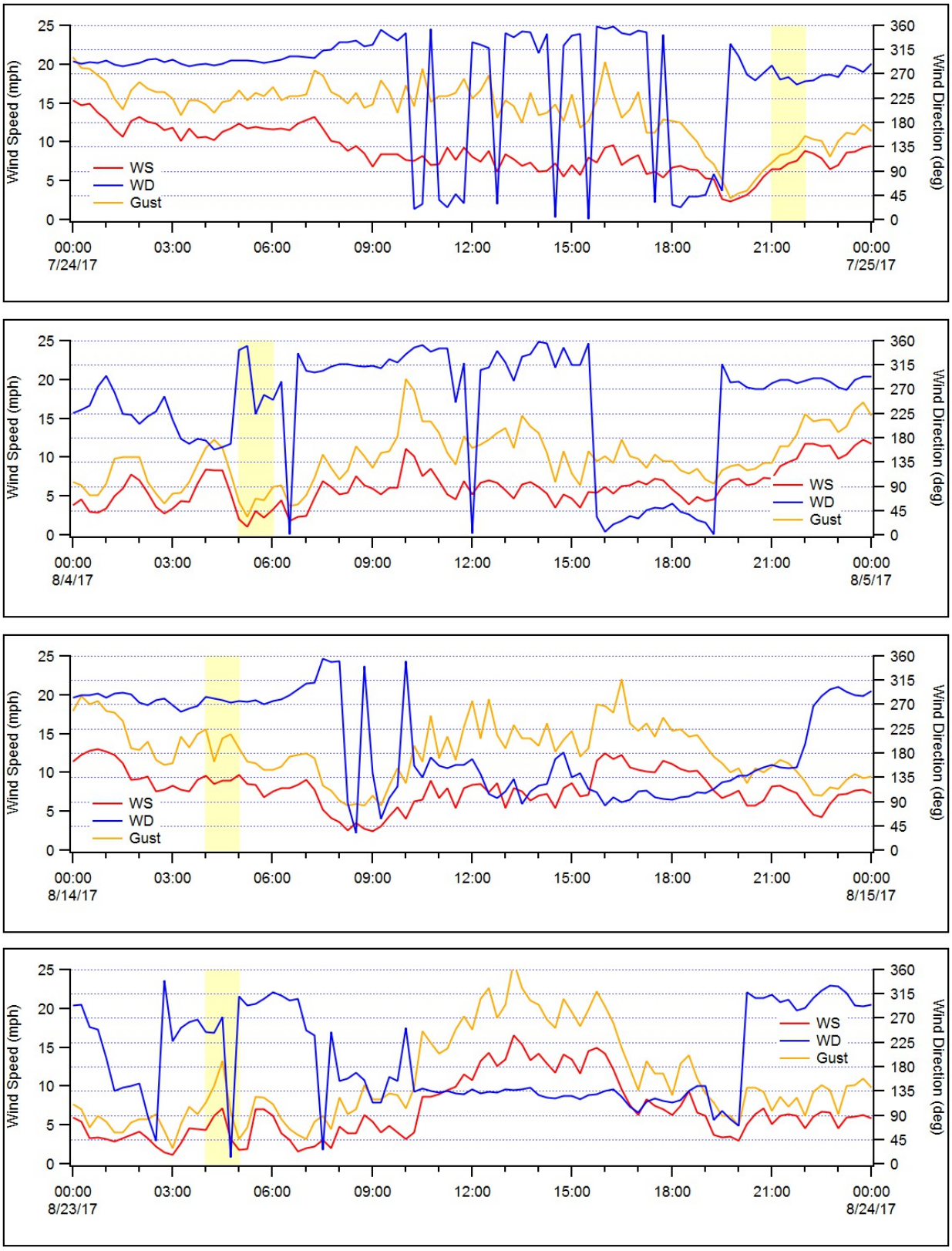

Figure 4.9. Wind Speed, Wind Gust, and Wind Direction at the HMN 200 East Station (#6) for the Four Selected Picarro Ammonia Measurement Dates

4.3.1 July 24, 2017 Ammonia Case

The ammonia volumetric concentration contours for the 9:30 PM and 10:00 PM model time periods are presented in Figure 4.10. Taken together, these two time periods represent the hour-long period from 9:00 PM to 10:00 PM. The highest concentration contour level is 1 ppb for the 9:30 period, and 10 ppb (with a very small contour) for the 10:00 period. This indicates that the APGEMS-TF model is underestimating the plume concentration relative to the measurement of 85 ppb, either as a result of dispersion or an underestimate of the source term. Based on the highest concentration regions from this simulation, the Picarro measurements were likely to the east of the Hanford Waste Treatment and Immobilization Plant (located within the cluster of buildings located to the east of the tank farms).

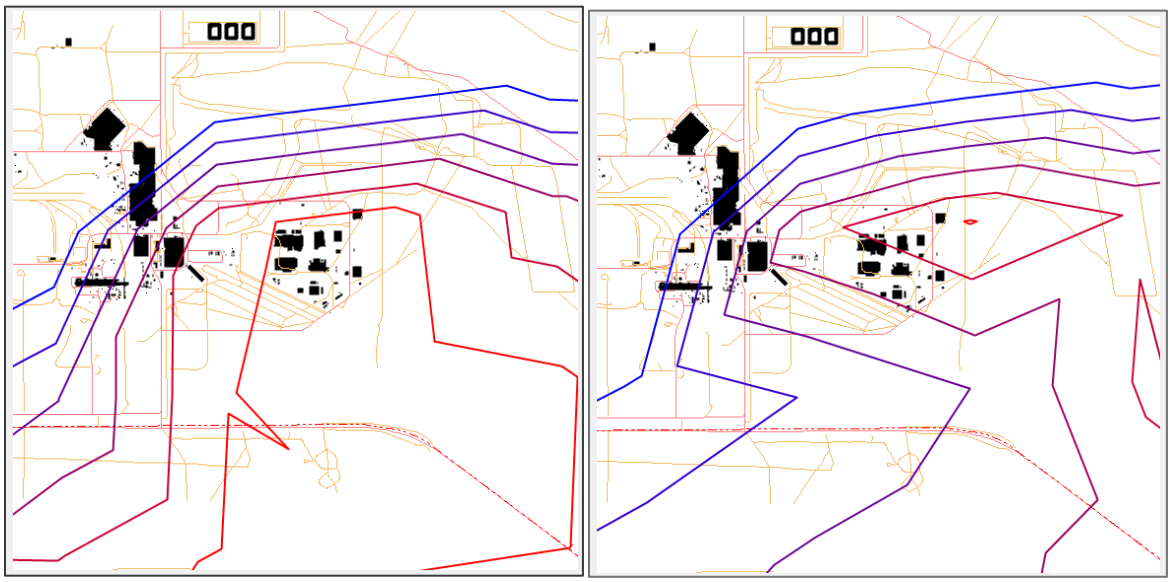

Figure 4.10. Ammonia Volumetric Concentration Contours at 9:30 PM (left panel) and 10:00 PM (right panel) on July 24, 2017. Contour levels shown range from 10 ppq to 1 ppb on the left panel, and 100 ppq to 10 ppb on the right panel.

4.3.2 August 4, 2017 Ammonia Case

The ammonia volumetric concentration contours for the 5:30 AM and 6:00 AM model time periods are presented in Figure 4.11. Note that the simulation was started at 5:00 AM, rather than an hour prior, as was done for other simulations, due to missing meteorological data during the 4:00 to 5:00 hour. This simulation start time likely contributes to a more boxy and somewhat smaller plume for the 5:30 AM period. The highest concentration contour level is 1 ppb for the 5:30 AM period, and 10 ppb for the 6:00 AM period. As was the case with the July 24 period, this indicates that the APGEMS-TF model is underestimating the plume concentration relative to the 35 ppb measurement. The highest concentrations for this simulation are generally within the 200 East Area tank farms (with some east-west width) and to the north. Based on this simulation, the Picarro measurements may have been to the north or east of the A corridor tank farms.

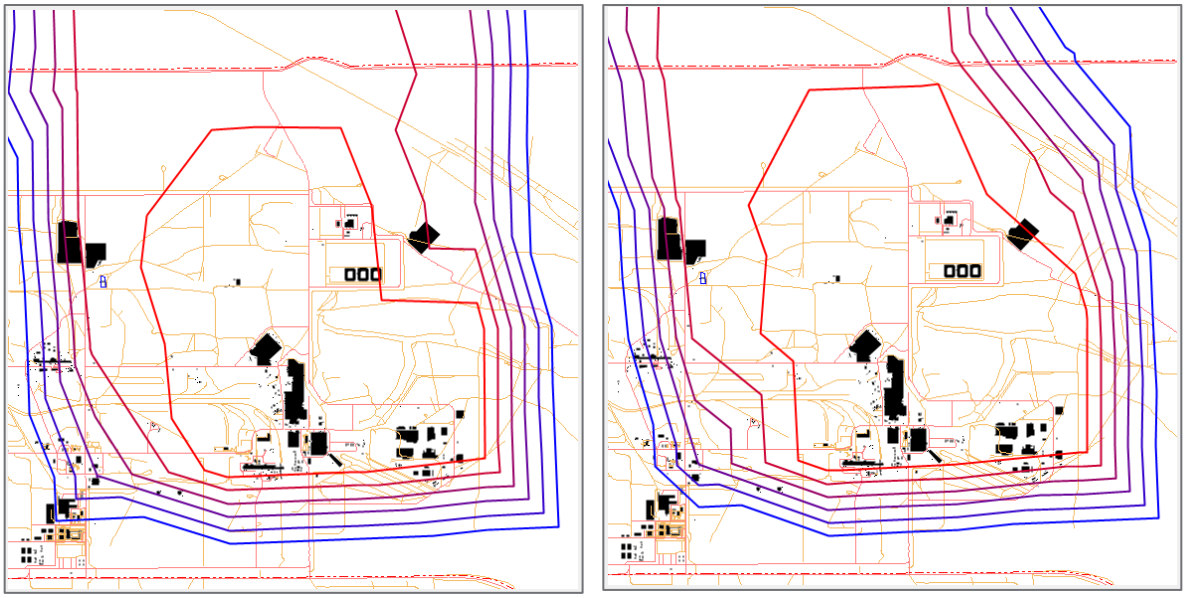

Figure 4.11. Ammonia Volumetric Concentration Contours at 5:30 AM (left panel) and 6:00 AM (right panel) on August 4, 2017. Contour levels shown range from 100 ppq to 10 ppb on the left panel, and 100 ppq to 10 ppb on the right panel.

4.3.3 August 14, 2017 Ammonia Case

The ammonia volumetric concentration contours for the 4:30 AM and 5:00 AM model time periods are presented in Figure 4.12. The highest concentration contour level is 10 ppb for the 4:30 AM period and 1 ppb for the 5:30 AM period. In this case, the Picarro measurement was a background concentration of 8 ppb, so the measurement location may have been outside of the highest concentrate contour location. Based on primarily the 4:30 AM simulation result, the Picarro measurement location may have been to the northeast or east of the 200 East Area tank farms.

