August 1, 2024

New York State Department of Environmental Conservation
232 Golf Course Road
Warrensburg, New York 12885
Attention: James Hogan III, PE; Regional Air Pollution Control Engineer

RE: ESMI of New York; Application ID:5-5330-00038/00027, Batch Number: 1018418

Dear Mr. Hogan,

ESMI of New York (ESMI), a Clean Earth Company, is submitting the following responses and attachments to comments received from the New York State Department of Environmental Conservation (NYSDEC) via emailed letter, letter dated June 5, 2024. The comments provided in the letter were in reference to responses submitted by ESMI on April 15, 2024.

The NYSDEC June 5, 2024 letter can be referenced in Attachment A of this document.
.

NYSDEC Comment 1: Summation of Comment

- The emissions must be modeled using the default air dispersion modeling options, without the Method 1 deposition component of the plume. Please provide the updated modeling protocol and reports using the correct modeling method. (Last sentence of the Comment 1.)

ESMI Response 1:

- The updated *Protocol for Emission Point Modeling Using AERMOD Software (AERMOD Protocol)* and *Summary of Emission Point Modeling Using AERMOD Software (AERMOD Summary)* are contained in Attachment B and Attachment C of this document, respectively.

  Please note that ESMI intended the *AERMOD Protocol*, *AERMOD Summary*, and the Application for a Solid Waste Management Permit, Research, Development, and Demonstration Permit (Project Application), dated December 29, 2023 would be viewed and referenced as a single document.

NYSDEC Comment 2: Summation of Comment

- That expanded evaluation/analyses may not be possible and/or warranted going into this proposed 2- week RD&D project, but it would be necessary, upon obtaining the results of the testing required to be performed, for the facility to be granted DEC's approval to continue these process operations beyond that short RD&D project time-period. (last sentence of Comment 2.)

ESMI Response 2:

- ESMI noted in the Project Application on document page 12, page number 8, Air Resources Section, the following:
    - "PFAS results will be utilized to calculate PFAS mass placed into the TDU and, when compared to PoP Test results, calculate destruction removal efficiencies (DRE's) for PFAS. Actual emissions and calculated DRE's will be compared to the potential to emit (PTE) calculations and DRE's utilized in the facility Modeling to determine if the model should be re-run based on the measured data or whether the projected emissions were representative of the actual emissions. Measured emissions will then be compared to State and Federal guidelines (should Federal guidelines exist) to determine compliance."
- ESMI has updated the *AERMOD Summary*, page number 1, last paragraph, noting "Clean Earth will model, as noted in the Project application (page number 8), PFAS compounds for which emissions were measured should measurements and compounds differ from those in this model."

NYSDEC Comment 3: Summation of Comment:

- Please explain how the PFAS destruction efficiencies of the RD&D project operations (estimated to range from 99.90-99.99°/o) were determined. Additional documentation supporting that specified PFAS destruction efficiency range for the facility's thermal treatment system and the source(s) used to make the determination(s) must be provided, including references used to arrive at this indicated destruction efficiency range.

ESMI Response 3:

- ESMI submitted quotations and links to reference documents related to destruction efficiencies in the Project Application as noted below:
    - Document page 8, page number 4, Secondary Treatment Unit (STU) Section, including footnotes 7, 8, and 9.
    - Document page 12 and 13, page number 8 and number 9, Applications of thermal desorption to PFAS Treatment including footnotes 15 and 16
    - Document page 20 and 21, page number 13 and number 14; Attachment B, listed active document links
- ESMI, in evaluation of the available science and testing referenced, utilized destruction removal efficiencies (DRE's) of 99.9% and 99.99%. These values represent the lower of the referenced DRE's. Lower DRE's generate higher emission totals.

  *AERMOD Summary*, Table 3 notes that at a DRE of 99.9%, the summation of the modeled PFAS compounds is 0.005% of the AGC for PFOA. Based on these results, ESMI did not believe it was necessary to model at the higher DRE's represented in the referenced documents or at the tested DRE of the ESMI secondary treatment unit (page number 4, Secondary Treatment Unit).

- ESMI has updated the *AERMOD Summary*, page number 4, Section 3.1, last paragraph noting "Reference to destruction efficiencies applicable to thermal desorption are included in the following Project application sections; Secondary Treatment Unit (page number 4), Applications of thermal desorption to PFAS Treatment (page number 8), Attachment B (page number 13)."

NYSDEC Comment 4:

- Page 40, Table 4 from your April 15 submittal: Please correct the column title "Max Annual Dispersion" to "Max Annual Dispersion Concentration."

ESMI Response 4:

- *AERMOD Summary*, Table 3 was updated accordingly. Please note that due to the removal of data associated with deposition, the data is now contained in Table 3.

NYSDEC Comment 5, 5a, and 5b: Summation of Comment:

- Please update Table 2 accordingly. (Last sentence of Comment 5.)

ESMI Response 5:

- *AERMOD Summary*, Table 3 was updated accordingly. Please note that due to the removal of data associated with deposition, the data is now contained in Table 3.

ESMI looks forward to continuing collaborating with the State to develop a research project that will assist all parties in identifying scientific data to support management practices for PFAS contaminated soils in New York State. Should you have any questions on this document, its contents, or require additional information, please do not hesitate to contact us.

Sincerely,

Robert Martin

Digitally signed by Robert Martin
DN: cn=Robert Martin, o=Clean Earth, ou=Fort Edward, email=rmartin@harsco.com, c=US
Date: 2024.08.02 13:53:25 -04'00'

Robert Martin
Technical Director
P: 518.747.5500
E: rmartin@cleanearthinc.com

Attachment A

NYSDEC Letter Dated June 2, 2024

# NEW YORK STATE DEPARTMENT OF ENVIRONMENTAL CONSERVATION

**Office of Environmental Quality, Region 5**
232 Golf Course Road, Warrensburg, NY 12885
P: (518) 623-1200 | F: (518) 623-3603
www.dec.ny.gov

**Sent Via Email Only**

June 5, 2024

ENVIRONMENTAL SOIL MANAGEMENT INC,
Attn: Robert Martin
304 Towpath LN
Fort Edward NY, 12828-1754
rmartin@cleanearthinc.com

**Re: ESMI of New York (ESMI),**
**Facility ID: 5-5330-00038/00027**
**Fort Edward (T), Washington County**

Dear Robert Martin:

The department has the following comments to the responses submitted by you on April 15, 2024, for the Notice of Incomplete Application (dated March 15, 2024):

1. Page 1 from your April 15 submittal: The PFAS 'deposition' modeling methodology indicated in response Item # 2 is still not acceptable modeling assumptions. Method 1 is designed to calculate the deposition of particles with diameters greater than 10 µm. Most, if not all, of the emitted air contaminants will be smaller than 10 µm and will therefore have different gravitational settling velocities, aerodynamic resistance, etc. The emissions must be modeled using the default air dispersion modeling options, without the Method 1 deposition component of the plume. Please provide the updated modeling protocol and reports using the correct modeling method.

2. Page 11, last paragraph from your April15 submittal: The EPA test methods for measuring PFAS Compounds both in the soil and air media have expansive analyte lists. As such, there will be many more PFAS compounds that the DEC will require to be "evaluated" than the limited amount listed out in this paragraph. That expanded evaluation/analyses may not be possible and/or warranted going into this proposed 2-week RD&D project, but it would be necessary, upon obtaining the results of the testing required to be performed, for the facility to be granted DEC's approval to continue these process operations beyond that short RD&D project time-period.

    a. Therefore, rather than being so prescriptive with only these individual PFAS Compounds being identified, it'd be better just to use the encompassing term of "PFAS" or "PFAS Compounds" in general to allow the flexibility for the evaluation of all the PFAS that will be able to be measured, as will be required at some time.
    b. Alternatively, the first sentence of this paragraph could be edited to something such as the following: "*The PFAS contaminants will be evaluated including, but not limited to, the following USEPA regulated PFAS compounds.*"

3. Page 14, the 2nd Paragraph of Section 3.1 from your April 15 submittal: (*Note, this is the first occurrence, but which is also indicated in many additional locations throughout the document*): Please explain how the PFAS destruction efficiencies of the RD&D project operations (estimated to range from 99.90–99.99%) were determined. Additional documentation supporting that specified PFAS destruction efficiency range for the facility's thermal treatment system and the source(s) used to make the determination(s) must be provided, including references used to arrive at this indicated destruction efficiency range.

4. Page 40, Table 4 from your April 15 submittal: Please correct the column title "Max Annual Dispersion" to "Max Annual Dispersion Concentration."

5. Page 156, Table 2 from your April 15 submittal: The NYSDOH-derived interim AGC for $CF_4$ is 330 µg $m^{-3}$, and not the 0.33 µg $m^{-3}$ listed. So, the maximum annual dispersion concentration for $CF_4$ was calculated to be 1.6×10E-5% of its AGC, and not the 0.02% that's indicated. Please update the PDF Page 156 Table 2 accordingly.

    a. The maximum annual dispersion concentration (see previous comment above) for $CF_4$ is indicated to be 1.74E-05% of its AGC in Table 4 on PDF Page 40, which differs from the value listed in the previous bullet above. Please update the maximum annual dispersion concentration accordingly.

    b. The notation that the $CF_4$ AGC listed has *not* formally *accepted by the NYSDEC* is incorrect. The NYSDEC has adopted the CF4 AGC value.

If you have any questions regarding this, please contact Yasmini Patel at 518-623-1217 or yasmini.patel@dec.ny.gov.

Sincerely,

James E. Hogan III

James E. Hogan III, P.E.
Regional Air Pollution Control Engineer
Region 5, Division of Air Resources

YP:ja

ec: Y. Patel/File
B. Magee

Attachment B

Protocol for Emission Point Modeling Using AERMOD Software

July 2023
Updated August 2024

# Protocol for Emission Point Modeling Using AERMOD Software

## Clean Earth LLC
## 304 Towpath Lane
## Village of Fort Edward,
## Washington County, New York

*Prepared for:*

CLEAN EARTH LLC
304 Towpath Lane
Fort Edward, New York 12828

*Prepared by:*

C.T. MALE ASSOCIATES
50 Century Hill Drive
Latham, New York 12110
(518) 786-7400
FAX (518) 786-7299

*C.T. Male Project No.: 22.2756*

**PROTOCOL FOR EMISSION POINT MODELING USING AERMOD SOFTWARE**
**CLEAN EARTH LLC, 304 TOWPATH LANE**
**VILLAGE OF FORT EDWARD, WASHINGTON COUNTY, NEW YORK**

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## 1.0 PROJECT OVERVIEW

Clean Earth LLC (Clean Earth) owns and operates an existing facility permitted under an Air State Facility Permit issued by the New York State Department of Environmental Conservation (NYSDEC), Permit ID 5-5330-00038/00021. The permit is listed as being issued under the facility name of "Environmental Soil Management of New York LLC dba ESMI A Clean Earth Company". The facility is in the process of preparing for requesting authorization to treat Per- and polyfluoroalkyl substances (PFAS) contaminated media. The work is being completed for the Clean Earth facility located at 304 Towpath Lane in the Village of Fort Edward, Washington County, New York. This protocol has been prepared to conduct air dispersion modeling of the facility's proposed operations to estimate the level of impact associated with PFAS emissions from the facility.

Under this protocol, the air dispersion modeling will be completed in accordance with generally accepted modeling practices and will utilize software which runs the current version of the United States Environmental Protection Agency's (USEPA) AERMOD software as detailed in Section 2. Estimated contaminant-specific hourly and annual maximum hourly concentrations will be derived from the model and will be based on a range of PFAS control efficiency for the soil treated at the facility.

The contaminants to be evaluated include the following USEPA regulated Per- and polyfluoroalkyl substances (PFAS) compounds; perfluorooctanoic acid (PFOA), perfluorooctane sulfonate (PFOS), perfluorononanoic acid (PFNA), perfluorohexane sulfonate (PFHxS), and perfluorobutane sulfonate (PFBS). This analysis will also include dispersion modeling of Hydrogen Fluoride (HF) and Carbon Tetrafluoride ($CF_4$) per the request of the NYSDEC.

## 2.0 MODELING SOFTWARE

### 2.1 Selection of AERMOD Software

In accordance with NYSDEC Policy DAR-10: NYSDEC Guidelines on Dispersion Modeling Procedures for Air Quality Impact Analysis, this protocol intends to follow the Division of Air Resources' recommended dispersion modeling procedures for conducting ambient impact analyses. By following these procedures, the protocol also follows the USEPA approved methodologies, as incorporated in Appendix W of 40 CFR Part 51 regulations. In performing such assessments, a set of recommended and acceptable procedures has been defined by USEPA and NYSDEC to assist source applicants to assure the proper application of the modeling analysis. As detailed within DAR-10, source analyses at major sources should adhere strictly to the requirements and preferred modeling procedures described in the USEPA Guidelines, with the added requirements of NYSDEC on the application of AERMOD.

### 2.2 Description of AERMOD Software

AERMOD is a regulatory steady-state plume modeling system with three separate components: AERMOD (Dispersion Model), AERMAP (Terrain Preprocessor), and AERMET (Meteorological Preprocessor). AERMAP characterizes the terrain, and generates receptor grids for the AERMOD dispersion model, while AERMET provides AERMOD with the meteorological information it needs to characterize the planetary boundary layer.

AERMET uses meteorological data and surface characteristics to calculate boundary layer parameters (e.g., mixing height, friction velocity, etc.) needed by AERMOD. This data is representative of the meteorology in the modeling domain.

AERMAP uses gridded terrain data for the modeling area to calculate a representative terrain-influence height associated with each receptor location. The gridded data is supplied to AERMAP in the format of the Digital Elevation Model (DEM) data from the United States Geological Survey (USGS). The terrain preprocessor can also be used to compute elevations for both discrete receptors and receptor grids.

In developing AERMOD, AERMIC adopted design criteria to yield a model with desirable regulatory attributes. It was felt that the model should: 1) provide reasonable concentration estimates under a wide variety of conditions with minimal discontinuities; 2) be user friendly and require reasonable input data and computer resources as is the case with the ISCST3 model; 3) capture the essential physical processes while remaining fundamentally simple; and, 4) accommodate modifications with ease as the science evolves.

In order to provide consideration to downwash, cavity impacts, and building wakes and eddies, the software incorporates a feature known as the Building Profile Input Program (BPIP). The BPIP incorporates a program that calculates building heights (BH) and projected building widths (PBW), and is designed to determine whether or not a stack is being subjected to wake effects from a structure or structures, and may lead to different BH and PBW values than those calculated for GEP. These calculations are performed only if a stack is being influenced by structure wake effects.

The current version of AERMOD, version 23132 will be used to complete the proposed Air Dispersion Modeling. If a newer version of AERMOD is released during the review period for this protocol, the most current version would be used in place of 23132.

## 3.0 SUMMARY OF MODEL INPUTS

### 3.1 Facility Modeling Parameters

Design data for the facility will be used as the basis for running the model in conjunction with the anticipated maximum operations which would involve thermal treatment of PFAS containing soil through thermal desorption. The model input data includes emission point parameters (stack location, stack base elevation, emission rate, stack height, stack exit temperature, stack gas velocity and stack diameter), as well as existing building footprints and heights. The model is capable of being run using specific area settings (i.e., urban or rural settings), and will utilize the rural setting based on the layout of the facility and surrounding area. The modeling will be performed using the default air dispersion modeling options. Deposition will not be included as part of this modeling.