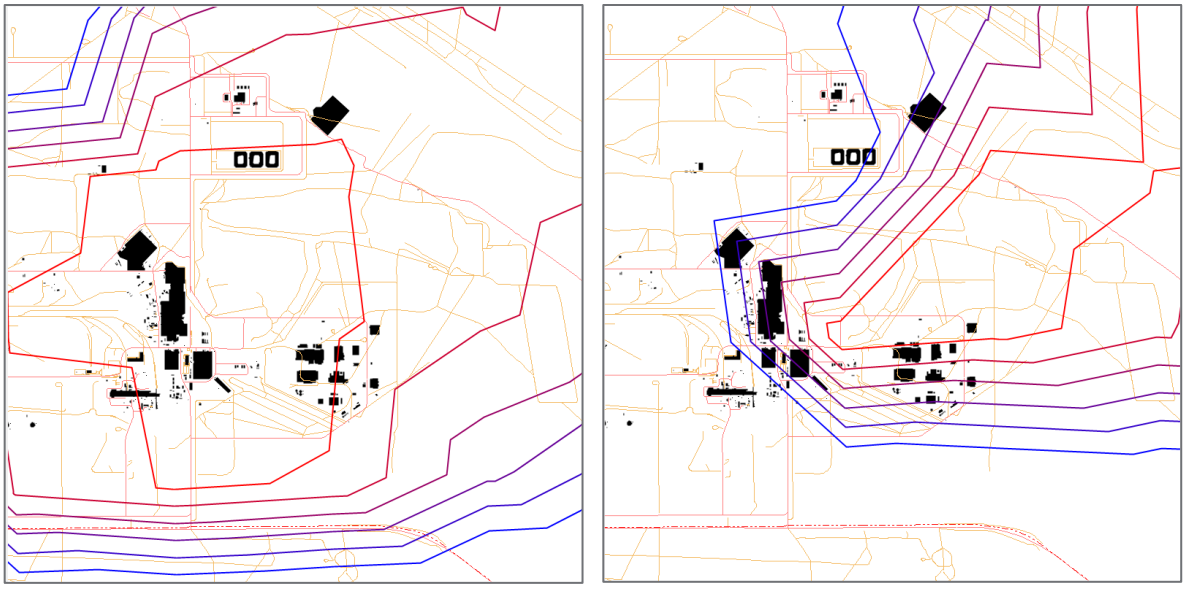

Figure 4.12. Ammonia Volumetric Concentration Contours at 4:30 AM (left panel) and 5:00 AM (right panel) on August 14, 2017. Contour levels shown range from 100 ppq to 10 ppb in the left panel, and 10 ppq to 1 ppb in the right panel.

4.3.4 August 23, 2017 Ammonia Case

The ammonia volumetric concentration contours for the 4:30 AM and 5:00 AM model time periods are presented in Figure 4.13. The highest concentration contour level is 10 ppb for each of the time periods presented, in comparison to the 35 ppb Picarro measurement. As was seen in the other time periods, this indicates that the APGEMS-TF model is underestimating the concentration of the plume relative to the measurements, primarily due either to excess diffusion or underestimated emission rates. Based on this simulation, the Picarro measurement location is estimated to be to the northeast or east of the 200 East Area tank farms.

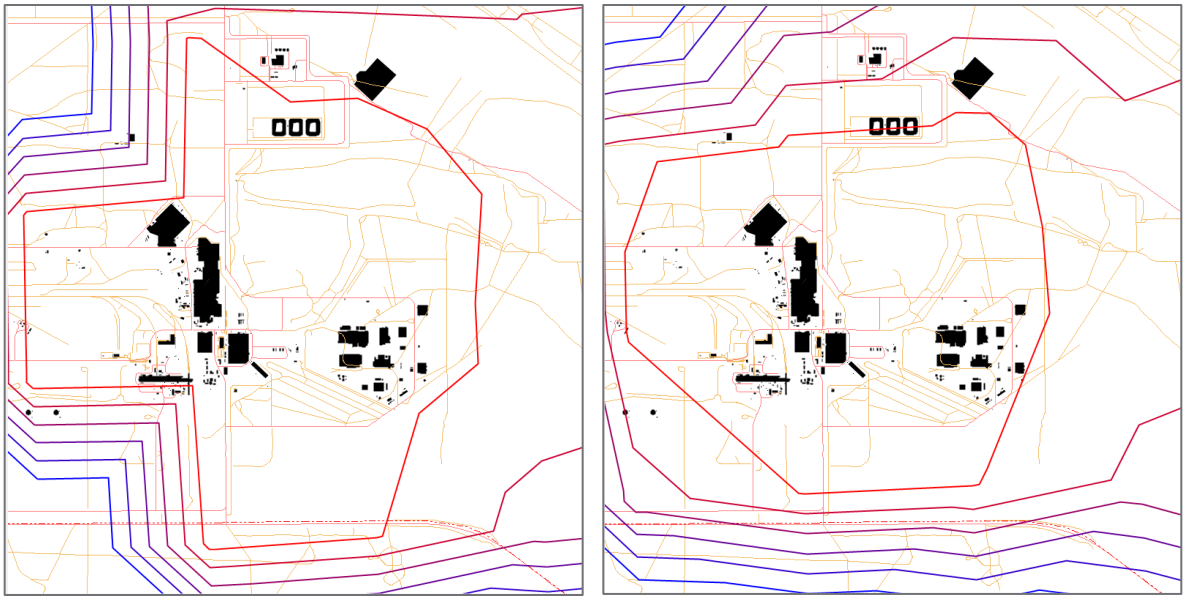

Figure 4.13. Ammonia Volumetric Concentration Contours at 4:30 AM (left panel) and 5:00 AM (right panel) on August 23, 2017. Contour levels shown range from 100 ppq to 10 ppb.

4.3.5 Speculated Location of Site 4A

The four simulations of Picarro ammonia measurement periods for the "blind" modeling exercise described above point to measurement locations that may have been to the north, northeast, and east of the 200 East tank farms. The background measurement date, August 14, 2017 provides a contrast to the other cases to indicate areas where concentrations may have been too high to be a candidate for the measurement location. Combining the simulations themselves, as well as the meteorological data from the nearby 200 East HMN Station, we conclude that the Picarro measurement location, Site 4A, was most likely within the bounds of the figures presented in this section, and to the east of the Hanford Waste Treatment and Immobilization Plant, most likely off of one of the nearby roads that are east or immediately northeast of that facility. After the blind model runs were performed, the model team was informed that the measurements were made along the east fence to the Waste Treatment and Immobilization Plant, which was within the area identified by the model team as the potential measurement location.

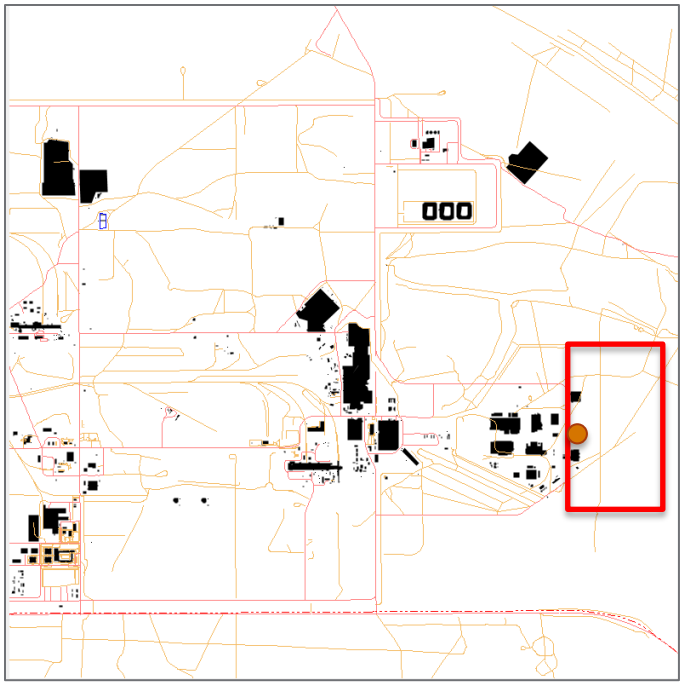

Figure 4.14. Speculated Location (red rectangle) of the Site 4A Picarro Ammonia Measurement Site, along with the Actual Measurement Site (orange marker)

5.0 Model Summary and Future Development

The APGEMS-TF model was developed during fiscal year 2018 to address specific requirements for dispersion model use in the Hanford tank farms. The original APGEMS model, which was designed for radiological emissions, was restructured to treat chemical emissions from one or more emission points. The core elements of the model, such as the meteorological pre-processor and puff model itself, were not altered under this project. Instead, existing model outputs have been adapted to produce results that are customized for tank farms users. This includes the presentation of concentration contours in units of ppm/ppb/ppt, as well as concentration contours expressed as a fraction of the OEL for each chemical.

The model runs with time steps as small as 15 minutes, with a default value of 30 minutes. The model is currently structured to use the HMN data, which delivers 15 min averaged values of variables such as wind speed, wind direction, temperature, dew point, and pressure. In-farm meteorological data (e.g., the Coastal meteorological station or the Lufft meteorological station, deployed by WRPS) are not currently incorporated for model use because the equipment are not operational at this time. When data are available, WRPS will produce 15 min averages of the necessary meteorological variables to append to the Hanford-provided telemetry file, and PNNL will modify the XML file to allow the model to recognize these additional stations.

The performance of the puff model itself is accepted as a reasonable approximation of the plume position and concentration at distances beyond 100 m. The model is employed at the Hanford EOC to respond to radiological emission events on the Hanford Site, and is part of the DOE SCAPA CAM Toolbox.[1] Since this model has been developed for use as an emergency response model, it is designed to balance the need to have sufficient detail to plan an appropriate response to an event, against the need to provide a solution quickly so that appropriate responses may be employed without delay. For any single emission scenario, the model produces output within several seconds. However, with the inclusion of multiple emission sources, each with multiple chemical emissions, the model run-time will increase.

The APGEMS-TF model includes a prepopulated list of emission positions within the 200 East Area of the Hanford Site, along with chemical emission rate estimates for those positions for a selected list of chemicals for each location. This is meant to allow users to quickly set up a model simulation with relatively conservative emission rates. Each chemical emission is defined with an emission rate in units of g/s. Future model development activities under consideration for APGEMS-TF include automatic and time-varying definition of emission rates based on stack monitoring data collected from spectroscopic measurement equipment, which is expected to be deployed on stacks within the 200 East Area.

Test cases described in this report demonstrate the capabilities and limitations of the APGEMS-TF version 1.0 model. The model is an appropriate tool for modeling chemical emissions within and around the tank farms, although the current version exhibits unrealistically large plumes in the nearest several kilometers of the sources when multiple emission points are modeled, which is a result of the relatively coarse grid employed to combine the multiple emission results. This model result will be resolved with the development of APGEMS-TF version 1.1, to be released in FY18. Some screen shots or file naming conventions presented in this document will be different in APGEMS-TF version 1.1 as a result of further development activities.

Additional development activities that are considered for the APGEMS-TF model include the capability to use forecast data, rather than real-time site measurement data, as well as regular, automatic simulations

[1] The Subcommittee on Consequence Assessment and Protective Actions is to be restructured, and will consolidated under a newly established Subcommittee on Technical Analysis and Response Support (STARS).

using either the most recent meteorological data or a combination of recent meteorological data with the forecast data for the current day. These activities, if pursued, are expected to occur during fiscal year 2019. In addition, a web tool is envisioned to allow users to use the model through a web interface, potentially using the real-time stack monitor data, meteorological data, and forecast data.

6.0 References

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Appendix A

List of Chemicals of Potential Concern

Appendix A

List of Chemicals of Potential Concern

The Air Pollutant Graphical Environmental Modeling System-Tank Farms (APGEMS-TF) model contains a chemical database for users to select in establishing user-defined emissions. The database contains the latest list of 61 chemicals of potential concern (see Table A.1).

Table A.1. Chemicals of Potential Concern that Are Included in APGEMS-TF (from Way, 2017)

Nr	Agent	CAS #	OEL	Units	MW
Inorganic Compounds					
1	Ammonia	7664-41-7	25	ppm	17.0306
2	Nitrous oxide	10024-97-2	50	ppm	44.0127
3	Mercury	7439-97-6	25	ug/m^3	200.59
Hydrocarbons					
4	1,3-Butadiene	106-99-0	1	ppm	54.0924
5	Benzene	71-43-2	0.5	ppm	78.1147
6	Biphenyl	92-52-4	0.2	ppm	154.2135
Alcohols					
7	1-Butanol	71-36-3	20	ppm	74.1237
8	Methanol	67-56-1	200	ppm	32.0424
Ketones					
9	2-Hexanone	591-78-6	5	ppm	100.1619
10	3-Methyl-3-butene-2-one	814-78-8	0.02	ppm	84.1189
11	4-Methyl-2-hexanone	105-42-0	0.5	ppm	114.189
12	6-Methyl-2-heptanone	928-68-7	8	ppm	128.2161
13	3-Buten-2-one	78-94-4	0.2	ppm	70.0918
Aldehydes					
14	Formaldehyde	50-00-0	0.3	ppm	30.0264
15	Acetaldehyde	75-07-0	25	ppm	44.0535
16	Butanal	123-72-8	25	ppm	72.1077
17	2-Methyl-2-butenal	1115-11-3	0.03	ppm	84.1189
18	2-Ethyl-hex-2-enal	645-62-5	0.1	ppm	126.2001
19	2-Propenal	107-02-8	0.1	ppm	56.0647
Furans and Substituted Furans					
20	Furan	110-00-9	1	ppb	68.0758
21	2,3-Dihydrofuran	1191-99-7	1	ppb	70.0918
22	2,5-Dihydrofuran	1708-29-8	1	ppb	70.0918
23	2-Methylfuran	534-22-5	1	ppb	82.1029
24	2,5-Dimethylfuran	625-86-5	1	ppb	96.13
25	2-Ethyl-5-methylfuran	1703-52-2	1	ppb	110.1571
26	4-(1-Methylpropyl)-2,3-dihydrofuran	34379-54-9	1	ppb	126.2001
27	3-(1,1-Dimethylethyl)-2,3-dihydrofuran	34314-82-4	1	ppb	126.2001

Table A.1 (cont'd)

Nr	Agent	CAS #	OEL	Units	MW
28	2-Pentylfuran	3777-69-3	1	ppb	138.2113
29	2-Heptylfuran	3777-71-7	1	ppb	166.2655
30	2-Propylfuran	4229-91-8	1	ppb	110.1571
31	2-Octylfuran	4179-38-8	1	ppb	180.2926
32	2-(3-Oxo-3-phenylprop-1-enyl)furan	717-21-5	1	ppb	198.2234
33	2-(2-Methyl-6-oxoheptyl)furan	51595-87-0	1	ppb	194.276
Phthalates					
34	Diethyl Phthalate	84-66-2	5	mg/m^3	222.2429
Nitriles					
35	Acetonitrile	75-05-8	20	ppm	41.0529
36	Propanenitrile	107-12-0	6	ppm	55.0799
37	Butanenitrile	109-74-0	8	ppm	69.107
38	Pentanenitrile	110-59-8	6	ppm	83.1341
39	Hexanenitrile	628-73-9	6	ppm	97.1612
40	Heptanenitrile	629-08-3	6	ppm	111.1883
41	2-Methylene butanenitrile	1647-11-6	0.3	ppm	81.1182
42	2,4-Pentadienenitrile	1615-70-9	0.3	ppm	79.1023
Amines					
43	Ethylamine	75-04-7	5	ppm	45.08
Nitrosamines					
44	N-Nitrosodimethylamine	62-75-9	0.3	ppb	74.0818
45	N-Nitrosodiethylamine	55-18-5	0.1	ppb	102.14
46	N-Nitrosomethylethylamine	10595-95-6	0.3	ppb	88.11
47	N-Nitrosomorpholine	59-89-2	0.6	ppb	116.12
Organophospates and Organophosphonates					
48	Tributylphosphate	126-73-8	0.2	ppm	266.3204
49	Dibutylbutylphosphonate	78-46-6	0.007	ppm	250.3209
Halogenated Hydrocarbons					
50	Chlorinated Biphenyls	2051-60-7	1	mg/m^3	188.6585
51	2-Fluoropropene	1184-60-7	0.1	ppm	60.0717
Pyridines					
52	Pyridine	110-86-1	1	ppm	79.1023
53	2, 4-Dimethylpyridine	108-47-4	0.5	ppm	107.1564
Organonitrites					
54	Methyl nitrite	624-91-9	0.1	ppm	61.0405
55	Butyl nitrite	544-16-1	0.1	ppm	103.1218
Organonitrates					
56	Butyl nitrate	928-45-0	2.5	ppm	119.1212
57	1,4-Butanediol, dinitrate	3457-91-8	0.05	ppm	180.1181
58	2-Nitro-2-methylpropane	594-70-7	0.3	ppm	103.1218
59	1,2,3-Propanetriol, 1,3-dinitrate	623-87-0	0.05	ppm	182.0905

Table A.1 (cont'd)

Nr	Agent	CAS #	OEL	Units	MW
Isocyanates					
60	Methyl isocyanate	624-83-9	20	ppb	57.0523
Organometallic					
61	Dimethyl mercury	593-74-8	0.01	mg/m^3	230.6594

Appendix B

Emission Rates and Data Sources

Appendix B

Emission Rates and Data Sources

The emission rates that are prepopulated in the Air Pollutant Graphical Environmental Modeling System-Tank Farms (APGEMS-TF) model are listed in Table B.1. These rates were developed based on a survey of various concentration data sources, combined with stack and passive breather flow rates to develop a mass flow rate for each emission location considered. Table B.2 summarizes the data sources that were consulted for each emission location. Tank Farms Data Access and Visualization (DAV) Explorer data are also presented in Figure B.1, Figure B.2, Figure B.3, and Figure B.4.

Table B.1. Summary of Emission Rates for Emission Locations included in APGEMS-TF

Emission Location	Chemical	Emission Rate (g/s)
242-A Evaporator Stack	Ammonia	0.01
	Mercury	4.9E-6
	NDMA	3.49E-6
AP Stack	Ammonia	0.040
	Mercury	2.41E-5
	NDMA	3.71E-5
AW Stack	Ammonia	0.0165
	Furan	2.78E-6
	Mercury	1.63E-4
	NDMA	3.31E-4
	Nitrous oxide	0.059
AN Stack	Ammonia	0.0456
	Mercury	4.52E-4
	Formaldehyde	2.77E-4
	Furan	1.82E-5
	Nitrous oxide	0.0501
	Nitrosomethyethylamine	3.12E-6
	Nitrosomorpholine	1.95E-6
AY/AZ Stack	Ammonia	0.0596
	Formaldehyde	1E-5
	Furan	3.11E-6
	Mercury	0.0113
	NDMA	2.84E-6
	Nitrous oxide	0.018

Table B.1. (contd)

Emission Location	Chemical	Emission Rate (g/s)
A Farm Passive Breather Filters (PBFs)	Ammonia	5.68E-4
	Mercury	2.83E-7
	NDMA	1.04E-3
	Nitrous oxide	1.45E-7
AX Farm PBFs	Ammonia	0.0012
	2,3-dihydrofuran	5.59E-8
	Formaldehyde	8.33E-7
	Mercury	1.67E-6
	NDMA	7.19E-8
	N-Nitrosomorpholine	2.01E-7
	Nitrous oxide	4.36E-4
C Farm PBFs	Ammonia	2.49E-4
	2,3-dihydrofuran	1.1E-9
	Formaldehyde	1.89E-7
	Furan	4.95E-8
	Mercury	4.17E-7
	NDMA	1.88E-6
	Nitrosodiethylamine	2.17E-6
	Nitrosomethylethylamine	1.27E-7
	Nitrous oxide	3.46E-4

Table B.2. Summary of Data Sources Used to Develop Emission Rates

Emission Location	Chemical	VCZ Report	SWIHDS	Cartridge	DAV	Other[(a)]
242-A Evaporator Stack	Ammonia	NA	NA	NA	NA	Connor
	Mercury	NA	NA	NA	NA	Connor
	NDMA	NA	NA	NA	NA	Connor
AP Stack	Ammonia	X	NA	X	X	QRA
	Mercury	X	NA	X	X	QRA
	NDMA	X	NA	X	X	QRA
AW Stack	Ammonia	X	NA	X	X	QRA
	Furan	X	NA	X	X	QRA
	Mercury	X	NA	X	X	QRA
	NDMA	X	NA	X	X	QRA
	Nitrous Oxide	X	NA	NA	NA	NA

Table B.2. (contd)

Emission Location	Chemical	VCZ Report	SWIHDS	Cartridge	DAV	Other[(a)]
AN Stack	Ammonia	X	NA	X	X	NA
	Mercury	X	NA	X	X	NA
	Formaldehyde	X	NA	X	X	NA
	Furan	X	NA	X	X	NA
	Nitrous Oxide	X	NA	NA	NA	NA
	Nitrosomethyethylamine	X	NA	X	X	NA
	Nitrosomorpholine	X	NA	X	X	NA
AY/AZ Stack[b]	Ammonia	X	NA	X	X	NA
	Formaldehyde	X	NA	X	X	NA
	Furan	X	NA	X	X	NA
	Mercury	X	NA	X	X	NA
	NDMA	X	NA	X	X	NA
	Nitrous oxide	X	NA	NA	NA	NA
A Farm Passive Breather Filters (PBFs)	Ammonia	X	X	X	X	QRA
	Mercury	X	X	X	X	QRA
	NDMA	X	X	X	X	QRA
	Nitrous oxide	X	NA	NA	NA	QRA
AX Farm PBFs	Ammonia	X	X	X	X	NA
	2,3-dihydrofuran	X	NA	X	NA	NA
	Formaldehyde	X	X	X	X	NA
	Mercury	X	X	X	X	NA
	NDMA	X	X	X	X	NA
	N-Nitrosomorpholine	X	X	X	X	NA
	Nitrous oxide	X	NA	NA	X	NA
C Farm PBFs	Ammonia	X	NA	NA	X	NA
	2,3-dihydrofuran	X	NA	NA	X	NA
	Formaldehyde	X	NA	NA	X	NA
	Furan	X	NA	NA	X	NA
	Mercury	X	NA	NA	X	NA
	NDMA	X	NA	NA	X	NA
	Nitrosodiethylamine	X	NA	NA	X	NA
	Nitrosomethylethylamine	X	NA	NA	X	NA
	Nitrous oxide	X	NA	NA	NA	NA

(a) Other data sources include the Connor (2005) report as well as the Quantitative Risk Assessment (QRA) documents (Kenexis. 2017a, 2017b , 2017c).

(b) Separate data sources for AY and AZ concentrations were available, and the maximum between the two (when differences occurred).

VCZ = Vapor Control Zone; SWIHDS = Site Wide Industrial Hygiene Database System; Cartridge = cartridge testing data; DAV = Data Access and Visualization site (WRPS, 2018); NA = data not available under the given category.