In order to estimate anticipated facility emissions, destruction efficiencies of 99.90% and 99.99% will be used for PFAS in soil to be treated.

### 3.2 Receptor Area to be Modeled

The modeling will be conducted for the area in the vicinity of the site, with the receptors oriented in a Cartesian grid pattern set up following the initial receptor grid spacing suggested in DAR-10: NYSDEC Guidelines on Dispersion Modeling Procedures for Air Quality Impact Analysis:

- Receptor spacing of 25m along the facility property line;
- 25m receptor spacing from the center of the facility to the facility property line;
- 70m receptor spacing from the facility property line to 1km;
- 100m spacing from 1km to 2km; and
- 250m spacing from 2km to 5km.

A total of 4,001 receptors (including sensitive receptors) will be modeled under this scenario, covering an area of approximately 25,000,000 square meters (±6,178 acres), and includes areas mapped as Potential Environmental Justice Area (PEJA) Community 15000US361150801001 in the Village of Hudson Falls, and a small portion of PEJA Community 15000US361130705002 on the eastern edge of the City of Glens Falls.

As recommended in DAR-10, a 25m receptor spacing within the property boundaries is included as public access is not precluded by means of a fence or other physical barrier. All receptor data corresponds to the interpolated ground level elevation as assigned by AERMAP.

Online resources were consulted to identify the location of additional, discrete sensitive receptors such as schools, hospitals, parks, nursing homes and daycares within the modeling area. A summary of the sensitive receptors within 2 km of the site are summarized in Table 1. Figure 3 provides a depiction of the receptor grid including the sensitive receptors.

**Table 1 – List of Sensitive Receptors Within Modeling Area**

| Facility Name | Location (UTM Coordinates) | Approximate Distance from Facility (km) |
|---|---|---|
| Fort Edward Jr. Sr. High School | 614811.26m, 4792114.38m | 0.97 |
| School on Burgoyne | 615068.06m, 4793260.20m | 0.83 |
| Fort Edward Village Recreation | 615168.68m, 4791200.98m | 0.86 |
| Learning Express Family Daycare | 614061.73m, 4792415.84m | 1.75 |
| A Mother's Dream Daycare | 614550.77m, 4794149.78m | 1.80 |
| Fort Edward-Kingsbury Health Center | 614987.73m, 4791610.57m | 1.38 |
| Fort Edward Village Recreation | 615155.76m, 4792128.53m | 0.85 |
| Wedgewood Golf Club | 616233.14m, 4792572.79m | 0.85 |
| Mullen Park | 615253.85m, 4792023.77m | 0.85 |

### 3.3 AERMAP Data Input

The current version of AERMAP, version 18081 will be used to complete the proposed Air Dispersion Modeling. The AERMAP terrain preprocessor will utilize USGS 7.5

Minute Native Format DEM topographical data for the Hudson Falls, Fort Miller, Gansevoort, and Glens Falls, New York quadrangles, data which provides a resolution of 10 meters.

### 3.4 AERMET Data Input

The AERMET meteorological preprocessor will utilize surface and upper air data for the most recently available five year period from the NYSDEC, which includes the years 2017-2021. The National Weather Service (NWS) website indicates that climate data for the region of the project site is available from five regional climatology reporting locations: Albany, NY; Bennington, VT; Glens Falls, NY; Pittsfield, MA; and Poughkeepsie, NY. The Glens Falls location is closest to the site, and as such, was chosen as the most representative climate data for the facility. The meteorological data provided by the NYSDEC includes surface data for Glens Falls, and upper air data from Albany.

### 3.5 AERMOD Data Input

PFAS emissions estimates for on-site activities will be generated based on maximum material processing capacity for equipment on-site and will evaluate a range of performance of PFAS removal of the treatment system (99.90% and 99.99%). As the feed material will vary from project to project, data will be evaluated from existing PFAS containing soils as part of the input data.

Using the emission point data, the layout of the site buildings, the model will calculate the concentration of PFAS from the emissions from the emission point. The model will consider complex terrain through incorporating the AERMAP program into the modeling scenario. USGS topographical data will be imported into the modeling software to account for the complex terrain (i.e., those areas where the terrain exceeds the stack base elevation).

A "Representative" PFAS input of 0.1 g/s will be modeled as an arbitrary value and as a screening level to allow for emissions of contaminants to be estimated by scaling the "Representative" PFAS modeling results. This "Representative" PFAS value is not indicative of the actual estimated facility emissions or modeling results.

Stack parameters to be utilized in the dispersion modeling are shown in Table 2.

**Table 2 – Stack Parameters (from 2014 Stack Testing)**

| | |
|---|---|
| Stack Height | 55 feet |
| Stack Diameter | 3.67 feet |
| Flow Rate | 56,181 ACFM (average from stack test) |
| Exit Velocity | 88.68 feet/second (average from stack test) |
| Exit Temperature | 398°F |

## 4.0 SUMMARY OF MODELING RESULTS

The AERMOD modeling analysis will account for the operations currently contemplated for the facility, including operation of the facility's thermal desorption system for the treatment of PFAS containing soil. Modeling data will include the dimensions and footprints of the facility's buildings, as well as specific information relative to the emission point. The model will incorporate topographical data from the USGS, and meteorological data from Glens Falls and Albany Airports. A summary of the model results will be presented within the summary report, which will include graphical representations of the model output at 99.90% and 99.99%, respectively.

The results of the modeling software specific to air dispersion modeling will be compared to the AGC and SGC values for individual contaminants as determined by the NYSDEC, and as listed within the NYSDEC document titled "DAR-1 AGC/SGC Tables". As a conservative approach, the sum of the five (5) modeled PFAS compounds will be compared to the individual AGC for PFOA. $CF_4$ does not have an established AGC, and the value presented is based on the recommendation of the New York State Department of Health (NYSDOH) in their October 2023 assessment.

### 4.1 Locations of Maximum Concentration Receptors

The location of the receptor for the maximum concentration will be provided within the summary report. Isopleths indicating the results of the modeling demonstrating the concentrations of PFAS will also be included within the summary report.

## 5.0 REFERENCES

United States Environmental Protection Agency (ongoing) – American Meteorological Society / EPA Regulatory Model - AERMOD Modeling System currently located and documented at EPA Home>> Air & Radiation>> Technology Transfer Network>> Support Center for Regulatory Atmospheric Modeling>> Preferred/Recommended Models

# FIGURES


**MAP REFERENCE**

United States Geological Survey
7.5 Minute Series Topographic Map
Quadrangle: Hudson Falls, NY
Date: 2019


CIVIL ENGINEERING
ENVIRONMENTAL SERVICES
SURVEY SERVICES
LAND SERVICES
ARCHITECTURE
ENERGY & BUILDING SYSTEMS SERVICES
ELECTRICAL ENGINEERING

C.T. MALE ASSOCIATES
Engineering, Surveying, Architecture, Landscape Architecture & Geology, D.P.C.

50 CENTURY HILL DRIVE, LATHAM, NEW YORK 12110
PHONE (518) 786-7400 FAX (518) 786-7299

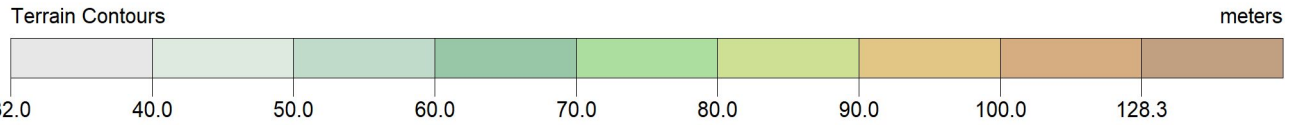

# FIGURE 1 SITE LOCATION MAP

## CLEAN EARTH, FORT EDWARD FACILITY

| | |
|---|---|
| VILLAGE OF FORT EDWARD | WASHINGTON COUNTY, NY |
| SCALE: 1" = ±2,000' | |
| DRAFTER: L.HAND | |
| PROJECT No. 22.2756 | |

PROJECT TITLE:

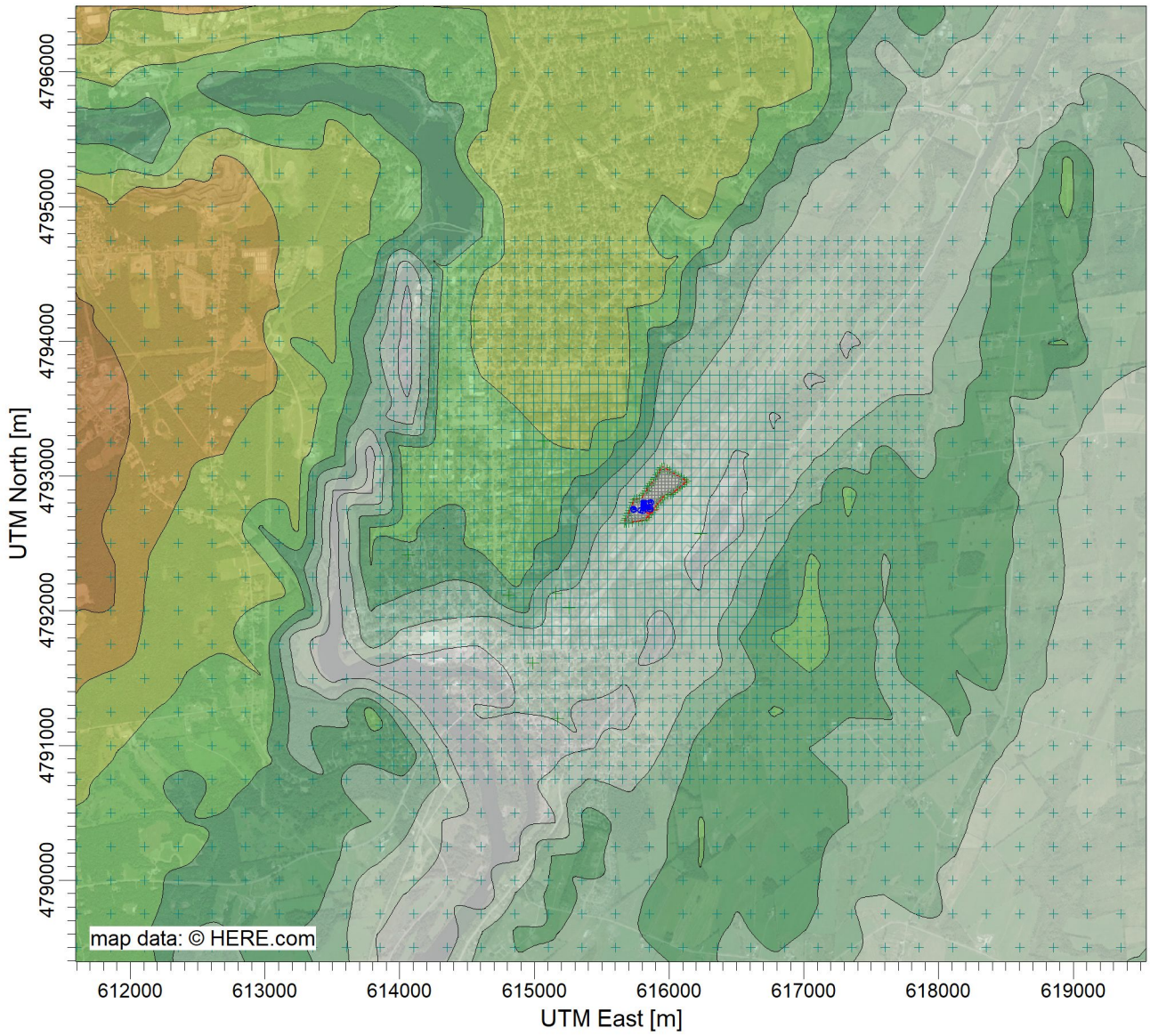
**Air Dispersion and Deposition Modeling - Clean Earth Fort Edward, NY Site**
**Facility Building, Emission Points, Elevations and Property Line**


| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| | **1** | **C.T. Male Associates** | |
| | RECEPTORS: | MODELER: | |
| | **4001** | **C.T. Male Staff** | |
| | | SCALE: 1:5,000<br>0 0.1 km | |
| | | DATE: | PROJECT NO.: |
| | | **5/8/2023** | **22.2756** |

PROJECT TITLE:

**Air Dispersion and Deposition Modeling - Clean Earth Fort Edward, NY Site**
**Receptor Grid Depiction**




Terrain Contours — meters

32.0 | 40.0 | 50.0 | 60.0 | 70.0 | 80.0 | 90.0 | 100.0 | 128.3

| | | | |
|---|---|---|---|
| COMMENTS: | SOURCES: **1** | COMPANY NAME: **C.T. Male Associates** | |
| | RECEPTORS: **4001** | MODELER: **C.T. Male Staff** | |
| | | SCALE: 1:50,000 — 0 — 2 km | |
| | | DATE: **5/8/2023** | PROJECT NO.: **22.2756** |

Attachment C

Summary of Emission Point Modeling Using AERMOD Software

December 2023
Updated August 2024

# Summary of Emission Point Modeling Using AERMOD Software

## Clean Earth LLC
## 304 Towpath Lane
## Village of Fort Edward,
## Washington County, New York

*Prepared for:*

CLEAN EARTH LLC
304 Towpath Lane
Fort Edward, New York 12828

*Prepared by:*

C.T. MALE ASSOCIATES
50 Century Hill Drive
Latham, New York 12110
(518) 786-7400
FAX (518) 786-7299

*C.T. Male Project No.: 22.2756*

**SUMMARY OF EMISSION POINT MODELING USING AERMOD SOFTWARE**
**CLEAN EARTH LLC, 304 TOWPATH LANE**
**VILLAGE OF FORT EDWARD, WASHINGTON COUNTY, NEW YORK**

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**SUMMARY OF EMISSION POINT MODELING USING AERMOD SOFTWARE**
**CLEAN EARTH LLC, 304 TOWPATH LANE**
**VILLAGE OF FORT EDWARD, WASHINGTON COUNTY, NEW YORK**

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ATTACHMENTS

## 1.0 PROJECT OVERVIEW

Clean Earth LLC (Clean Earth) owns and operates an existing facility permitted under an Air State Facility Permit issued by the New York State Department of Environmental Conservation (NYSDEC), Permit ID 5-5330-00038/00021. The permit is listed as being issued under the facility name of "Environmental Soil Management of New York LLC dba ESMI A Clean Earth Company". The facility is in the process of preparing for requesting authorization to treat Per- and polyfluoroalkyl substances (PFAS) contaminated media. The work is being completed for the Clean Earth facility located at 304 Towpath Lane in the Village of Fort Edward, Washington County, New York. This project conducted air dispersion modeling of the facility's proposed operations in order to estimate the level of impact associated with PFAS emissions from the facility.

In accordance with the previously prepared protocol, the air dispersion modeling was completed in accordance with generally accepted modeling practices and utilized software which runs the current version of the United States Environmental Protection Agency's (USEPA) AERMOD software as detailed in Section 2.

The contaminants evaluated relative to dispersion include the following USEPA regulated Per- and polyfluoroalkyl substances (PFAS) compounds; perfluorooctanoic acid (PFOA), perfluorooctane sulfonate (PFOS), perfluorononanoic acid (PFNA), perfluorohexane sulfonate (PFHxS), and perfluorobutane sulfonate (PFBS). Clean Earth will model, as noted in the Project application (page number 8), PFAS compounds for which emissions were measured should measurements and compounds differ from those in this model. This analysis also includes dispersion modeling of Hydrogen Fluoride (HF) and Carbon Tetrafluoride ($CF_4$) per the request of the NYSDEC.