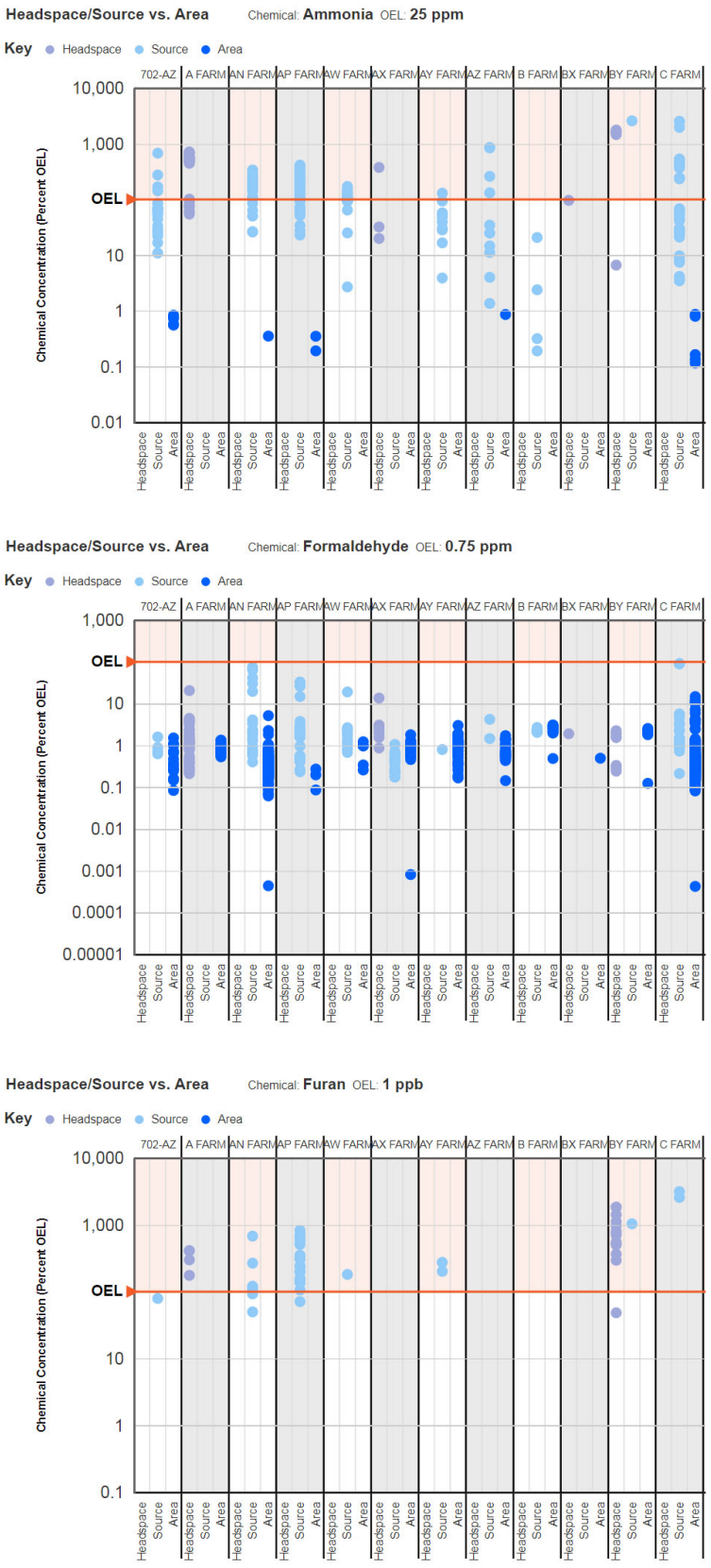

Figure B.1. DAV Summary Plots for Ammonia, Formaldehyde, and Furan (WRPS, 2018)

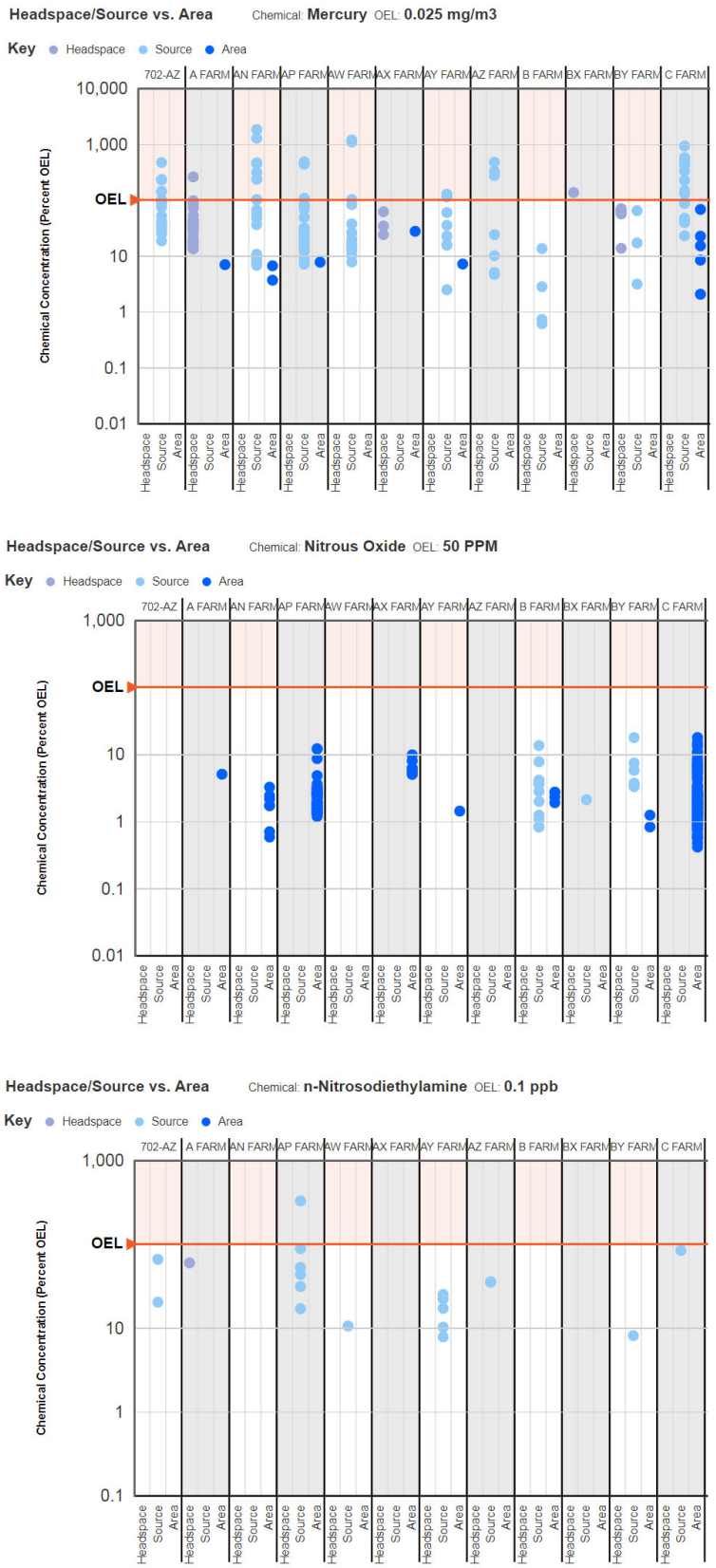

Figure B.2. DAV Summary Plots for Mercury, Nitrous Oxide, and n-Nitrosodiethylamine (WRPS, 2018)

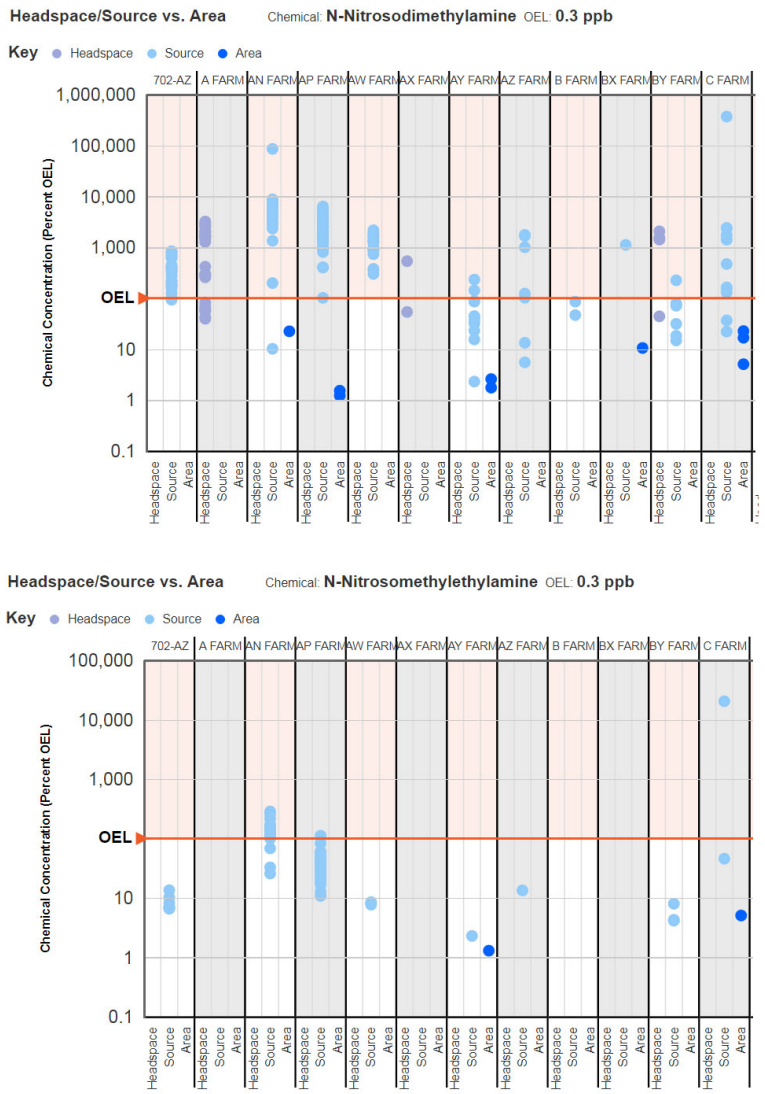

Figure B.3. DAV Summary Plots for n-Nitrosodimethylamine, and n-Nitrosodimethyethylamine (WRPS, 2018)