## 2.0 MODELING SOFTWARE

### 2.1 Selection of AERMOD Software

In accordance with NYSDEC Policy DAR-10: NYSDEC Guidelines on Dispersion Modeling Procedures for Air Quality Impact Analysis, this project followed the Division of Air Resources' recommended dispersion modeling procedures for conducting ambient impact analyses. By following these procedures, the protocol also followed the USEPA approved methodologies, as incorporated in Appendix W of 40 CFR Part 51 regulations. In performing such assessments, a set of recommended and acceptable procedures has been defined by USEPA and NYSDEC to assist source applicants to assure the proper application of the modeling analysis. As detailed within DAR-10, source analyses at major sources should adhere strictly to the requirements and preferred modeling procedures described in the USEPA Guidelines, with the added requirements of NYSDEC on the application of AERMOD.

### 2.2 Description of AERMOD Software

AERMOD is a regulatory steady-state plume modeling system with three separate components: AERMOD (Dispersion Model), AERMAP (Terrain Preprocessor), and AERMET (Meteorological Preprocessor). AERMAP characterizes the terrain, and generates receptor grids for the AERMOD dispersion model, while AERMET provides AERMOD with the meteorological information it needs to characterize the planetary boundary layer.

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In order to provide consideration to downwash, cavity impacts, and building wakes and eddies, the software incorporates a feature known as the Building Profile Input Program (BPIP). The BPIP incorporates a program that calculates building heights (BH) and projected building widths (PBW), and is designed to determine whether or not a stack is being subjected to wake effects from a structure or structures, and may lead to different BH and PBW values than those calculated for GEP. These calculations are performed only if a stack is being influenced by structure wake effects.

The current version of AERMOD, version 23132 was used to complete the Air Dispersion Modeling.

## 3.0 SUMMARY OF MODEL INPUTS

### 3.1 Facility Modeling Parameters

Design data for the facility was used as the basis for running the model in conjunction with the anticipated maximum operations which would involve thermal treatment of PFAS containing soil through thermal desorption. The model input data includes emission point parameters (stack location, stack base elevation, emission rate, stack height, stack exit temperature, stack gas velocity and stack diameter), as well as existing building footprints and heights. The model is capable of being run using specific area settings (i.e., urban or rural settings), and utilized the rural setting based on the layout of the facility and surrounding area. The modeling was performed using the default air dispersion modeling options. Deposition was not included as part of this modeling.

In order to estimate anticipated facility emissions, destruction efficiencies of 99.90% and 99.99% were used for PFAS in soil to be treated. A summary of dispersion modeling results with graphical representations of outputs are included in Attachment A and Attachment B for destruction efficiencies of 99.90% and 99.99%, respectively.

Reference to destruction efficiencies applicable to thermal desorption are included in the following Project application sections; Secondary Treatment Unit (page number 4), Applications of thermal desorption to PFAS Treatment (page number 8), Attachment B (page number 13).

### 3.2 Receptor Area Modeled

The modeling was conducted for the area in the vicinity of the site, with the receptors oriented in a Cartesian grid pattern set up following the initial receptor grid spacing suggested in DAR-10: NYSDEC Guidelines on Dispersion Modeling Procedures for Air Quality Impact Analysis:

- Receptor spacing of 25m along the facility property line;
- 25m receptor spacing from the center of the facility to the facility property line;
- 70m receptor spacing from the facility property line to 1km;
- 100m spacing from 1km to 2km; and
- 250m spacing from 2km to 5km.

A total of 4,001 receptors (including sensitive receptors) were modeled under this scenario, covering an area of approximately 25,000,000 square meters (±6,178 acres), and includes areas mapped as Potential Environmental Justice Area (PEJA) Community 15000US361150801001 in the Village of Hudson Falls, and a small portion of PEJA Community 15000US361130705002 on the eastern edge of the City of Glens Falls.

As recommended in DAR-10, a 25m receptor spacing within the property boundaries was included as public access is not precluded by means of a fence or other physical barrier. All receptor data corresponds to the interpolated ground level elevation as assigned by AERMAP.

Online resources were consulted to identify the location of additional, discrete sensitive receptors such as schools, hospitals, parks, nursing homes and daycares within the modeling area. A summary of the sensitive receptors within 2km of the site are summarized in Table 1. Figure 3 provides a depiction of the receptor grid including the sensitive receptors.

**Table 1 – List of Sensitive Receptors Within Modeling Area**

| Facility Name | Location (UTM Coordinates) | Approximate Distance from Facility (km) |
|---|---|---|
| Fort Edward Jr. Sr. High School | 614811.26m, 4792114.38m | 0.97 |
| School on Burgoyne | 615068.06m, 4793260.20m | 0.83 |
| Fort Edward Village Recreation | 615168.68m, 4791200.98m | 0.86 |
| Learning Express Family Daycare | 614061.73m, 4792415.84m | 1.75 |
| A Mother's Dream Daycare | 614550.77m, 4794149.78m | 1.80 |
| Fort Edward-Kingsbury Health Center | 614987.73m, 4791610.57m | 1.38 |
| Fort Edward Village Recreation | 615155.76m, 4792128.53m | 0.85 |
| Wedgewood Golf Club | 616233.14m, 4792572.79m | 0.85 |

| Facility Name | Location (UTM Coordinates) | Approximate Distance from Facility (km) |
|---|---|---|
| Mullen Park | 615253.85m, 4792023.77m | 0.85 |

### 3.3 AERMAP Data Input

The current version of AERMAP, version 18081 was used to complete the proposed Air Dispersion Modeling. The AERMAP terrain preprocessor will utilize USGS 7.5 Minute Native Format DEM topographical data for the Hudson Falls, Fort Miller, Gansevoort, and Glens Falls, New York quadrangles, data which provides a resolution of 10 meters.

### 3.4 AERMET Data Input

The AERMET meteorological preprocessor utilized surface and upper air data for the most recently available five year period from the NYSDEC, which includes the years 2017-2021. The National Weather Service (NWS) website indicates that climate data for the region of the project site is available from five regional climatology reporting locations: Albany, NY; Bennington, VT; Glens Falls, NY; Pittsfield, MA; and Poughkeepsie, NY. The Glens Falls location is closest to the site, and as such, was chosen as the most representative climate data for the facility. The meteorological data provided by the NYSDEC includes surface data for Glens Falls, and upper air data from Albany.

### 3.5 AERMOD Data Input

PFAS emissions estimates for on-site activities were generated based on maximum material processing capacity for equipment on-site and estimated destruction efficiencies of PFAS of the treatment system at 99.90% and 99.99% . As the feed material will vary from project to project, data was evaluated from existing PFAS containing soils as part of the input data.

Using the emission point data, the layout of the site buildings, the model calculated the concentration of PFAS from the emissions from the emission point. The model considered complex terrain through incorporating the AERMAP program into the modeling scenario. USGS topographical data was imported into the modeling software

to account for the complex terrain (i.e., those areas where the terrain exceeds the stack base elevation).

A "Representative" PFAS input of 0.1 g/s was also modeled as an arbitrary value and as a screening level to allow for emissions of contaminants to be estimated by scaling the "Representative" PFAS modeling results. This "Representative" PFAS value is not indicative of the actual estimated facility emissions or modeling results.

Stack parameters utilized in the dispersion modeling are shown in Table 2.

**Table 2 – Stack Parameters (from 2014 Stack Testing)**

| | |
|---|---|
| Stack Height | 55 feet |
| Stack Diameter | 3.67 feet |
| Flow Rate | 56,181 ACFM (average from stack test) |
| Exit Velocity | 88.68 feet/second (average from stack test) |
| Exit Temperature | 398°F |

## 4.0 SUMMARY OF MODELING RESULTS

The AERMOD modeling analysis accounts for the operations currently contemplated for the facility, including operation of the facility's thermal desorption system for the treatment of PFAS containing soil. Modeling data included the dimensions and footprints of the facility's buildings, as well as specific information relative to the emission point. The model incorporates topographical data from the USGS, and meteorological data from Glens Falls and Albany Airports. A summary of the model results is presented within the summary report in Attachments A and B, which also include graphical representations of the model output at 99.90% and 99.99% destruction efficiency, respectively.

The results of the modeling software specific to air dispersion modeling were subsequently compared to the AGC and SGC values for individual contaminants as determined by the NYSDEC, and as listed within the NYSDEC document titled "DAR-1 AGC/SGC Tables". A summary of the modeled maximum hourly concentration and annual concentrations, and a comparison of those values to the established SGC and AGC values are presented below. As a conservative approach, the sum of the five (5) modeled PFAS compounds was compared to the individual AGC for PFOA. $CF_4$ does not have an established AGC, and the value presented herein is based on the recommendation of the New York State Department of Health (NYSDOH) in their October 2023 assessment, included as Attachment C. The summary table shows that the modeled concentrations will not result in exceeding concentrations established by the NYSDEC or NYSDOH, which were developed to be protective of human health and the environment.

**Table 3 – Summary of Concentration Data from Modeling**

| Contaminant | Max Hourly Dispersion Concentration | SGC | % of SGC | Max Annual Dispersion Concentration | AGC | % of AGC |
|---|---|---|---|---|---|---|
| | All values in ug/m$^3$ | | | | | |
| Total Sampled PFAS (99.9% DRE, full receptor grid) | 2.75E-05 | N/A | N/A | 2.72E-07 | 0.0053[1] | 0.005% |
| Total Sampled PFAS (99.9% DRE, 1.5 mile endpoint) | 5.39E-06 | N/A | N/A | 7.08E-08 | 0.0053[1] | 0.001% |
| Hydrogen Fluoride (HF) | 1.26 | 5.6 | 23% | 0.0124 | 0.071 | 17% |
| Carbon Tetrafluoride ($CF_4$) | 5.28E-03 | N/A | N/A | 5.21E-05 | 330[2] | 1.74E-05% |

[1] – Individual AGC for PFOA

[2] – NYSDOH recommended AGC, formally accepted by the NYSDEC

### 4.1 Locations of Maximum Concentration Receptors

The location of the receptor for the maximum concentration is provided within the summary report. Isopleths indicating the results of the modeling demonstrating the concentrations of PFAS are also included within the summary report. None of the maximum concentration receptors was located in close proximity to any of the sensitive receptors. The maximum receptor for all model runs was located on-site, approximately 18 meters southwest of the emission point.

## 5.0 REFERENCES

United States Environmental Protection Agency (ongoing) – American Meteorological Society / EPA Regulatory Model - AERMOD Modeling System currently located and documented at EPA Home>> Air & Radiation>> Technology Transfer Network>> Support Center for Regulatory Atmospheric Modeling>> Preferred/Recommended Models

# Figure 1

## Site Location Map


**MAP REFERENCE**

United States Geological Survey
7.5 Minute Series Topographic Map
Quadrangle: Hudson Falls, NY
Date: 2019


CIVIL ENGINEERING
ENVIRONMENTAL SERVICES
SURVEY SERVICES
LAND SERVICES
ARCHITECTURE
ENERGY & BUILDING SYSTEMS SERVICES
ELECTRICAL ENGINEERING

C.T. MALE ASSOCIATES
Engineering, Surveying, Architecture, Landscape Architecture & Geology, D.P.C.

50 CENTURY HILL DRIVE, LATHAM, NEW YORK 12110
PHONE (518) 786-7400 FAX (518) 786-7299


# FIGURE 1 SITE LOCATION MAP

## CLEAN EARTH, FORT EDWARD FACILITY

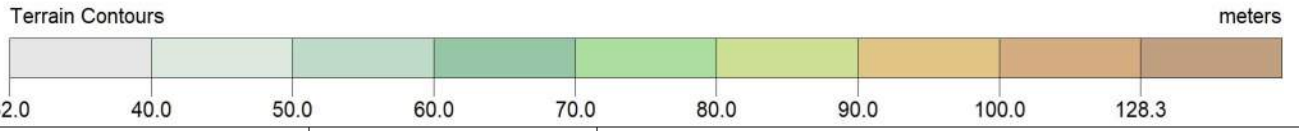
| | |
|---|---|
| VILLAGE OF FORT EDWARD | WASHINGTON COUNTY, NY |
| SCALE: 1" = ±2,000' | |
| DRAFTER: L.HAND | |
| PROJECT No. 22.2756 | |

# Figure 2

## Facility Buildings, Emission Points, Elevation and Property Line Map

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Facility Building, Emission Points, Elevations and Property Line**

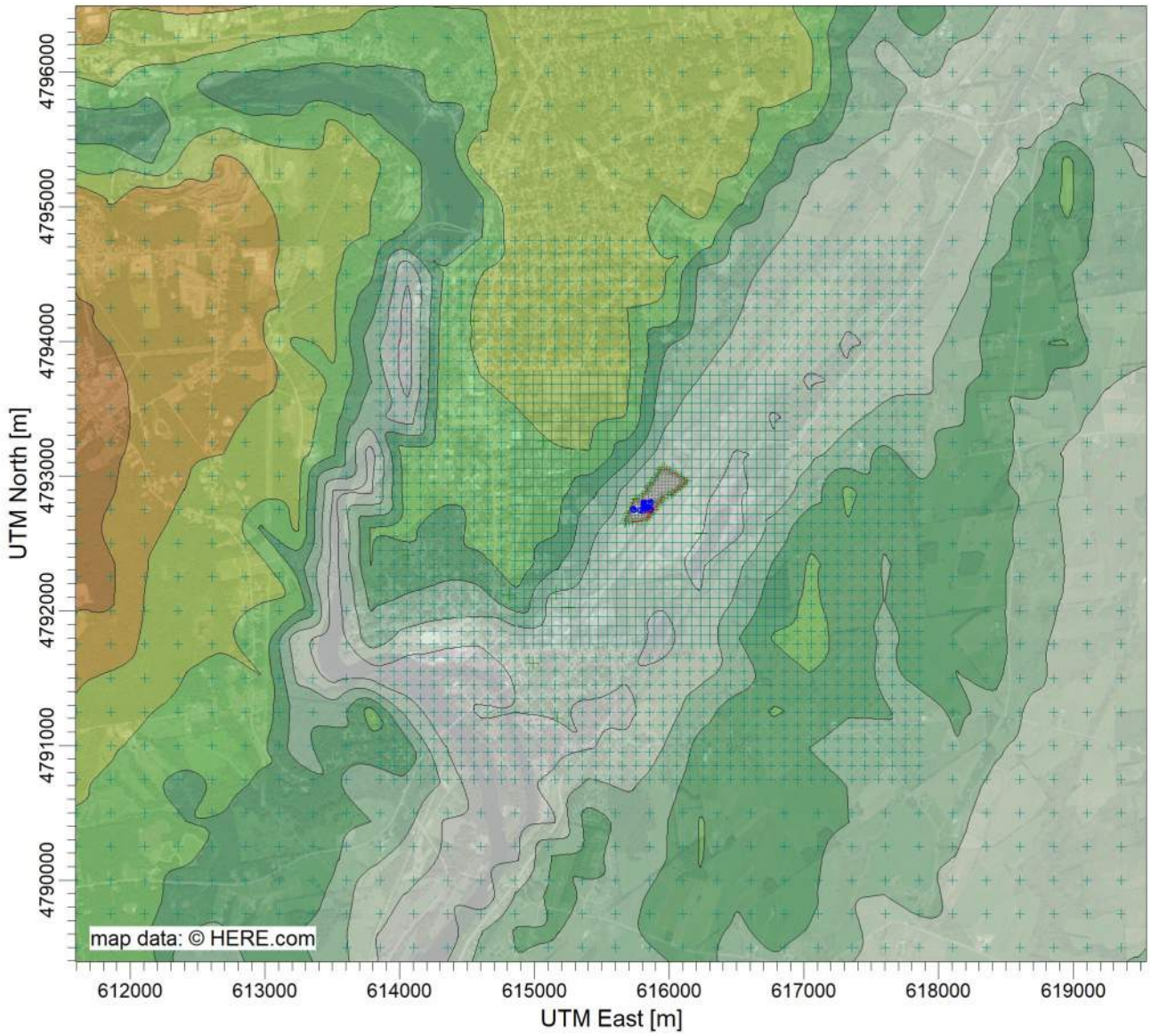

| | | | |
|---|---|---|---|
| COMMENTS: | SOURCES: **1** | COMPANY NAME: **C.T. Male Associates** | |
| | RECEPTORS: **4001** | MODELER: **C.T. Male Staff** | |
| | | SCALE: 1:5,000   | |
| | | DATE: **5/8/2023** | PROJECT NO.: **22.2756** |