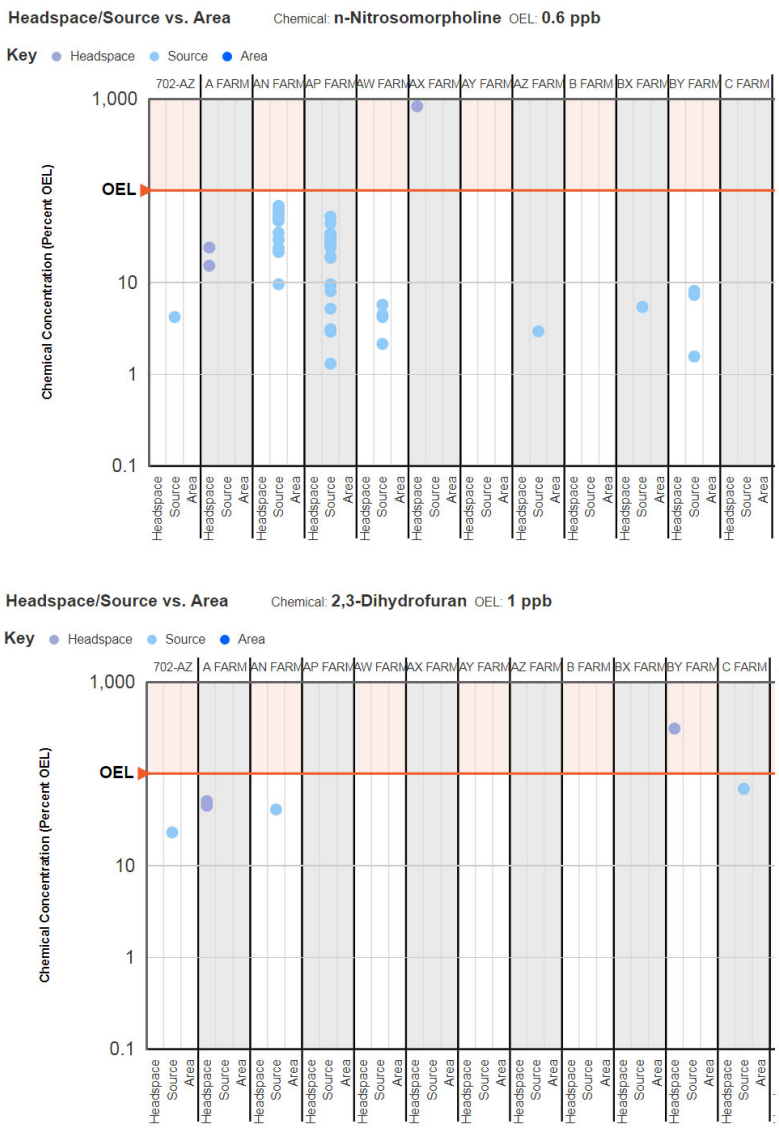

Figure B.4. DAV Summary Plots for n-Nitrosomorpholine, and 2,3-Dihydrofuran (WRPS, 2018)

Appendix C

Quick Launch Guide

Appendix C

Quick Launch Guide

C.1 Installation

The Air Pollutant Graphical Environmental Modeling System-Tank Farms (APGEMS-TF) software may be installed on a Windows-based workstation that has access to the necessary meteorological data. To install the APGEMS-TF software, run the setup.exe file provided in the installation package (see Figure C.1).

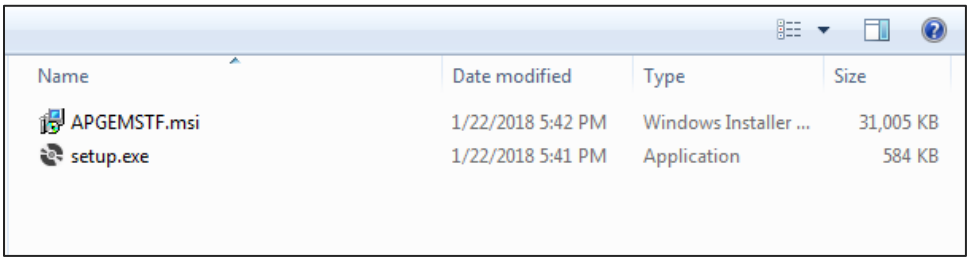

Figure C.1. Installation Files for APGEMS-TF

C.2 Starting APGEMS-TF

To launch the APGEMS-TF software, navigate to the Windows Start Menu to view "All Programs." A new folder called "APGEMS TF" will be listed, and within that folder, an application called "APGEMS for Tank Farms" will be included. Alternatively, a desktop shortcut called "APGEMS for Tank Farms" is available. Clicking on the icon/text will launch the software.

C.3 Model Display Elements

When APGEMS-TF is launched, the Main Menu (Figure C.2) screen is opened on the workstation. This screen allows users to access existing APGEMS-TF run files, configure the folder to read meteorological data, and perform simulation setup. The "Hide Options" button hides the items below the Menu Elements (Release Start Date, Calendar, Release Start Time, etc.). The "Help" button includes two items: "About" provides a screen with version information, and "User's Guide" provides the APGEMS v2 User's Guide. A dedicated User's Guide for APGEMS-TF has not been developed; a significant portion of the APGEMS v2 User's Guide provides information that is relevant to APGEMS-TF.

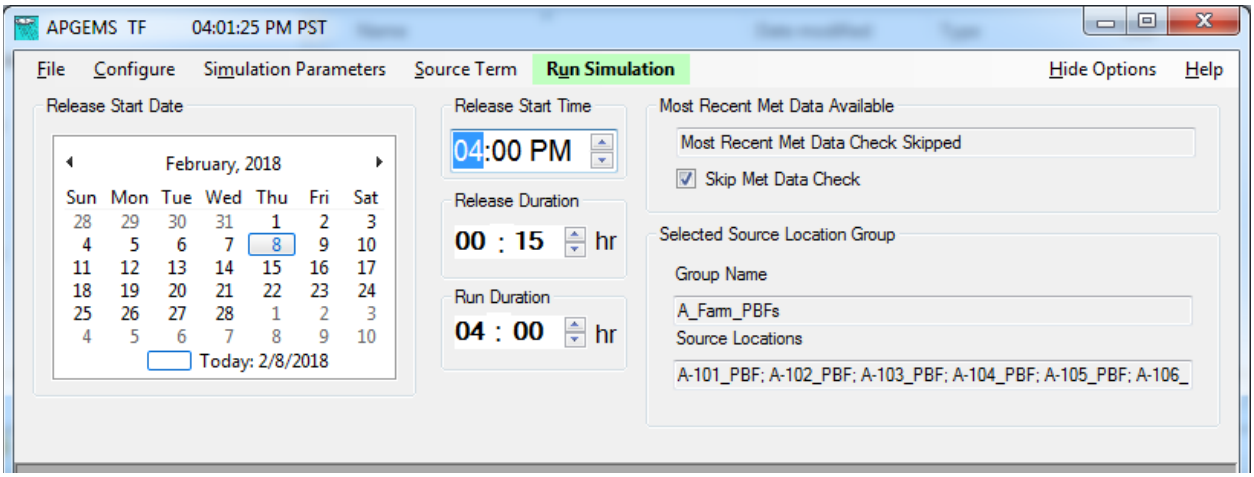

Figure C.2. APGEMS-TF Main Menu

C.3.1 Menu Elements

C.3.1.1 File

The "File" menu allows users to open an existing APGEMS-TF run file, view the error log, or exit the software.

C.3.1.2 Configure

The "Configure" menu allows users to select the directories used by APGEMS-TF, Map Properties, and Meteorological Stations. A user may wish to modify elements under the three tabs within the "Configuration" window when the software is first installed on a workstation, but no additional changes are typically made during subsequent uses of the application.

The "Directories" dialog box (Figure C.3) shows the file directories, which are prepopulated for most of the data types during APGEMS-TF installation. The "incoming real meteorological data" folder location may be verified or modified from within the "Directories" dialog box by placing the cursor within the box, clicking on "Browse," and selecting a folder location.

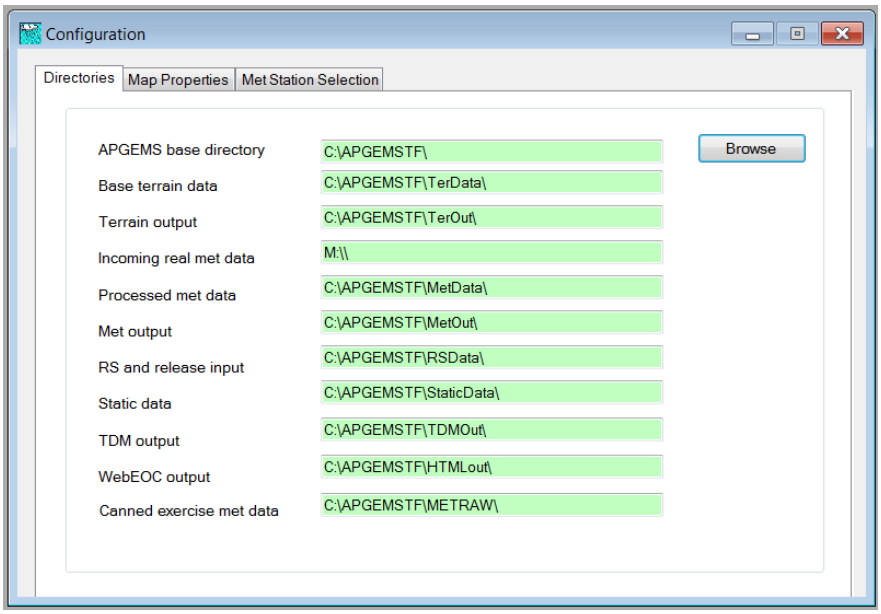

Figure C.3. APGEMS-TF Configuration Dialog Box for Directories

The "Map Properties" dialog box (Figure C.4) contains properties for the map layers that are included with the APGEMS-TF installation. Typically, these properties are not changed by the user, but some users may wish to alter colors, add layers, or remove layers.

The "Met Station Selection" dialog box (Figure C.5) contains a list of the surface meteorological stations as well as the elevated stations (tall towers) that are used by the model. If a user wishes to remove specific stations from the analysis, un-selecting specific stations from the list in this dialog box will remove them from the computation of the gridded meteorological field.