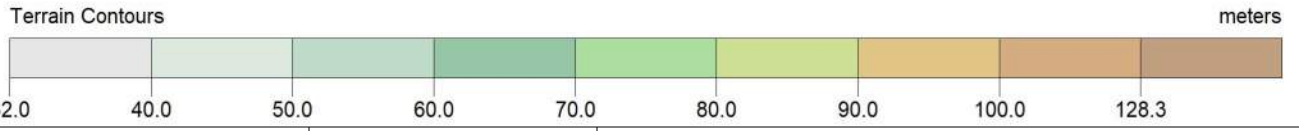
# Figure 3

## Receptor Grid Depiction Map

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Receptor Grid Depiction**




| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| | **1** | **C.T. Male Associates** | |
| | RECEPTORS: | MODELER: | |
| | **4001** | **C.T. Male Staff** | |
| | | SCALE: 1:50,000 | |
| | | 0 2 km | |
| | | DATE: | PROJECT NO.: |
| | | **5/8/2023** | **22.2756** |

# Attachment A

## Summary of Dispersion Modeling Results and Graphical Representations of Output at 99.90% Destruction Efficiency

| Compound | CAS# | Soil Concentration (in ppb) | Emission Rate based on 99.90% DRE (in g/s) | Dispersion Results (in ug/m^3) | | File Name |
|---|---|---|---|---|---|---|
| | | | | Maximum Hourly | Maximum Annual | |
| **Perfluorobutane Sulfonate (PFBS)** | 375-73-5 | 0.085 | 6.42589E-10 | 2.61465E-08 | 2.58169E-10 | PFBS9990 |
| **Perfluorooctanoic acid (PFOA)** | 335-67-1 | 4.482 | 3.38833E-08 | 1.37869E-06 | 1.36131E-08 | PFOA9990 |
| **Perfluorononanoic acid (PFNA)** | 375-95-1 | 2.061 | 1.55809E-08 | 6.33975E-07 | 6.25984E-09 | PFNA9990 |
| **Perfluorohexanesulfonic acid (PFHxS)** | 335-46-4 | 0.220 | 1.66317E-09 | 6.76733E-08 | 6.68202E-10 | PFHS9990 |
| **Perfluorooctanesulfonic acid (PFOS)** | 1763-23-1 | 58.793 | 4.44467E-07 | 1.80851E-05 | 1.78571E-07 | PFOS9990 |
| **Sum of all PFAS Compounds[2]** | N/A | 89.485 | 6.76495E-07 | 2.75261E-05 | 2.71791E-07 | PFAS9990 |
| **Sum of all PFAS Compounds (1.5 mile endpoint)[2]** | N/A | 89.485 | 6.76495E-07 | 5.39259E-06 | 7.08090E-08 | PFASENDP |
| **Hydrogen Fluoride (HF)[3]** | 7664-39-3 | N/A | 3.08737E-02 | 1.25623 | 1.24039E-02 | HF |
| **Carbon Tetrafluoride ($CF_4$)[4]** | 75-73-0 | N/A | 1.29685E-04 | 5.27681E-03 | 5.21029E-05 | CF4 |
| **"Representative" PFAS at 0.1 g/s** | N/A | N/A | 0.1 | 4.06893 | 4.01764E-02 | CEFE2023 |

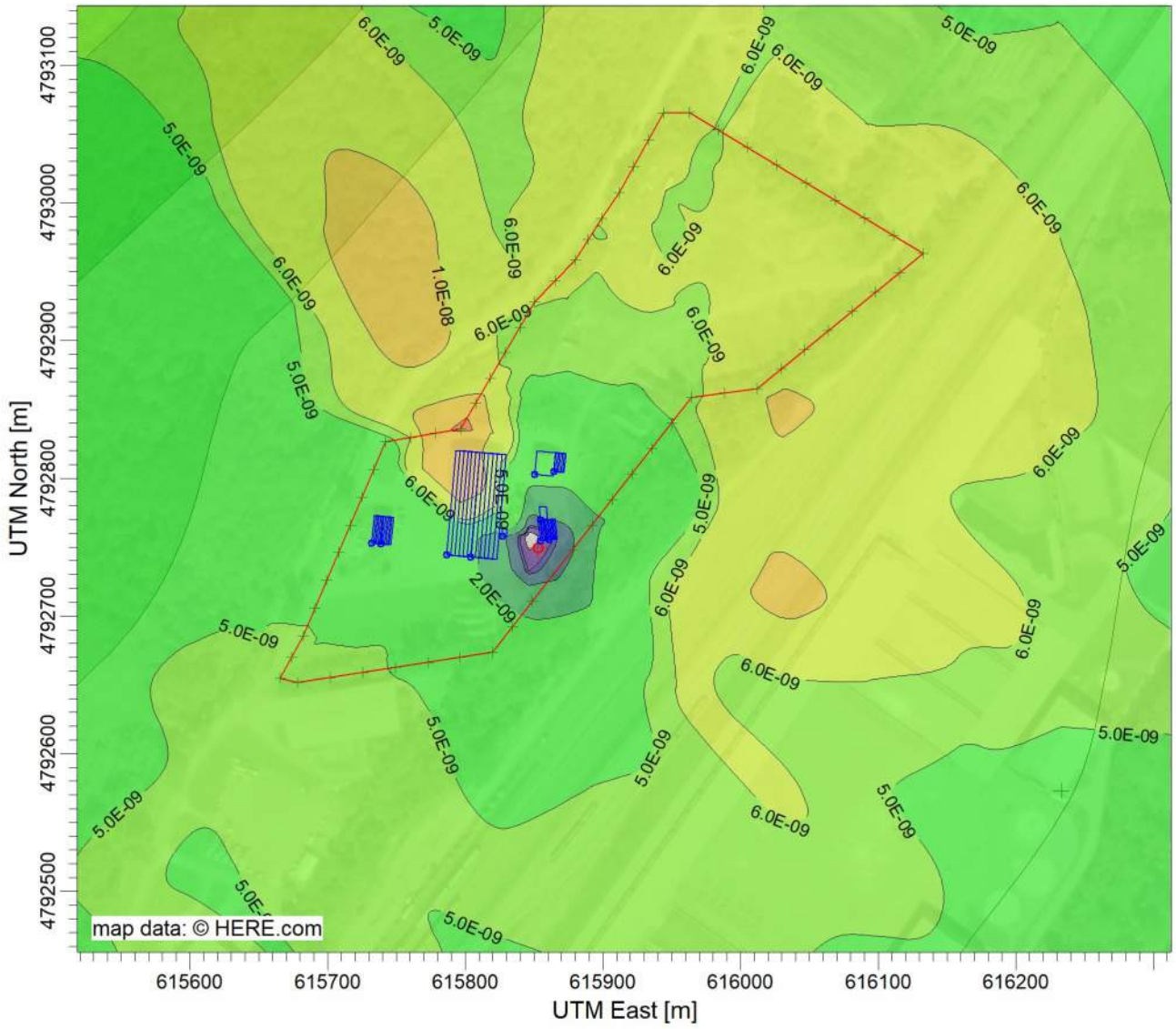
[1] - Sum of all sampled PFAS compounds.

[2] - Calculated emission rate based on conversion of all fluorine within PFAS compounds to hydrofluoric acid.

[3] - Calculated emission rate based on the following article:
Jonathan D. Krug, Paul M. Lemieux, Chun-Wai Lee, Jeffrey V. Ryan, Peter H. Kariher, Erin P. Shields, Lindsay C. Wickersham, Martin K. Denison, Kevin A. Davis, David A. Swensen, R. Preston Burnette, Jost O.L. Wendt & William P. Linak (2022) Combustion of C1 and C2 PFAS: Kinetic modeling and experiments, Journal of the Air & Waste Management Association, 72:3, 256-270, DOI: 10.1080/10962247.2021.2021317

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

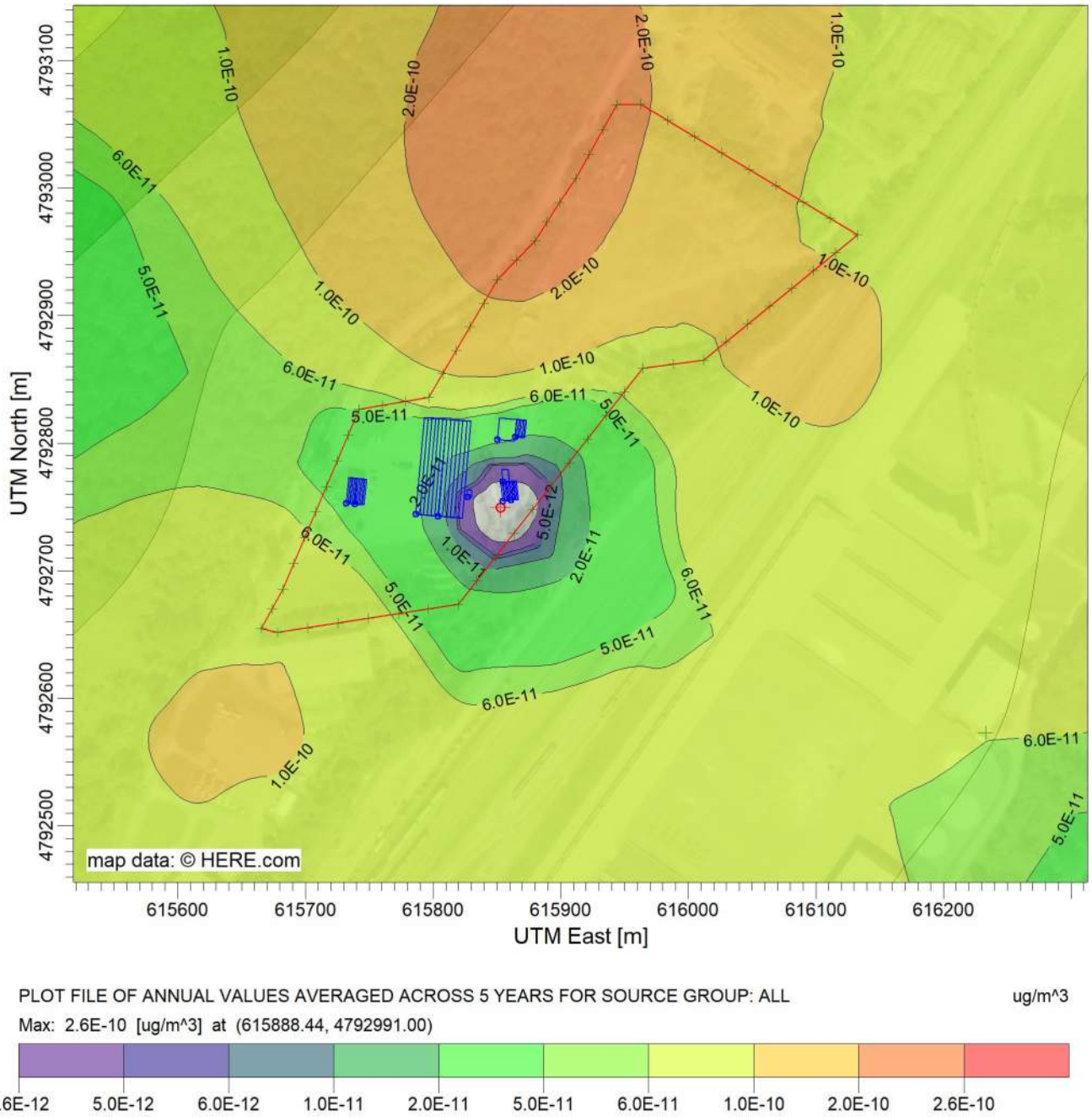
Max: 2.6E-08 [ug/m^3] at (615796.68, 4792835.91)

2.6E-10 5.0E-10 6.0E-10 1.0E-09 2.0E-09 5.0E-09 6.0E-09 1.0E-08 2.0E-08 2.6E-08

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorobutane Sulfonate (CAS No. 375-73-5) with Incoming Soil Concentration to Facility at 0.085 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**2.6E-08 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

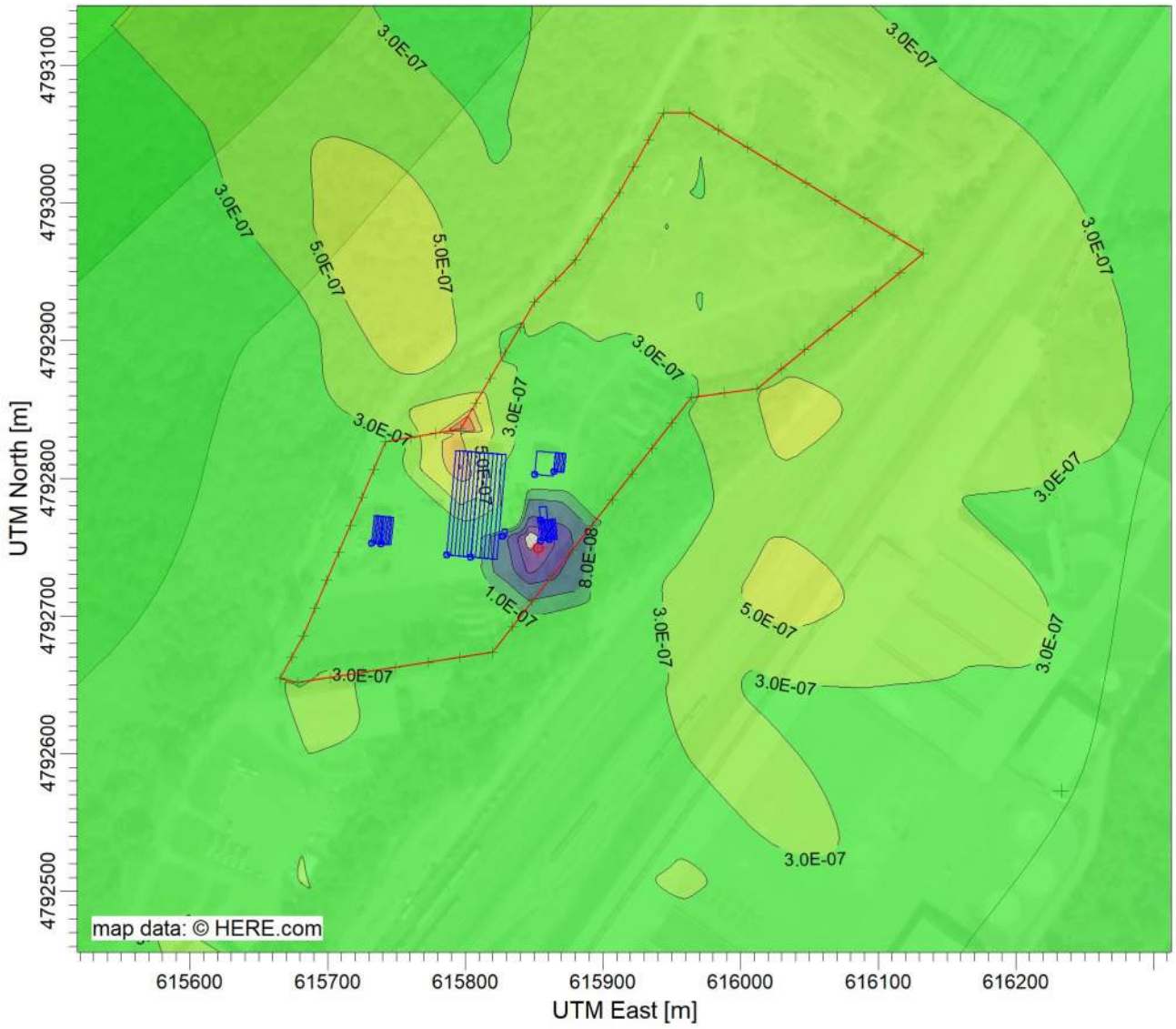
Max: 2.6E-10 [ug/m^3] at (615888.44, 4792991.00)

2.6E-12 5.0E-12 6.0E-12 1.0E-11 2.0E-11 5.0E-11 6.0E-11 1.0E-10 2.0E-10 2.6E-10

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorobutane Sulfonate (CAS No. 375-73-5) with Incoming Soil Concentration to Facility at 0.085 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**2.6E-10 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

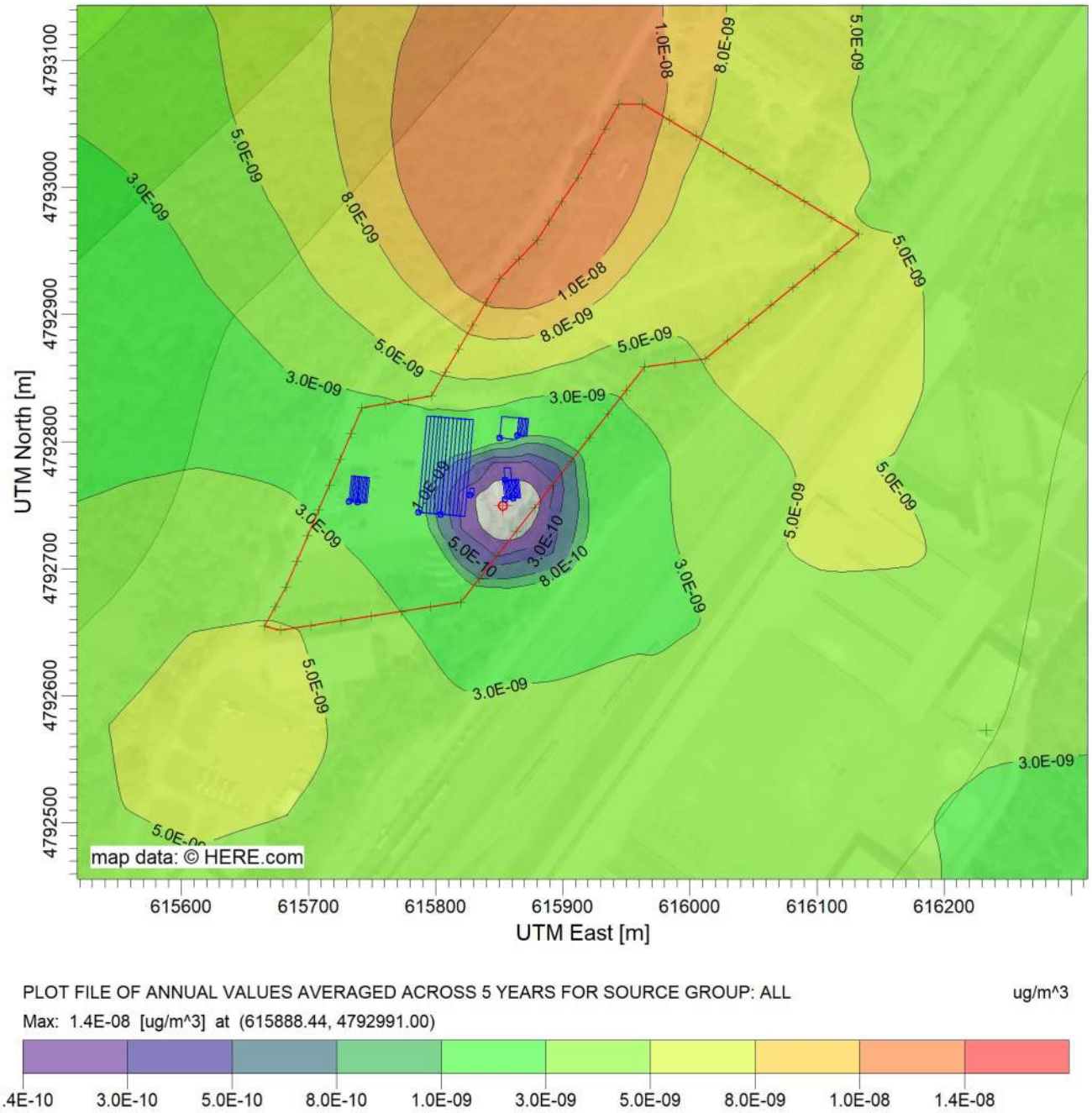
Max: 1.4E-06 [ug/m^3] at (615796.68, 4792835.91)

1.4E-08 3.0E-08 5.0E-08 8.0E-08 1.0E-07 3.0E-07 5.0E-07 8.0E-07 1.0E-06 1.4E-06

| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Perfluorooctanoic Acid (CAS No. 335-67-1) with Incoming Soil Concentration to Facility at 4.482 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.4E-06 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

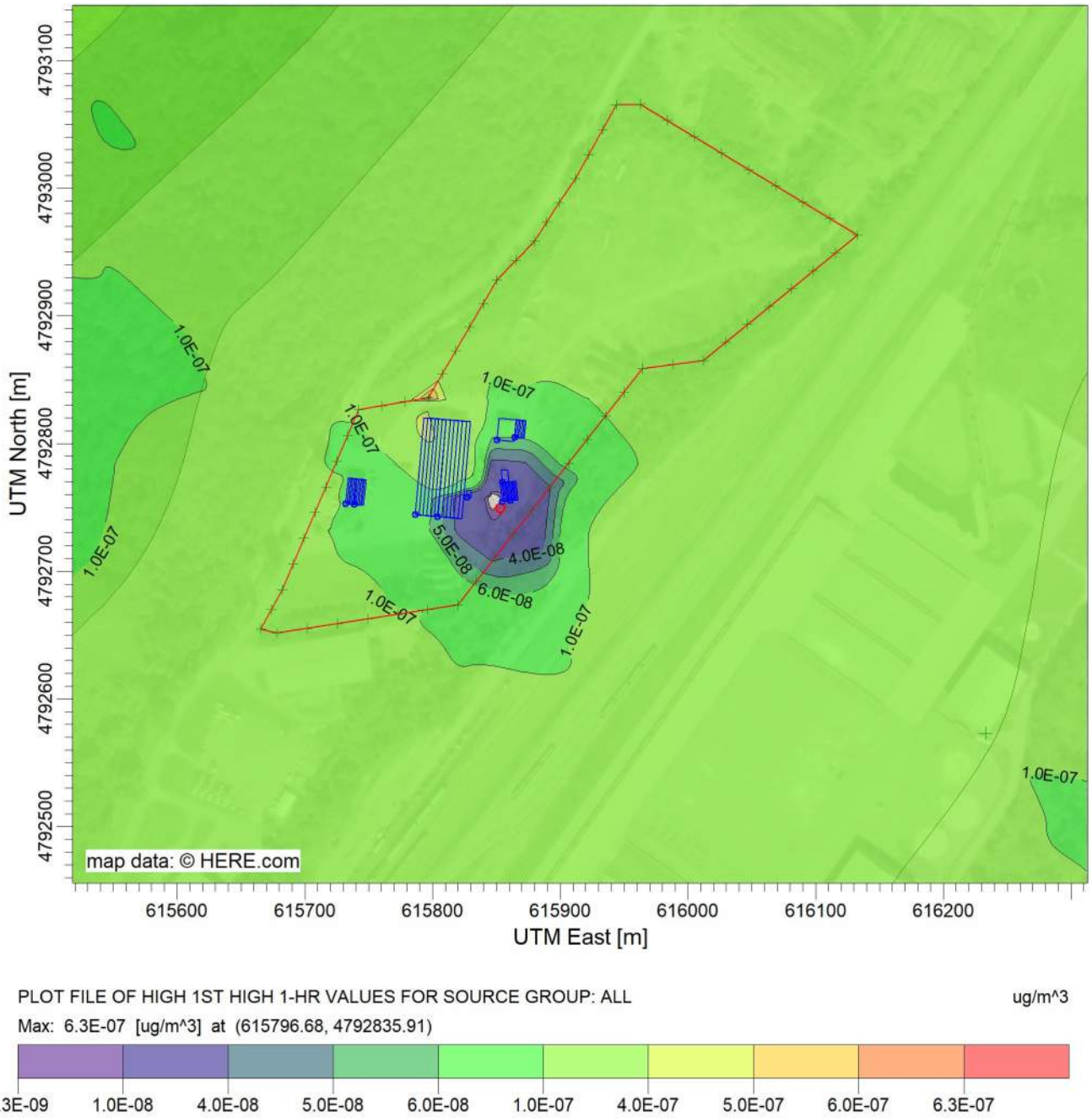
Max: 1.4E-08 [ug/m^3] at (615888.44, 4792991.00)




| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Perfluorooctanoic Acid (CAS No. 335-67-1) with Incoming Soil Concentration to Facility at 4.482 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.4E-08 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

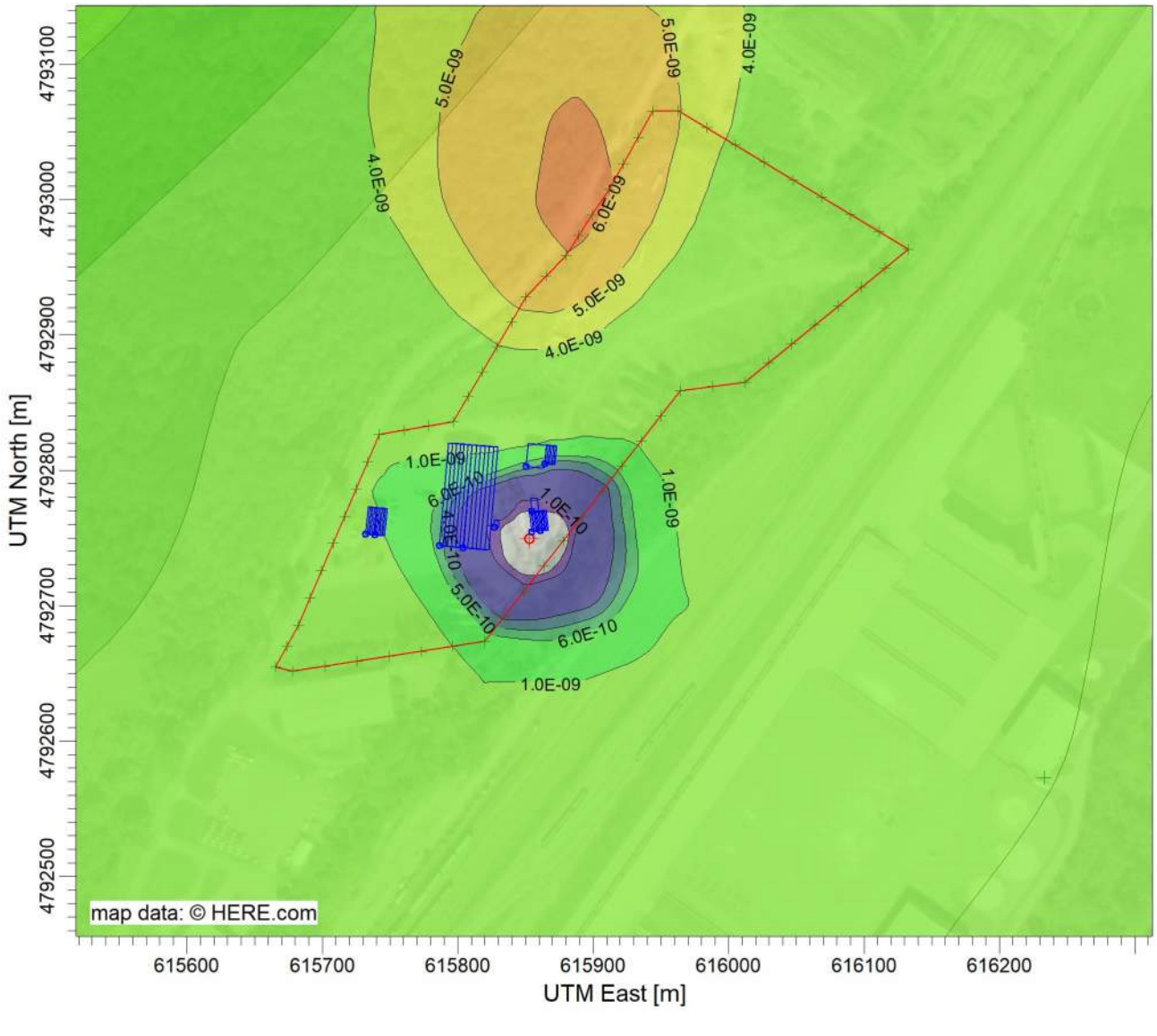
Max: 6.3E-07 [ug/m^3] at (615796.68, 4792835.91)

6.3E-09 1.0E-08 4.0E-08 5.0E-08 6.0E-08 1.0E-07 4.0E-07 5.0E-07 6.0E-07 6.3E-07

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorononanoic Acid (CAS No. 375-95-1) with Incoming Soil Concentration to Facility at 2.061 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**6.3E-07 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