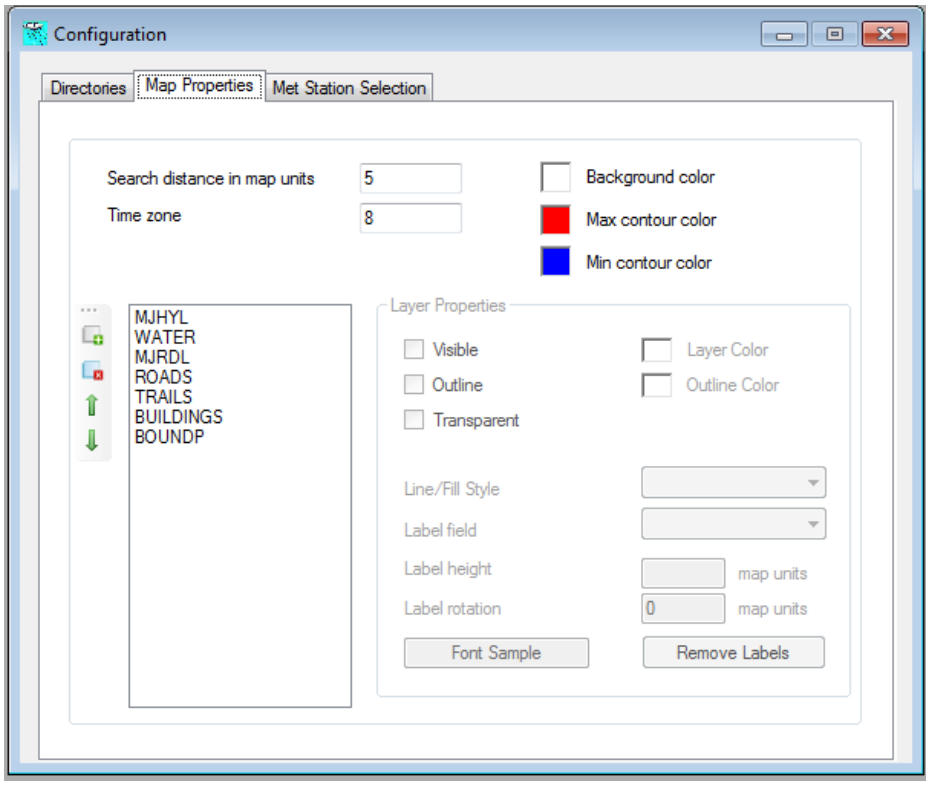

Figure C.4. APGEMS-TF Configuration Dialog Box for Map Properties

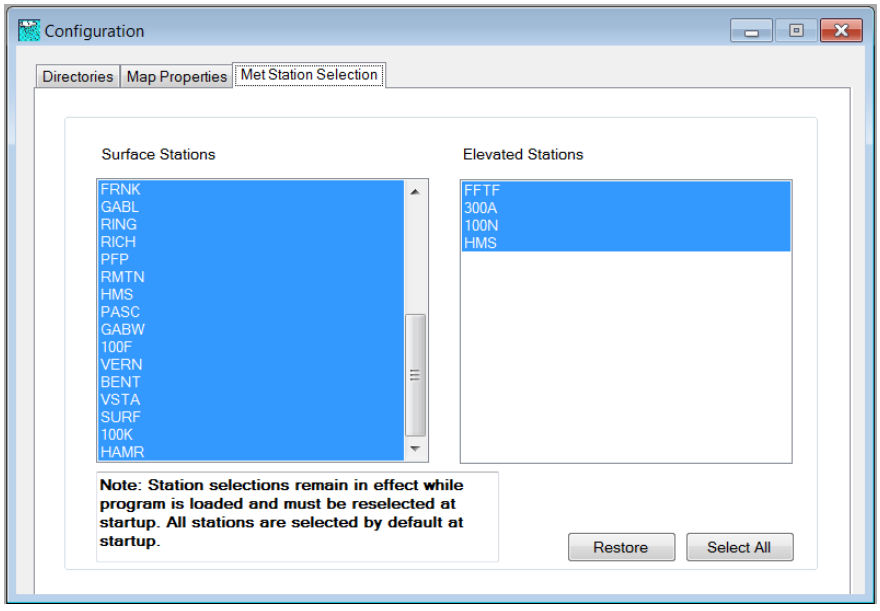

Figure C.5. APGEMS-TF Configuration Dialog Box for Met Station Selection

C.3.1.3 Simulation Parameters

The "Simulation Parameters" menu item allows users to define basic parameters concerning the simulation (Figure C.6). The "Output interval" may be defined as 15, 30, 60, or 120 minutes. The output interval defines the time difference between the start of the simulation and the subsequent output time,

and additional output times (less than the run duration). The "Inner domain size" is, by default, half of the outer domain size. A drop-down list is available to set the "Outer domain size" from 20 km to 200 km, in 20 km increments. The default value of 100 km is recommended for typical applications.

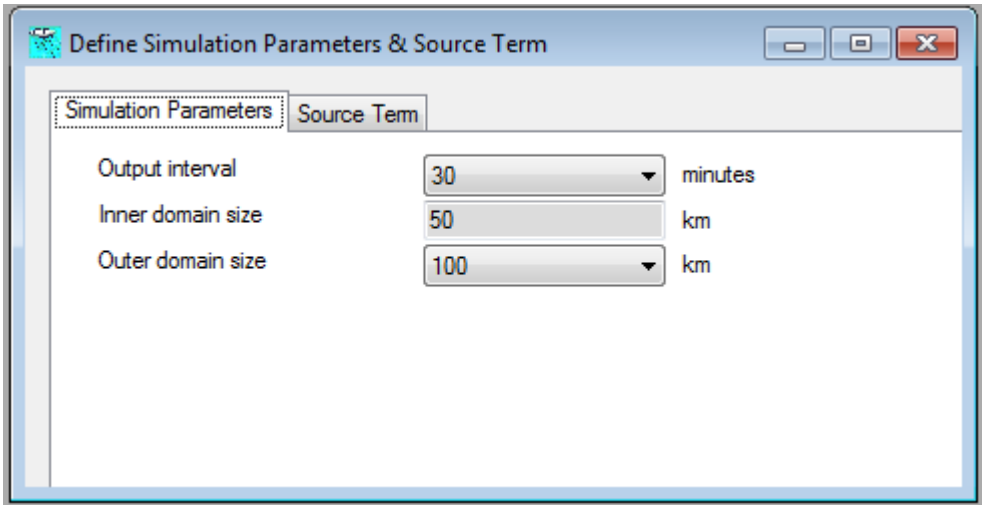

Figure C.6. APGEMS-TF Simulation Parameters Dialog Box

C.3.1.4 Source Term

The "Source Term" menu allows users to define the necessary characteristics of the source (Figure C.7). The drop-down list at the top of the window lists the name of the current "Tank Farm Source Location Group." Initially, this is populated with the first of the prepopulated groups. Either another prepopulated group may be selected from the drop-down list, or a New Source Group may be created using the button to the right of the drop-down list. A Source Group defines a group of one or more source locations to be used in the simulation.

The next box, labeled "Source Locations," is prepopulated with the source locations associated with the prepopulated source location group that is selected. However, for new user-defined source location groups, a new source location may be added by clicking the "Add Source Locations" button. This button opens up a new dialog box, as shown in Figure C.8. A list of locations is available for selection, or a user-defined location may be added by selecting the "Add Custom Location" button in the lower right-hand corner of the dialog box (Figure C.8. This opens a new window (Figure C.9) where the user may name a new release location and either select the location on the map or define State Plane northing and easting values. Selecting the "Done" button returns the user to the "Add Selected Source Location" dialog box (Figure C.8).

When one "Source Location" is highlighted in the list, release parameters for that "Source Location" may be defined in the next area of this dialog box. This includes the height of the release, the stack gas exit velocity, the stack gas exit temperature, and the stack diameter. The height of the release, along with the exit velocity and exit temperature defines the total release height for the emission. The "Save Release Parameters" button saves the values associated with the selected source location. With multiple source locations, unique source location release parameters may be specified for each location.

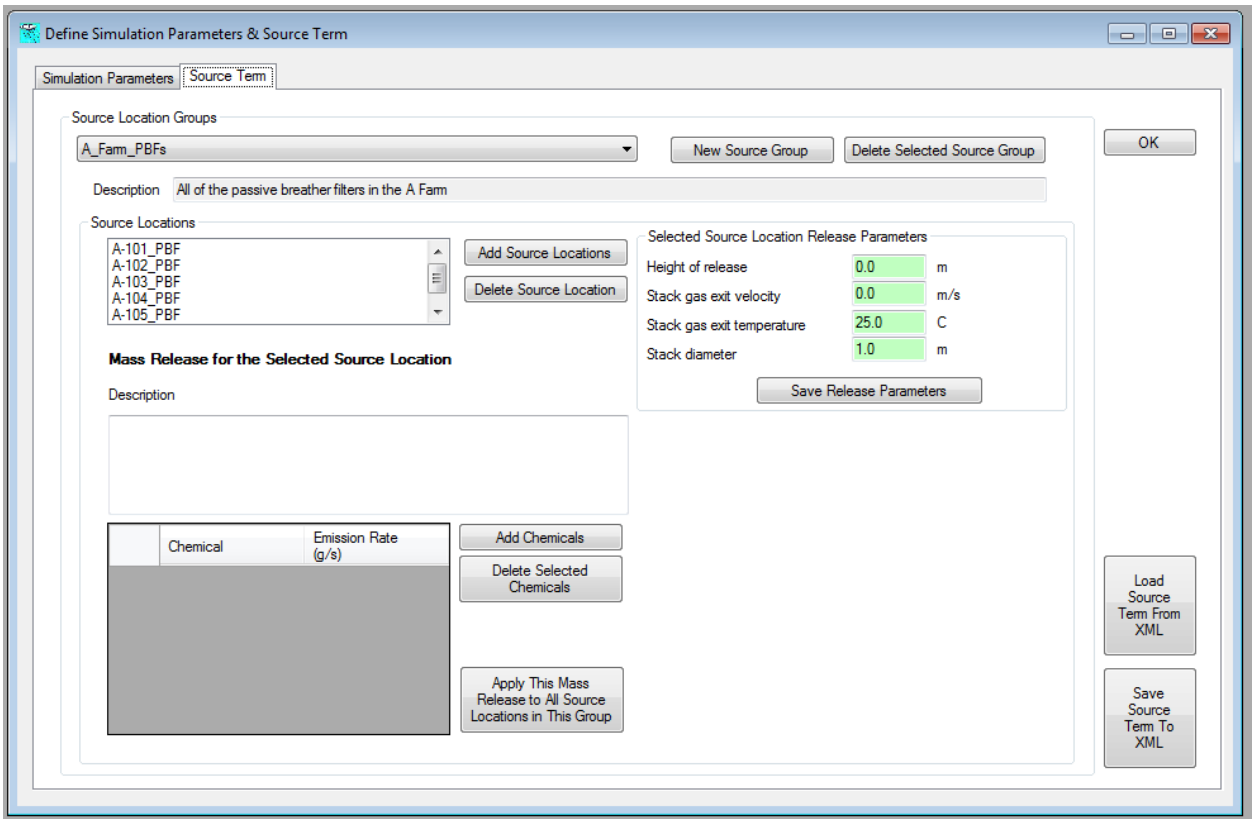

Figure C.7. APGEMS-TF Source Term Dialog Box

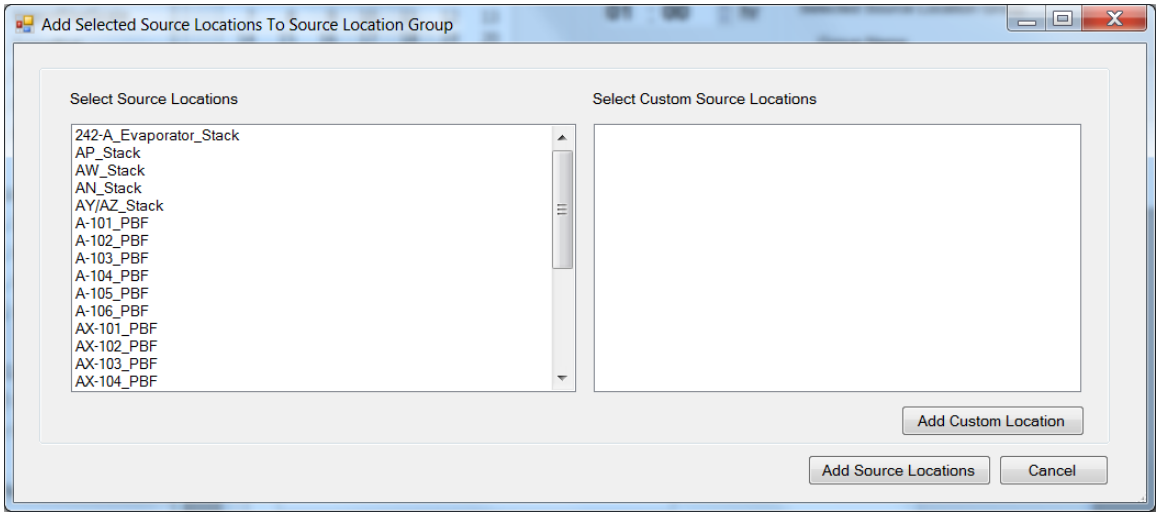

Figure C.8. APGEMS-TF Add Selected Source Location Dialog Box for Release Selection