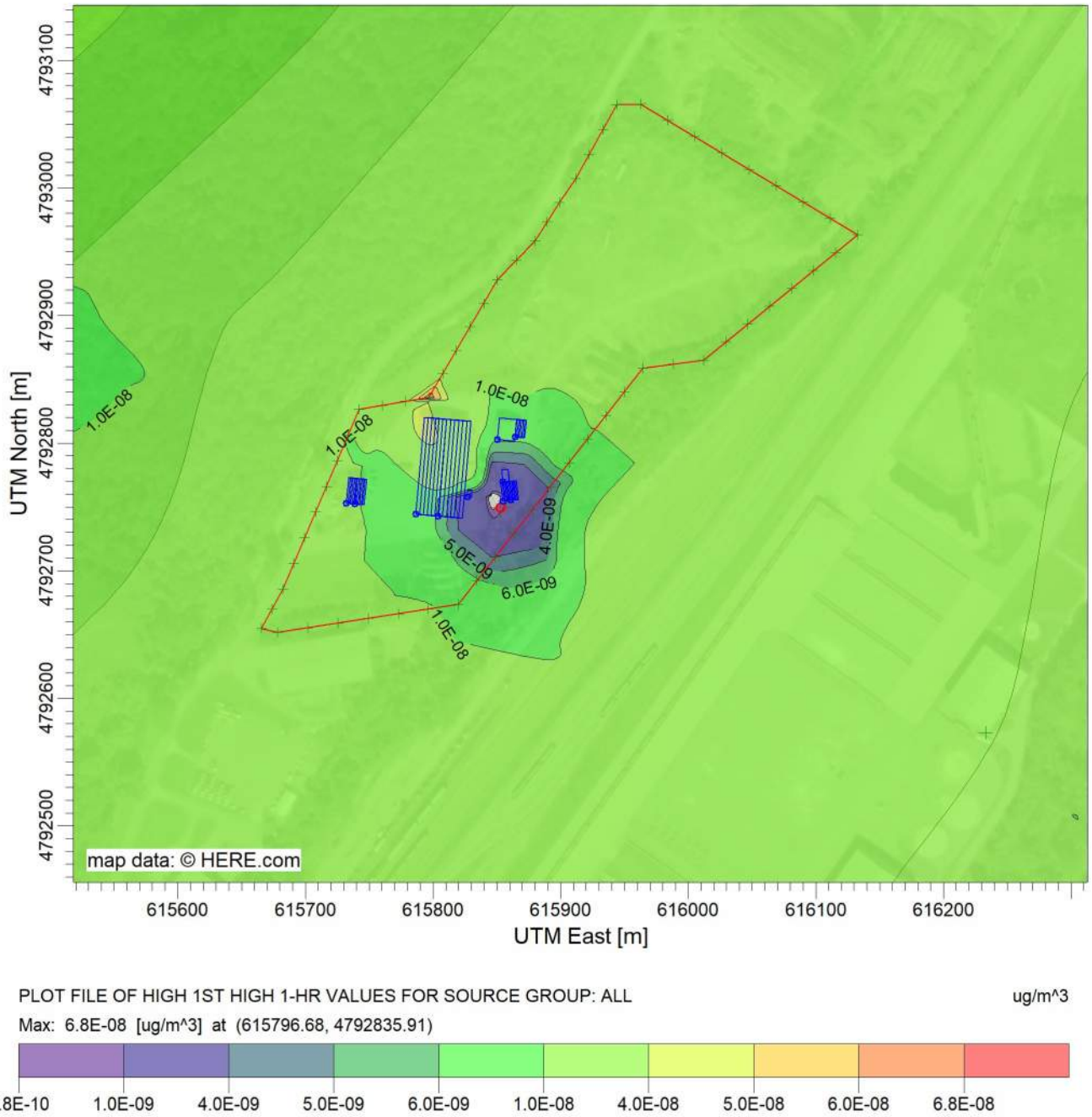
Max: 6.3E-09 [ug/m^3] at (615888.44, 4792991.00)

6.3E-11 1.0E-10 4.0E-10 5.0E-10 6.0E-10 1.0E-09 4.0E-09 5.0E-09 6.0E-09 6.3E-09

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorononanoic Acid (CAS No. 375-95-1) with Incoming Soil Concentration to Facility at 2.061 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**6.3E-09 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

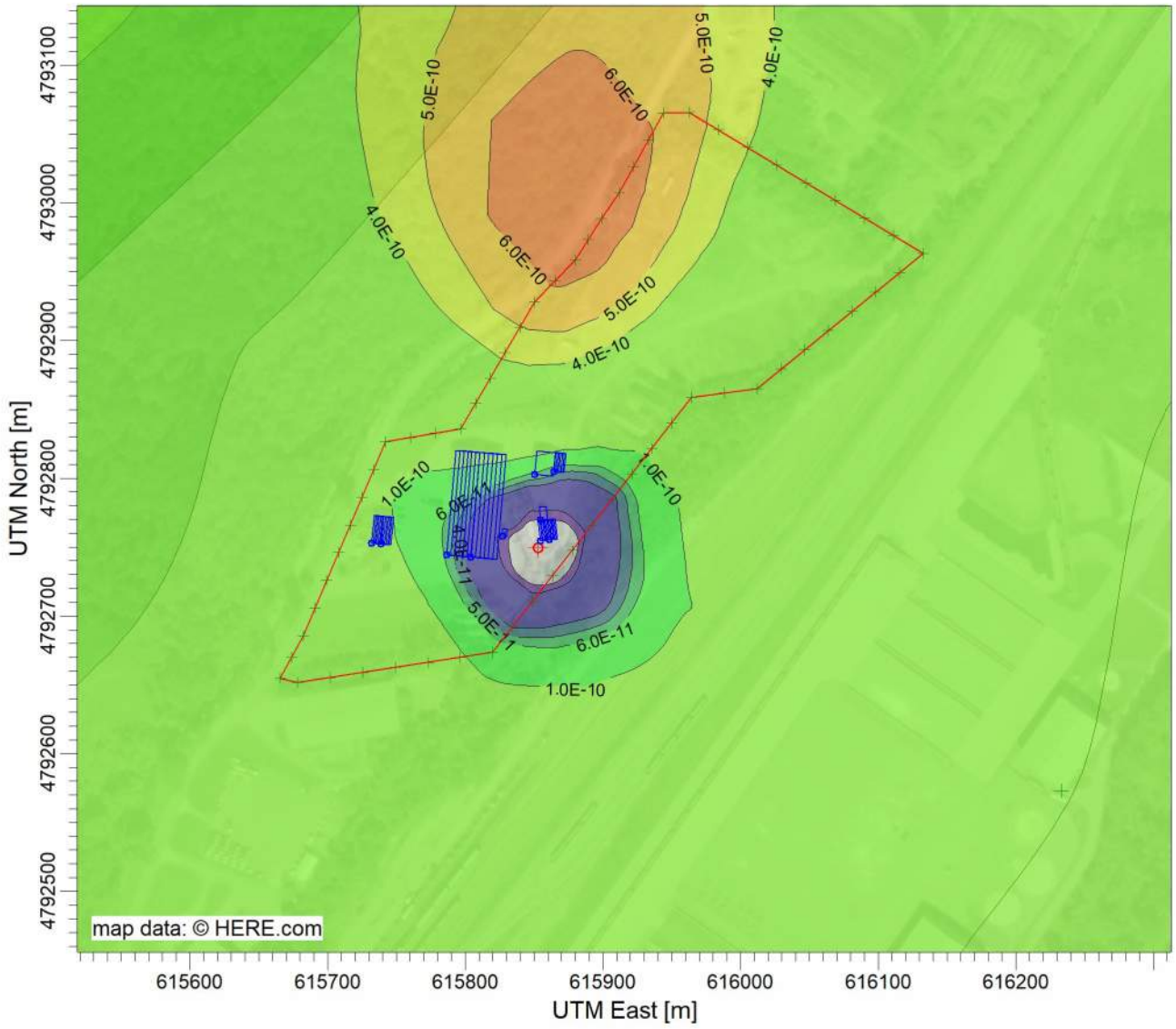
Max: 6.8E-08 [ug/m^3] at (615796.68, 4792835.91)

6.8E-10 1.0E-09 4.0E-09 5.0E-09 6.0E-09 1.0E-08 4.0E-08 5.0E-08 6.0E-08 6.8E-08

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorohexanesulfonic Acid (CAS No. 335-46-4) with Incoming Soil Concentration to Facility at 0.220 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**6.8E-08 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

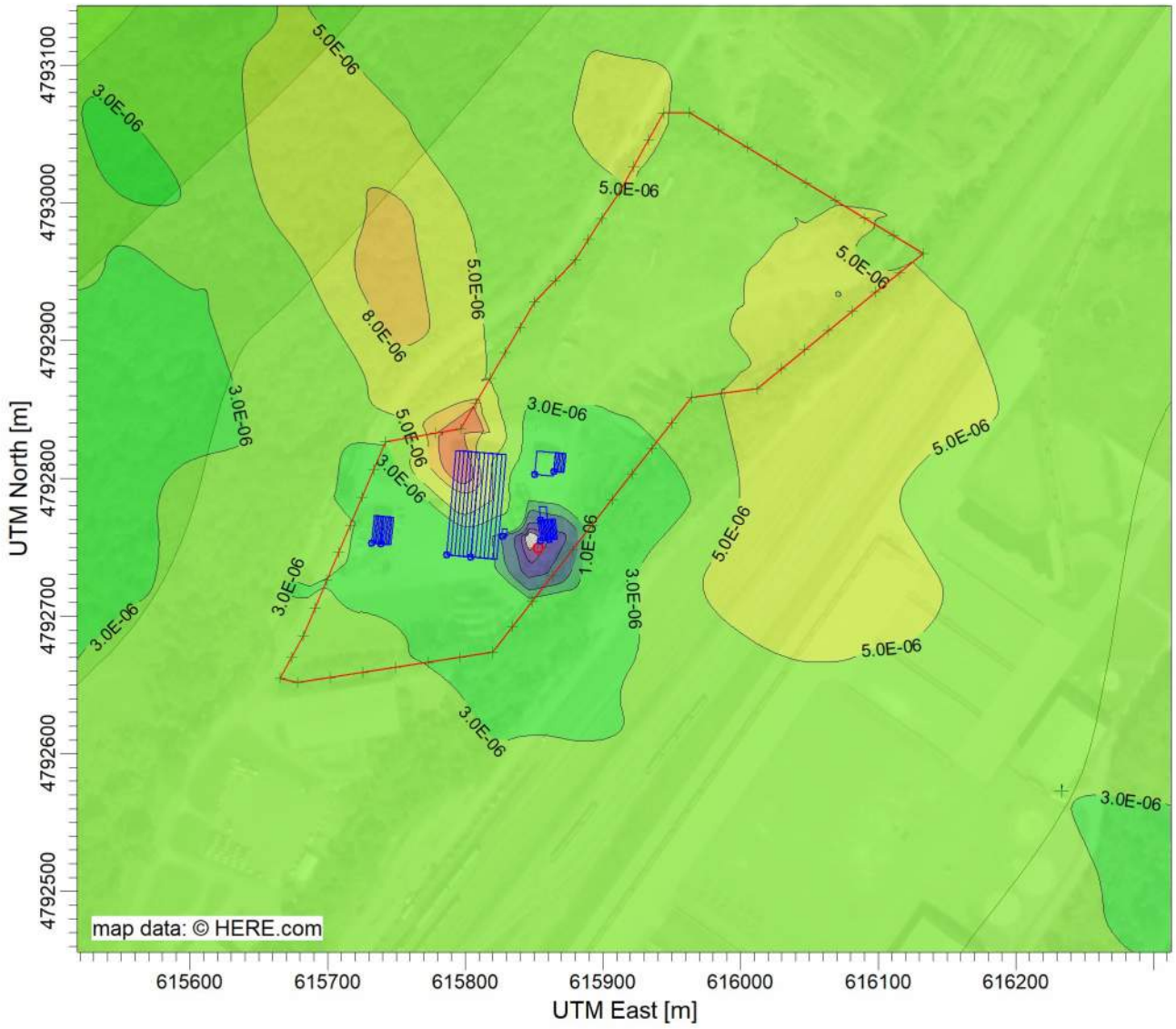
Max: 6.7E-10 [ug/m^3] at (615888.44, 4792991.00)

6.7E-12 1.0E-11 4.0E-11 5.0E-11 6.0E-11 1.0E-10 4.0E-10 5.0E-10 6.0E-10 6.7E-10

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorohexanesulfonic Acid (CAS No. 335-46-4) with Incoming Soil Concentration to Facility at 0.220 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**6.7E-10 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

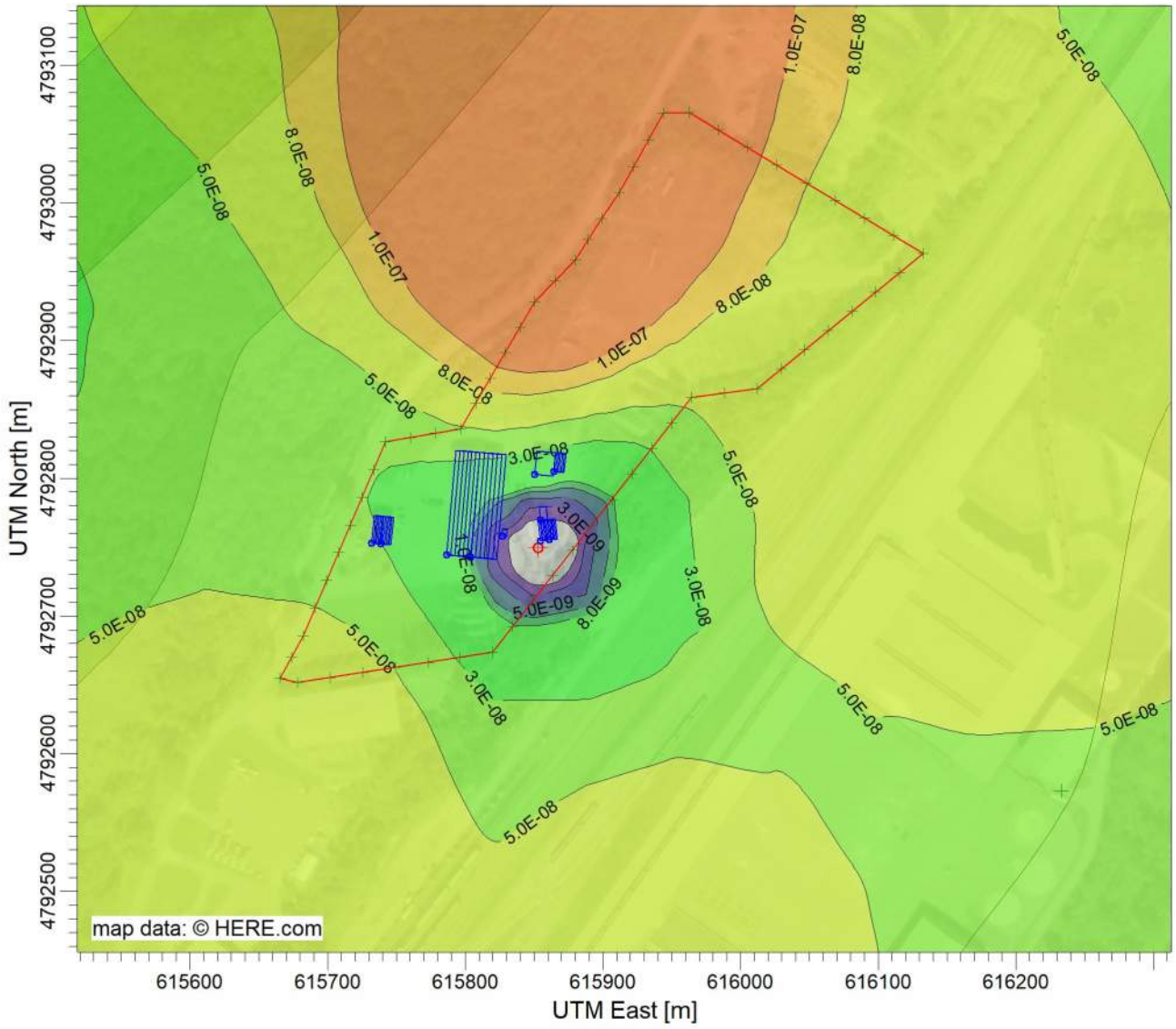
Max: 1.8E-05 [ug/m^3] at (615796.68, 4792835.91)

1.8E-07 3.0E-07 5.0E-07 8.0E-07 1.0E-06 3.0E-06 5.0E-06 8.0E-06 1.0E-05 1.8E-05

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorooctanesulfonic Acid (CAS No. 1763-23-1) with Incoming Soil Concentration to Facility at 58.793 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.8E-05 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

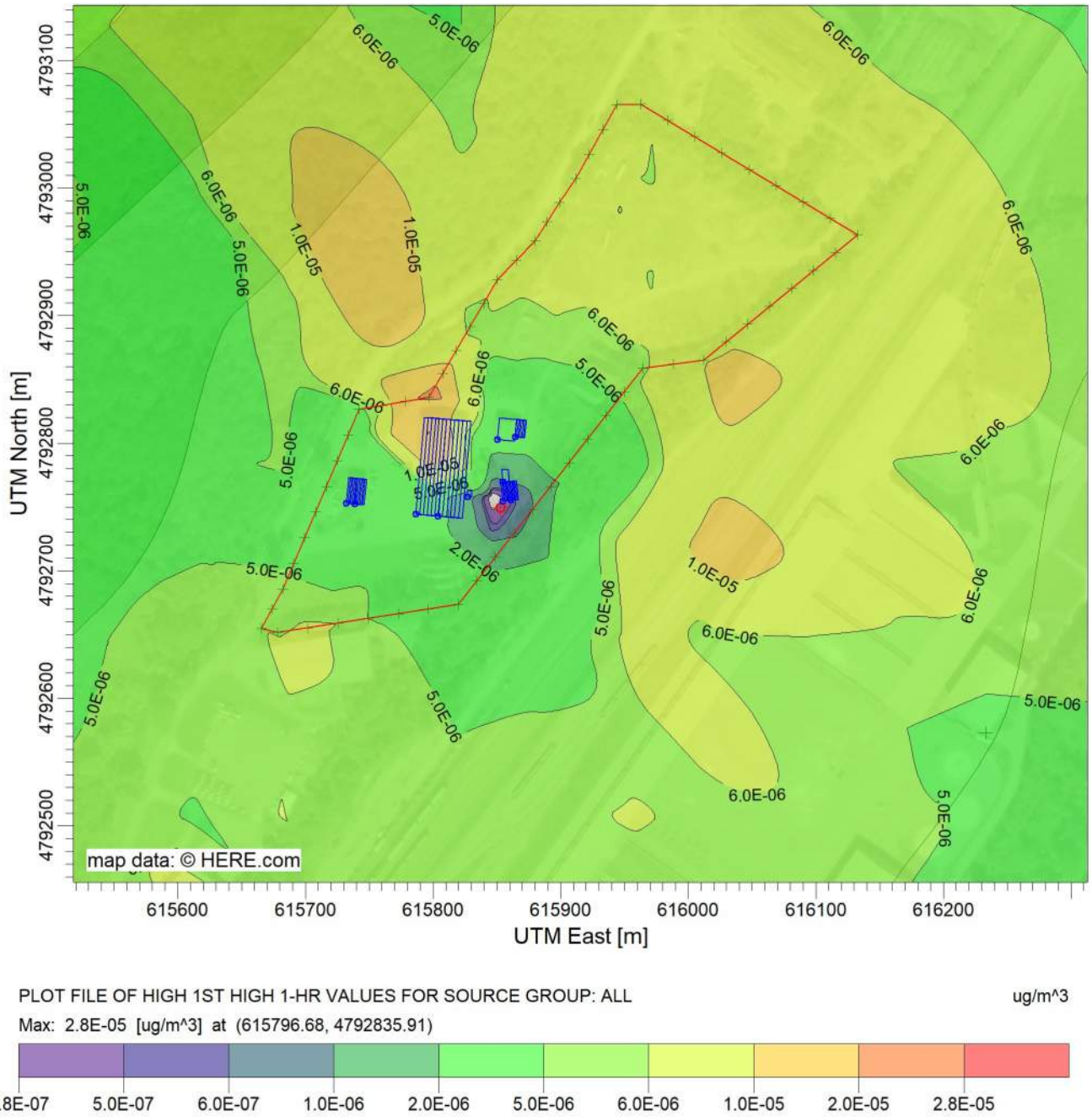
Max: 1.8E-07 [ug/m^3] at (615888.44, 4792991.00)

1.8E-09 3.0E-09 5.0E-09 8.0E-09 1.0E-08 3.0E-08 5.0E-08 8.0E-08 1.0E-07 1.8E-07

| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Perfluorooctanesulfonic Acid (CAS No. 1763-23-1) with Incoming Soil Concentration to Facility at 58.793 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.8E-07 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

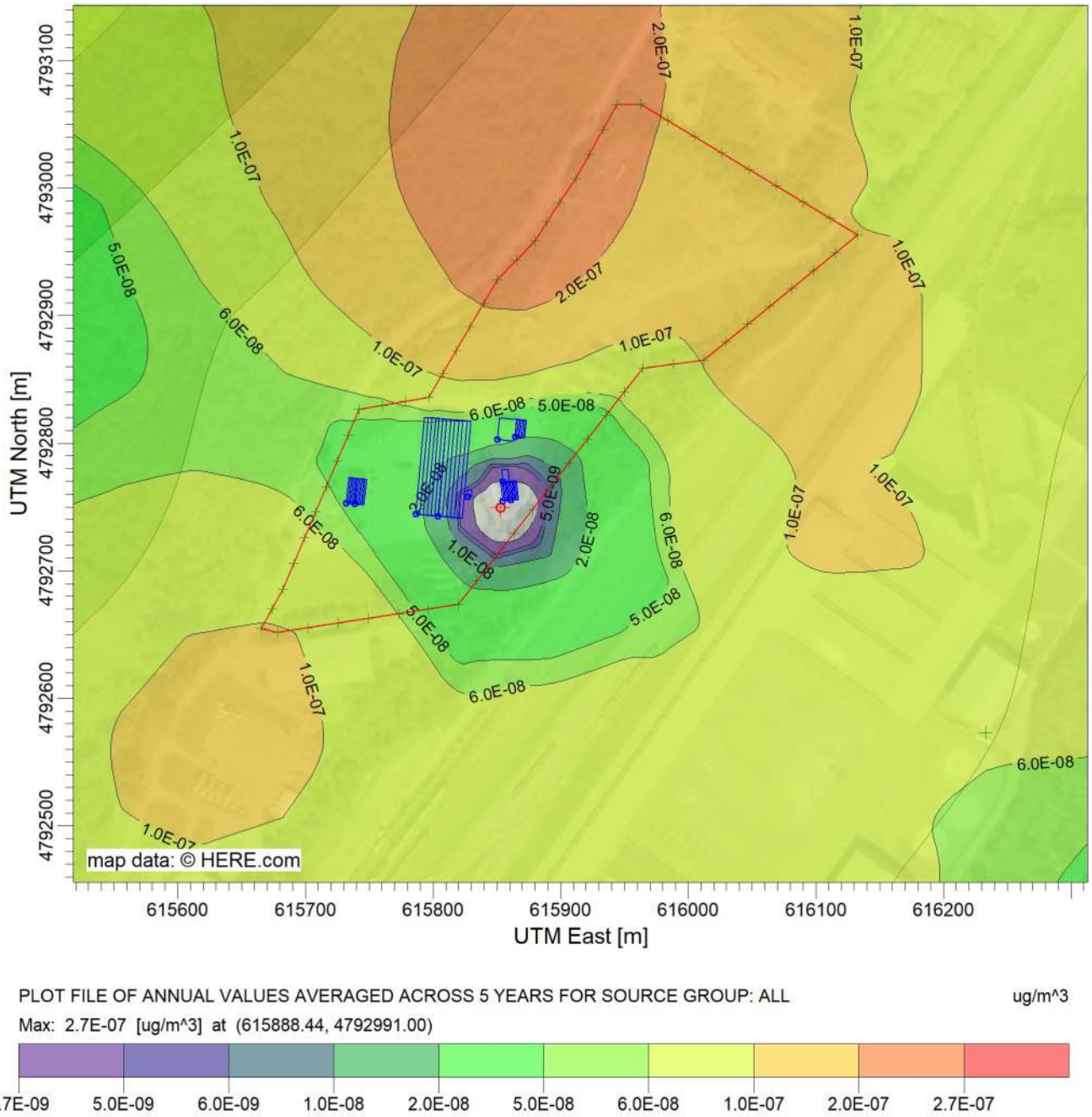
Max: 2.8E-05 [ug/m^3] at (615796.68, 4792835.91)




| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Sum of All PFAS Compounds with Incoming Soil Concentration to Facility at 89.485 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS: **4001** | MODELER: **C.T. MALE STAFF** | |
| | OUTPUT TYPE: **Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX: **2.8E-05 ug/m^3** | DATE: **7/15/2024** | PROJECT NO.: **22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.90% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

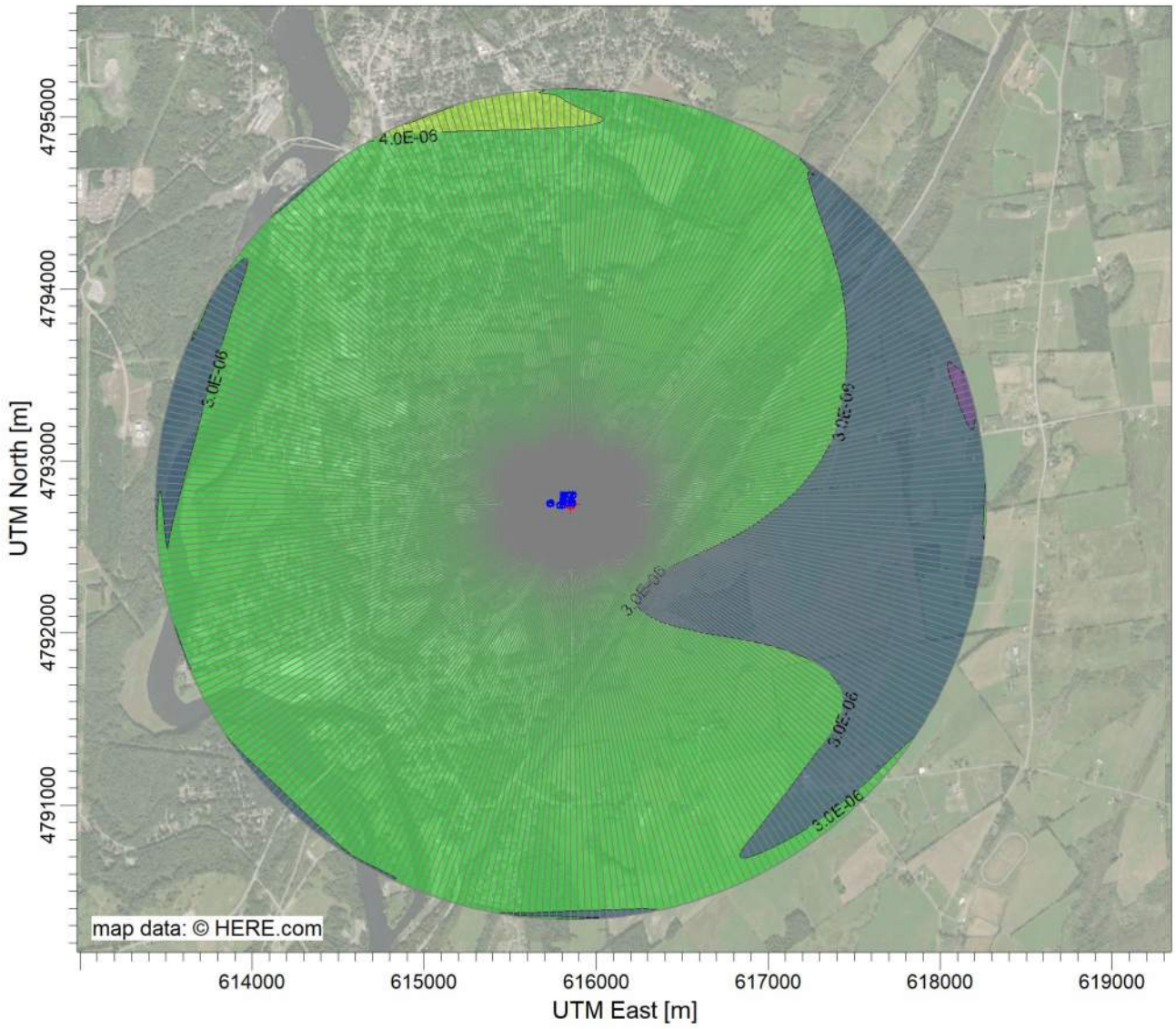
Max: 2.7E-07 [ug/m^3] at (615888.44, 4792991.00)




| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Sum of All PFAS Compounds with Incoming Soil Concentration to Facility at 89.485 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS: **4001** | MODELER: **C.T. MALE STAFF** | |
| | OUTPUT TYPE: **Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX: **2.7E-07 ug/m^3** | DATE: **7/15/2024** | PROJECT NO.: **22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.90% PFAS DRE - At 1.5 mile Endpoint**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