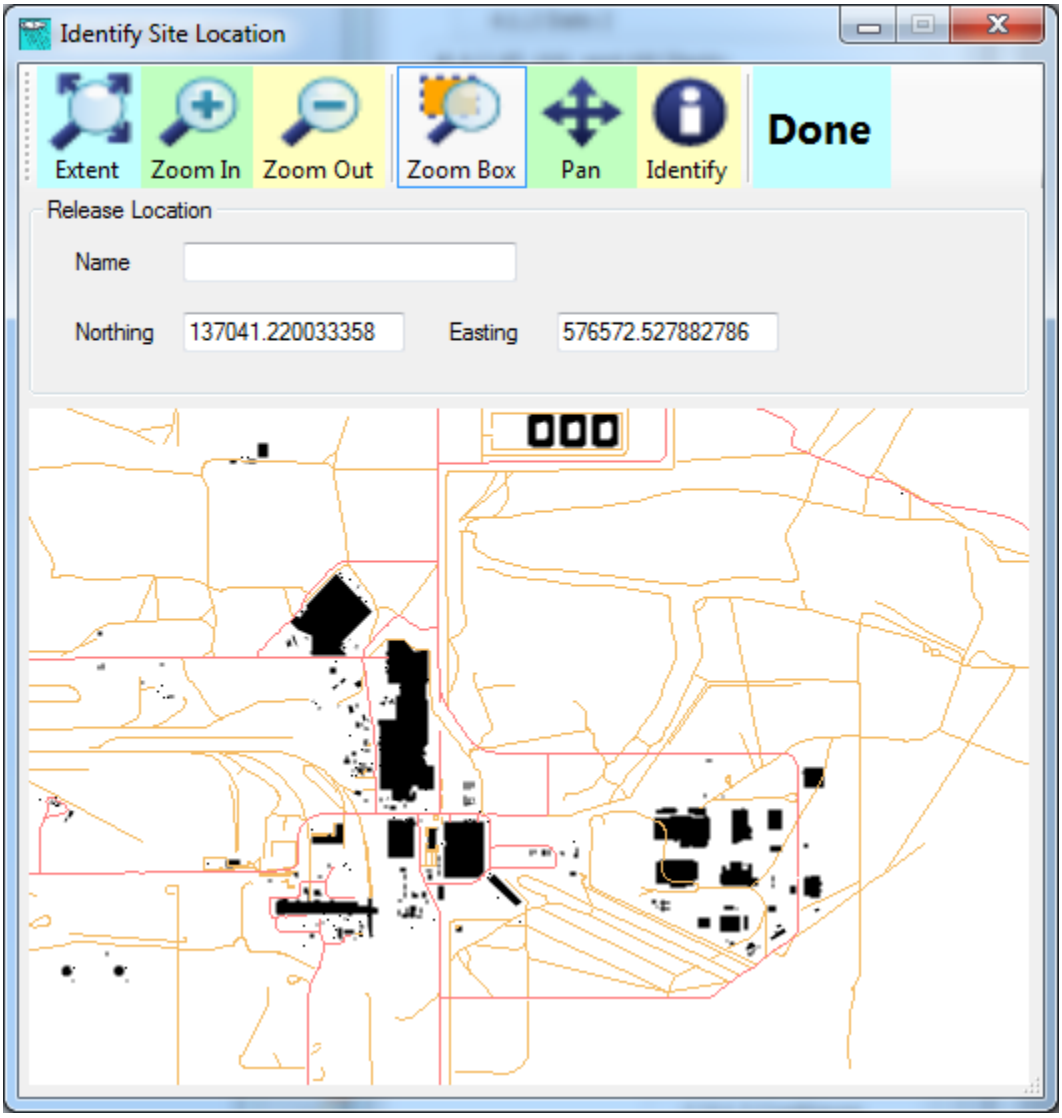

Figure C.9. APGEMS-TF Identify Site Location Dialog Box when Add Custom Location is Selected within the Add Selected Source Location Dialog Box

The final portion of the Source Term dialog box is the Mass Release for the Selected Source Location. For each Source Location selected from within the Source Location Group, a unique list of chemicals and associated emission rates may be defined. Note that, to ensure that each emission rate is saved for the current simulation, another emission rate box should be selected after the final emission rate is defined. This ensures that the software validates the user entry. As before, if a prepopulated Source Location Group with prepopulated Source Locations is selected, these mass release rates will be prepopulated with the values described in Section 2.3 and in Appendix B. If user-defined values are created, the "Save Source Term" button should be selected to save the values to the sourceterm.xml file. These variables will then be available for future simulations.

C.3.1.5 Run Simulation

The "Run Simulation" menu item does not open a dialog box; it is used to run the simulation. The result of selecting the "Run Simulation" button is described further below. Prior to selecting this button, the Release Start Date, Start Time, Duration, and Run Duration should be defined, as described below.

C.3.2 Release Start Date, Start Time, Duration, and Run Duration

The simulation release start date, release start time, release duration, and run duration are all set within the Main Menu window at the top of the user interface. To select the date for the simulation, click on the date on the calendar. To view different months, click on the small black arrows located on either side of the month and year title on the calendar. The release start time is located in the top center of the Main Menu, and may be modified either by typing into the box or using the arrows located to the right of the time box. Similarly, the release duration and run duration, which are located below the release start time, may be modified by typing into the box or using the arrows. Note that the release duration corresponds to the time over which the sources will be emitting chemicals, according to the emission rates listed in the Source Term dialog box, starting at the release start time. The run duration is the total period of time over which the model will run puff estimates, and can extend beyond the release duration period to observe dissipation of an emission that has been terminated.

C.4 Running the Model

Selecting the "Run Simulation" text (highlighted in green, Figure C.10) at the top of the Display Menu will execute the meteorological and puff models. A command-line window (Figure C.11) opens briefly while the model computations are performed, and closes when the model completes the computations successfully. The "Run Simulation" text may remain highlighted for a few seconds after the command-line window closes while the model output is processed for the graphical user interface. Typically, for a single emission location and single chemical emission, the model run-time is about 5 sec. Three emission locations with multiple chemicals at each location runs in about 30 sec.

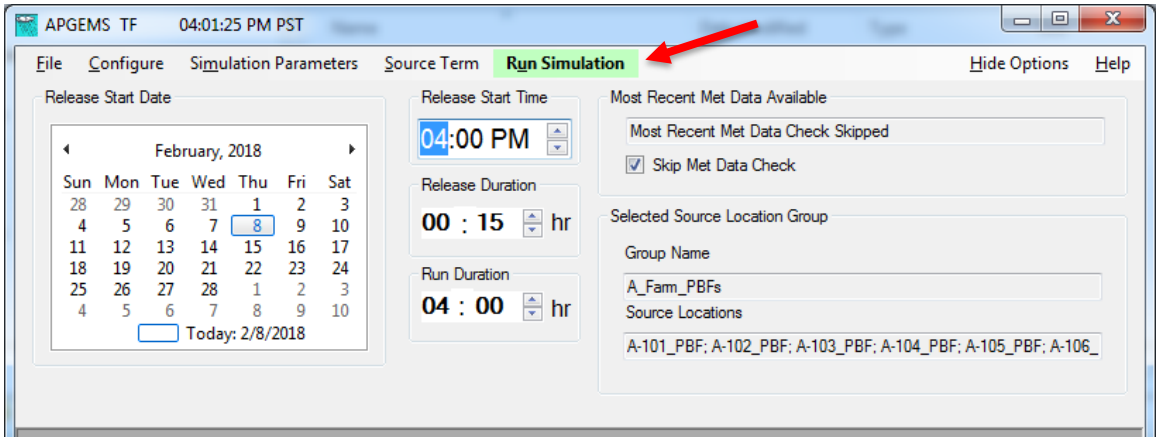

Figure C.10. Display Menu with Red Arrow to Indicate the "Run Simulation" Button

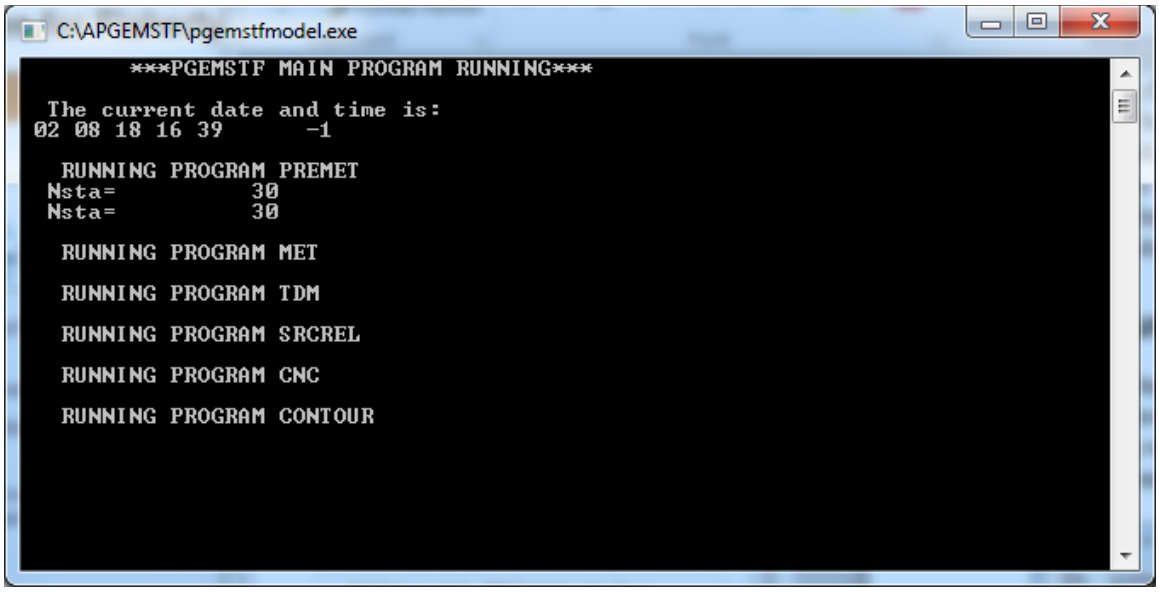

Figure C.11. Example Command-Line Window that Opens while the Model Is Being Executed

Common errors that a user is likely to encounter when running the model include an "Abnormal Termination" error or "Data Not Available" error. In the case of the abnormal program termination, additional details are needed to troubleshoot the cause, which may be found in the log (contained in APGEMSTF\logs). When data are not available for the start time of the simulation, the model will not produce an output file.

C.5 Model Output

When the model run is complete, the window will update with the plume contour result from the first time step of the simulation (Figure C.12). The default view when the contour results are first presented shows the overall map with contour levels for the first chemical modeled. A drop-down list, labeled "Contour Selection," allows users to change the contour presentation from mass per volume units (g/m^3), to either volumetric units (m^3/m^3, which also includes labels for the levels that correspond to ppm, ppb, and ppq levels), or Occupational Exposure Limit fractions. An additional drop-down list under the "Contour Selection" area contains the list of chemicals that were included in the simulation.

A separate drop-down list, labeled "Date & Time," allows users to step through each output time step. Alternatively, the "Animate" button, located near the top right of the window, may be used to automatically cycle through all of the available output time steps. When the animation is in progress, the button will change to "Stop Animation" to allow users to stop the animation. When a single output time is viewed, the contour intervals displayed may be modified by selecting or un-selecting specific contour intervals in the list. Note that some contour intervals that are selected (highlighted) may not exist in the output figure, because the highest contour level is defined by the first simulation time step, and subsequent time steps include the same list of contour intervals. The final item on the right-hand side of the output window is the contour width. The default width is 1, but typically, increasing the width to 2 allows users to distinguish the contour levels from the background features.

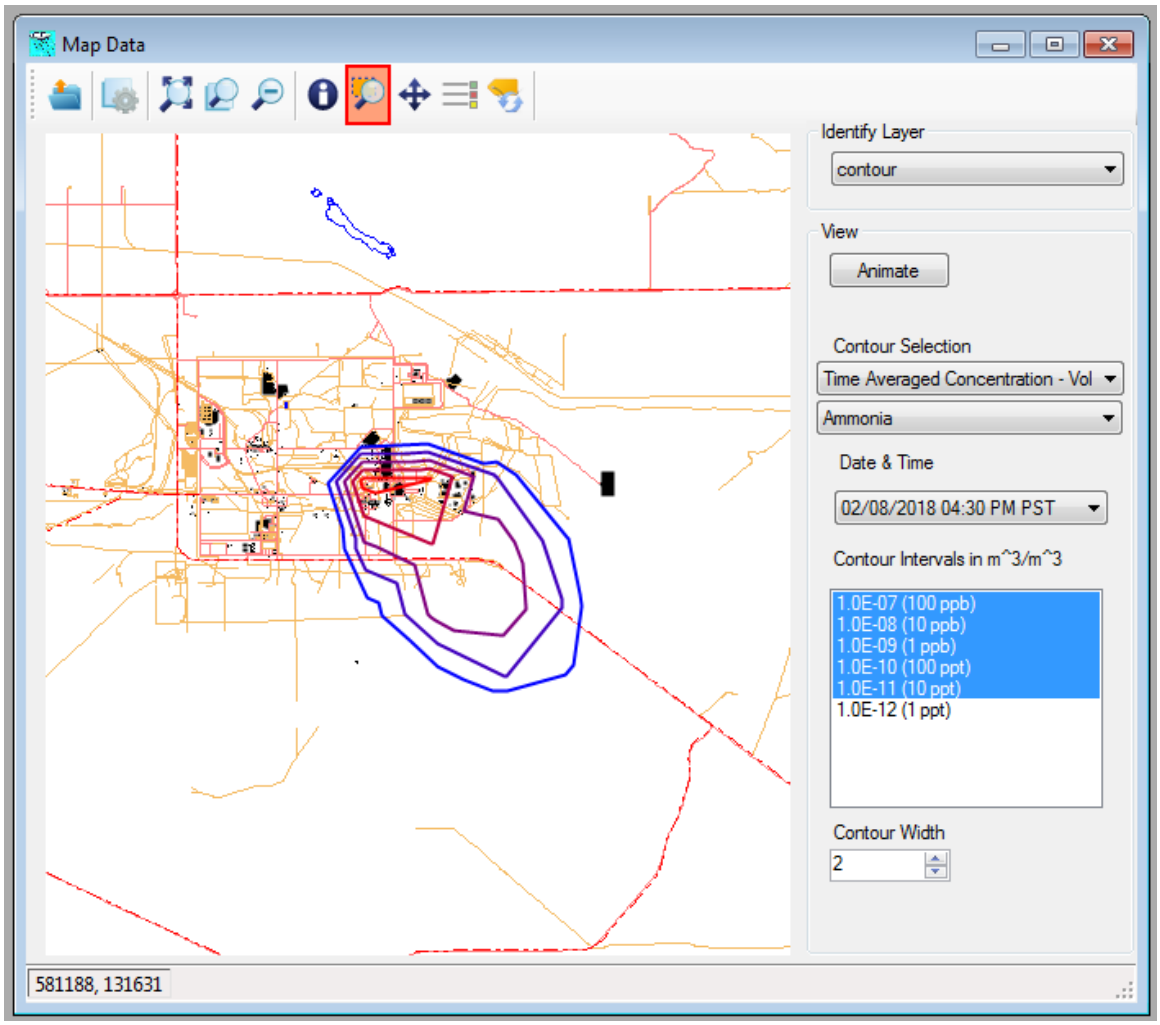

Figure C.12. Example of Model Output Results in the User Interface

The top portion of the output window contains tools to navigate the output window. The left-most icon, a folder with an arrow, is the "Open Run File" button. This opens the TFRSData folder, which allows users to open a previously performed simulation (same functionality as File\Open). The next icon, a sheet with a gear, is the "Map Properties" button. This opens the Configuration tab for the Map Properties, where users may modify the appearance of map layers.

The subsequent grouping of icons pertain to the zoom level on the map. The magnifying glass with arrows is the "Original Extent" button, which allows users to return to the default zoom level, showing the full map. The next icon, the magnifying glass over a sheet, is the "Zoom to Layer" button, which zooms the map view so that the selected layer fills the viewing area. Next, the magnifying glass with the "minus" sign is the "Zoom out" button, which zooms the map view out in step-wise increments. The lower-case "i" in the blue circle is the "Identify" button, which is used to provide information about the layer that is selected in the "Identify Layer" list when a user selects a point on the map. For example, when the "Contour" layer is selected, and the "Identify" button is selected, the user can click on one of the contour levels on the map and obtain the time, level, and coordinates of the point. Selecting other layers, such as ROADS or BUILDINGS primarily identifies the road or building name, along with information about the geographic information system layer. The magnifying glass with the dashed box is

the “Zoom box” button, which allows users to draw a box on the map to set a new zoom level. The blue arrows in a plus-sign orientation allow users to pan the image.

The final two buttons at the right-hand end of the top bar of the output window are the “Converted Coordinates” and “Contour Labels” buttons. The “Converted Coordinates” button, which looks like a list of three short lines with green, red, and yellow boxes on the end, allows a user to select a position on the map and find the UTM, Washington State Plane, and Latitude/Longitude coordinates. The “Contour Labels” button, which looks like a yellow tag with two small arrows along two arcs, adds contour values to the contours on the map. The zoom level may need to be adjusted so that the labels can be clearly associated with each contour line.

Appendix D

APGEMS-TF Model Ranking

Appendix D

APGEMS-TF Model Ranking

Table D.1. Real-Time Model Ranking for APGEMS and APGEMS-TF

Attribute	Weight (0-2)	APGEMS Score (0-2)	Weighted Model Score	APGEMS-TF Score (0-2)	Weighted Model Score
Release Height					
Ground-level release	2	2	4	2	4
Elevated release	2	1	2	1	2
Thermally buoyant	1	1	1	1	1
Momentum	1	1	1	1	1
Release Type					
Gas	2	2	4	2	4
Particles	0	1	0	1	0
Source Type(s)					
Point	2	1	2	1	2
Area	1	1	1	1	1
Volume	1	0	0	0	0
Line	0	0	0	0	0
Models multiple sources	1	0	0	1	1
Meteorological Inputs					
Time Varying	1	1	1	1	1
Spatially Varying	1	1	1	1	1
Real-Time Meteorology	2	2	4	2	4
Historical Meteorology	1	1	1	1	1
Treatment of Specific or Unique Conditions					
Inversion Layer	1	1	1	1	1
Fumigation	1	1	1	1	1
Low Wind Speed	2	0	0	0	0
Building Wake	2	1	2	1	2
Stack-tip Downwash	2	1	2	1	2
Dry deposition	0	1	0	1	0
Wet deposition	0	1	0	1	0
Terrain Capability					
Uneven terrain	2	2	4	2	4
Terrain steering	1	2	2	2	2

Table D.1 (contd)

Attribute	Weight (0-2)	APGEMS Score (0-2)	Weighted Model Score	APGEMS-TF Score (0-2)	Weighted Model Score
Receptor Types					
Discrete	2	1	2	1	2
Cartesian Grid	1	1	1	1	1
Polar Grid	1	1	1	1	1
Applicable Distance(s)					
≤ 100 m of release	2	1	2	1	2
100 m to 15,000 m	1	2	2	2	2
15,000 m to 50,000 m	0	1	0	1	0
≥ 50,000 m	0	0	0	0	0
Outputs					
Air Concentration	2	1	2	1	2
Ground Deposition	0	1	0	1	0
Output Type(s)					
Text	2	1	2	1	2
Chart	1	0	0	0	0
Contour Plots	1	1	1	1	1
Time Averages					
≤ 1 minute	2	0	0	0	0
> 1 minute	1	1	1	1	1
Usability					
User Interface	2	2	4	2	4
Ease of Use	2	2	4	2	4
Validation / Accuracy / Vetting of Methods	2	1	2	1	2
Runtime					
Fast Setup	2	2	4	2	4
Fast Execution	2	2	4	2	4
Maximum Score:	110	TOTAL:	66	TOTAL:	67

Table D.2. Worker Safety and Emergency Planning Model Ranking for APGESM and APGEMS-TF

Attribute	Weight (0-2)	APGEMS Score (0-2)	Weighted Model Score	APGEMS-TF Score (0-2)	Weighted Model Score
Release Height					
Ground-level release	2	2	4	2	4
Elevated release	2	1	2	1	2
Thermally buoyant	1	1	1	1	1
Momentum	1	1	1	1	1
Release Type					
Gas	2	2	4	2	4
Particles	0	1	0	1	0
Source Type(s)					
Point	2	1	2	1	2
Area	1	1	1	1	1
Volume	1	0	0	0	0
Line	0	0	0	0	0
Models multiple sources	1	0	0	1	1
Meteorological Inputs					
Time Varying	1	1	1	1	1
Spatially Varying	1	1	1	1	1
Real-Time Meteorology	0	2	0	2	0
Historical Meteorology	2	1	2	1	2
Treatment of Specific or Unique Conditions					
Inversion Layer	1	1	1	1	1
Fumigation	1	1	1	1	1
Low Wind Speed	2	0	0	0	0
Building Wake	2	1	2	1	2
Stack-tip Downwash	2	1	2	1	2
Dry deposition	0	1	0	1	0
Wet deposition	0	1	0	1	0
Terrain Capability					
Uneven terrain	2	2	4	2	4
Terrain steering	1	2	2	2	2

Table D.2 (contd)

Attribute	Weight (0-2)	APGEMS Score (0-2)	Weighted Model Score	APGEMS-TF Score (0-2)	Weighted Model Score
Receptor Types					
Discrete	2	1	2	1	2
Cartesian Grid	1	1	1	1	1
Polar Grid	1	1	1	1	1
Applicable Distance(s)					
≤ 100 m of release	2	0	0	0	0
100 m to 15,000 m	1	1	1	1	1
15,000 m to 50,000 m	0	1	0	1	0
≥ 50,000 m	0	0	0	0	0
Outputs					
Air Concentration	2	1	2	1	2
Ground Deposition	0	1	0	1	0
Output Type(s)					
Text	2	1	2	1	2
Chart	1	0	0	0	0
Contour Plots	1	1	1	1	1
Time Averages					
≤ 1 minute	2	0	0	0	0
> 1 minute	1	1	1	1	1
Usability					
User Interface	1	2	2	2	2
Ease of Use	1	2	2	2	2
Validation / Accuracy / Vetting of Methods	2	1	2	1	2
Runtime					
Fast Setup	1	2	2	2	2
Fast Execution	1	2	2	2	2
Maximum Score:	100	TOTAL:	52	TOTAL:	53

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