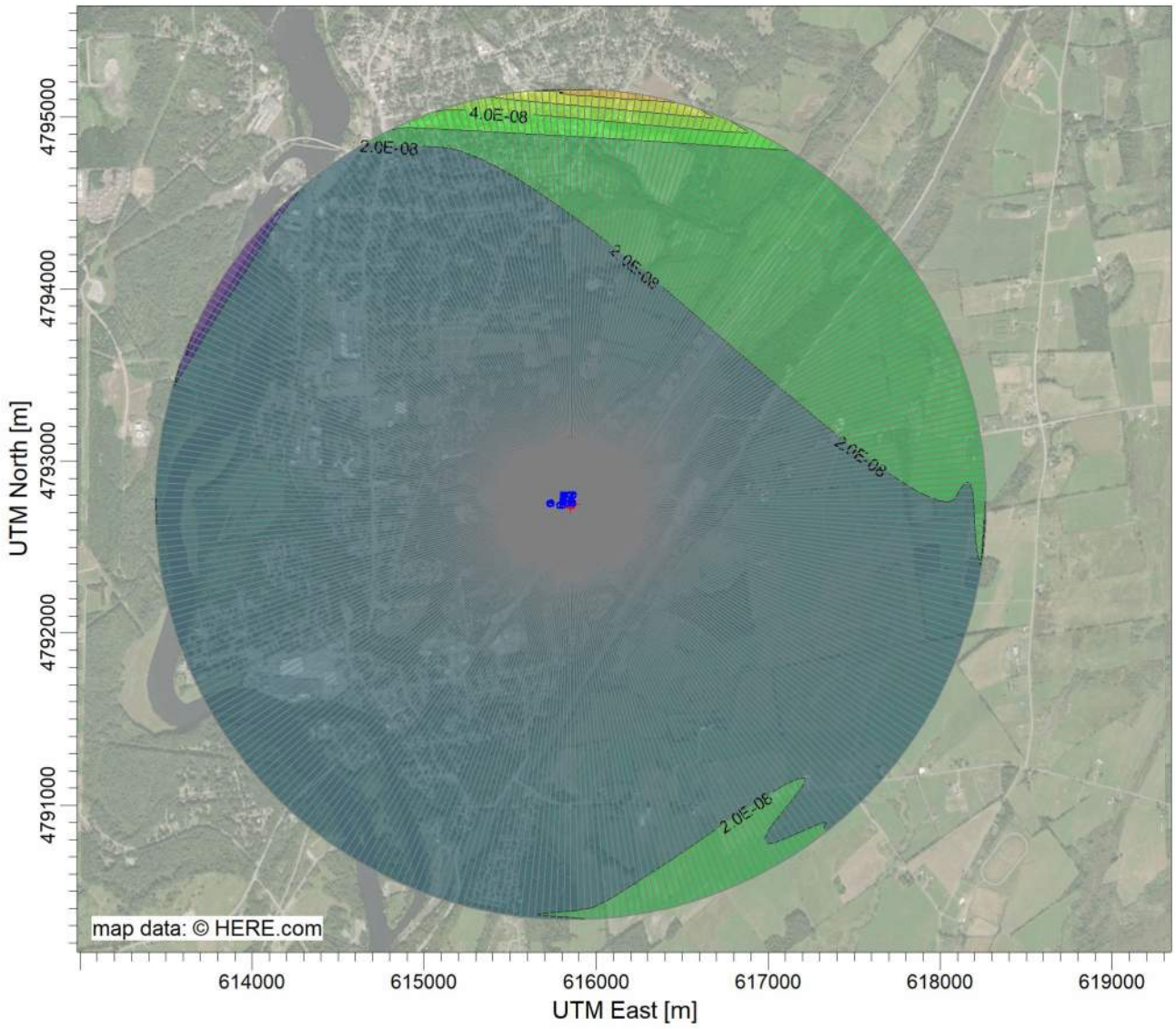
Max: 5.4E-06 [ug/m^3] at (614987.80, 4795003.24)

1.7E-06 2.0E-06 3.0E-06 4.0E-06 5.0E-06 5.4E-06

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Sum of All PFAS Compounds with Incoming Soil Concentration to Facility at 89.485 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**360** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:40,000<br>0 1 km | |
| | MAX:<br>**5.4E-06 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.90% PFAS DRE - At 1.5 mile Endpoint**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

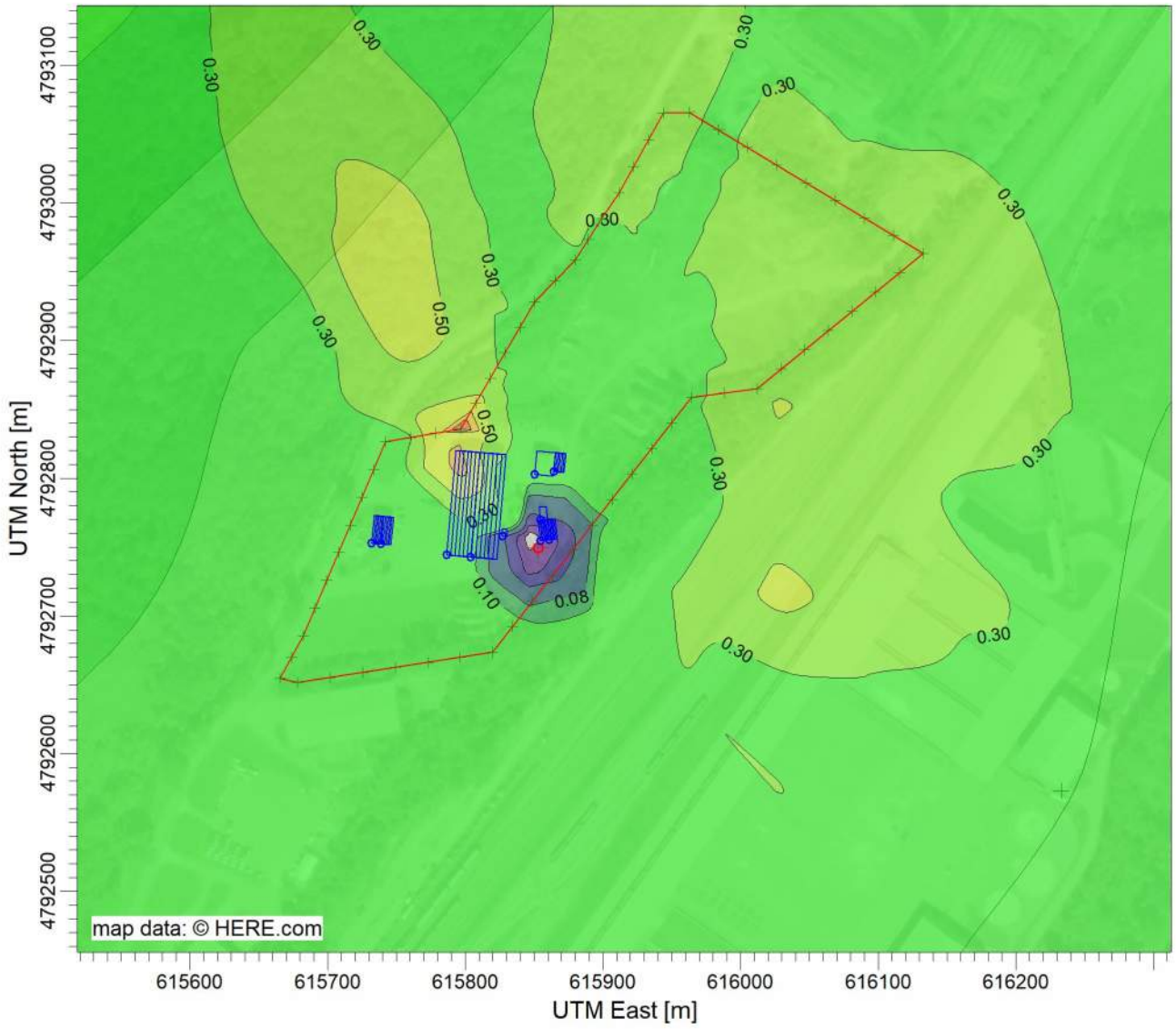
Max: 7.1E-08 [ug/m^3] at (616230.53, 4795133.86)

7.0E-09 9.0E-09 1.0E-08 2.0E-08 3.0E-08 4.0E-08 5.0E-08 6.0E-08 7.0E-08 7.1E-08

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Sum of All PFAS Compounds with Incoming Soil Concentration to Facility at 89.485 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**360** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:40,000<br>0 1 km | |
| | MAX:<br>**7.1E-08 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

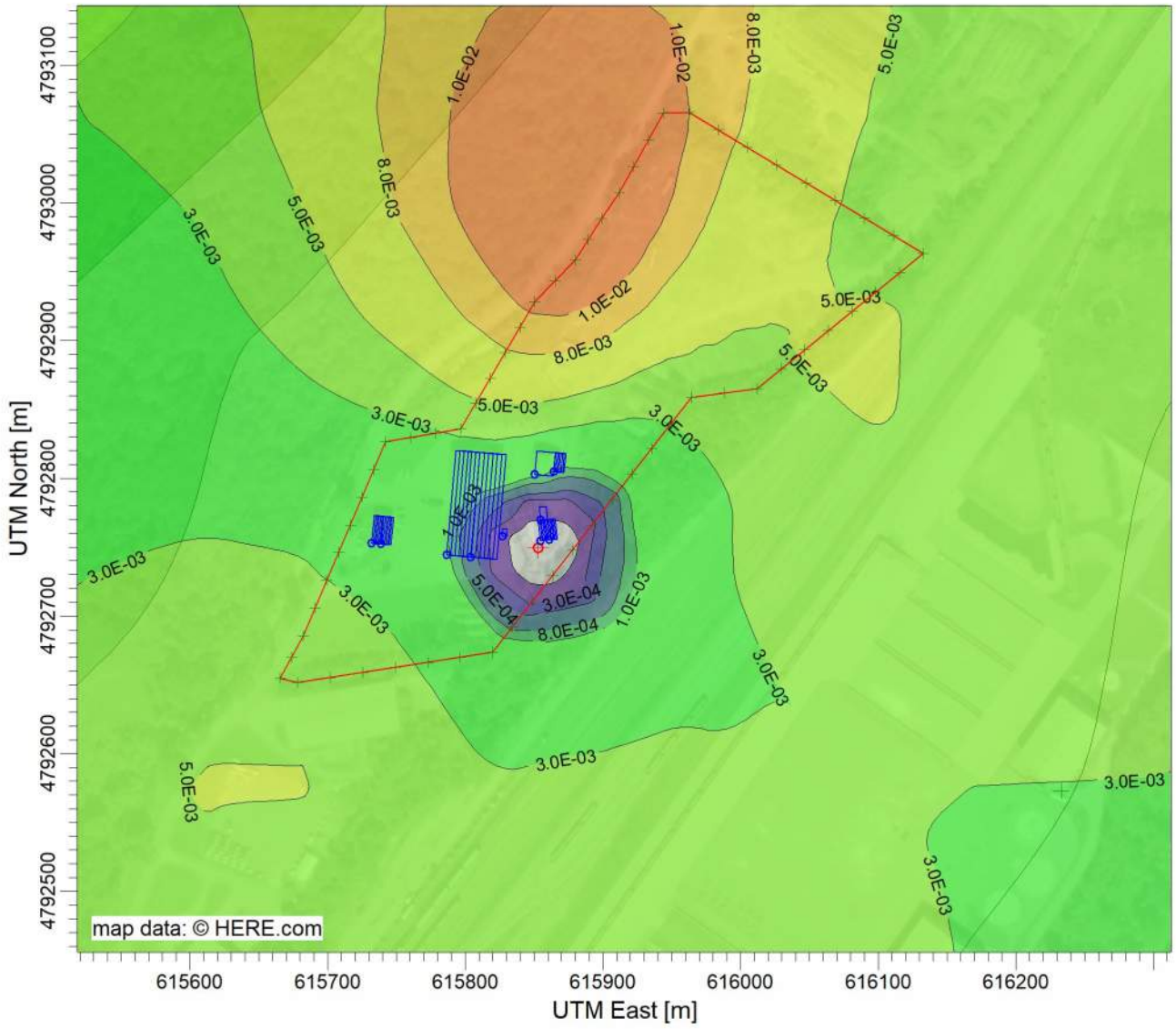
Max: 1.26 [ug/m^3] at (615796.68, 4792835.91)

0.01 0.03 0.05 0.08 0.10 0.30 0.50 0.80 1.00 1.26

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Hydrogen Fluoride (CAS No. 7664-39-3) based on conversion of all Fluoride within PFAS compounds to HF. | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.26 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

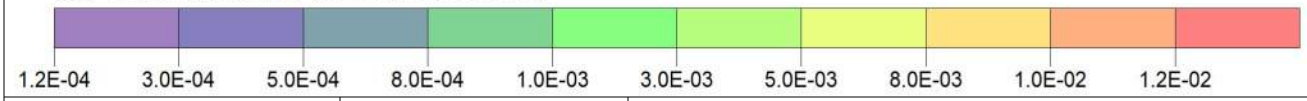
PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

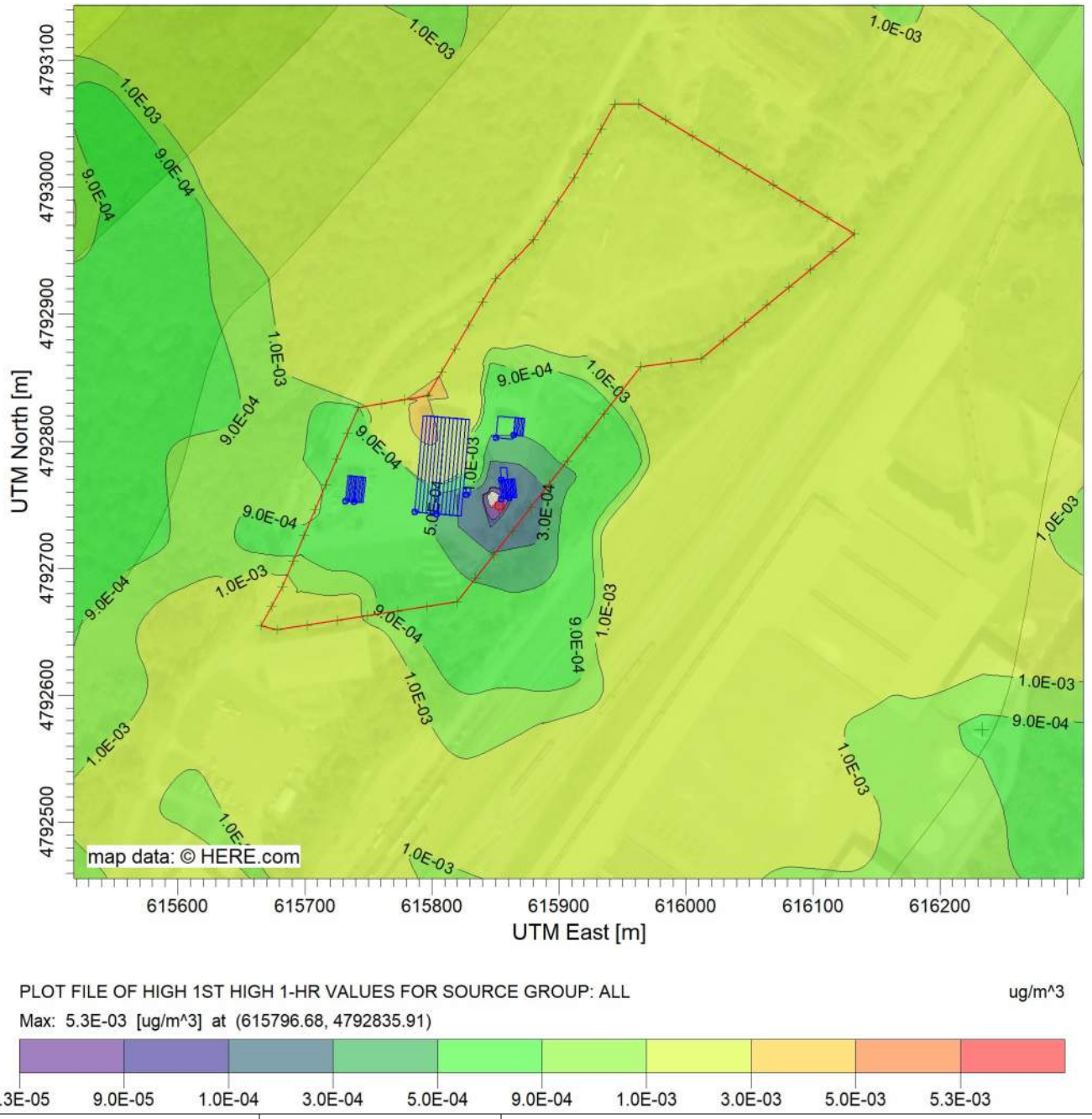
Max: 1.2E-02 [ug/m^3] at (615888.44, 4792991.00)




| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Hydrogen Fluoride (CAS No. 7664-39-3) based on conversion of all Fluoride within PFAS compounds to HF. | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.2E-02 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

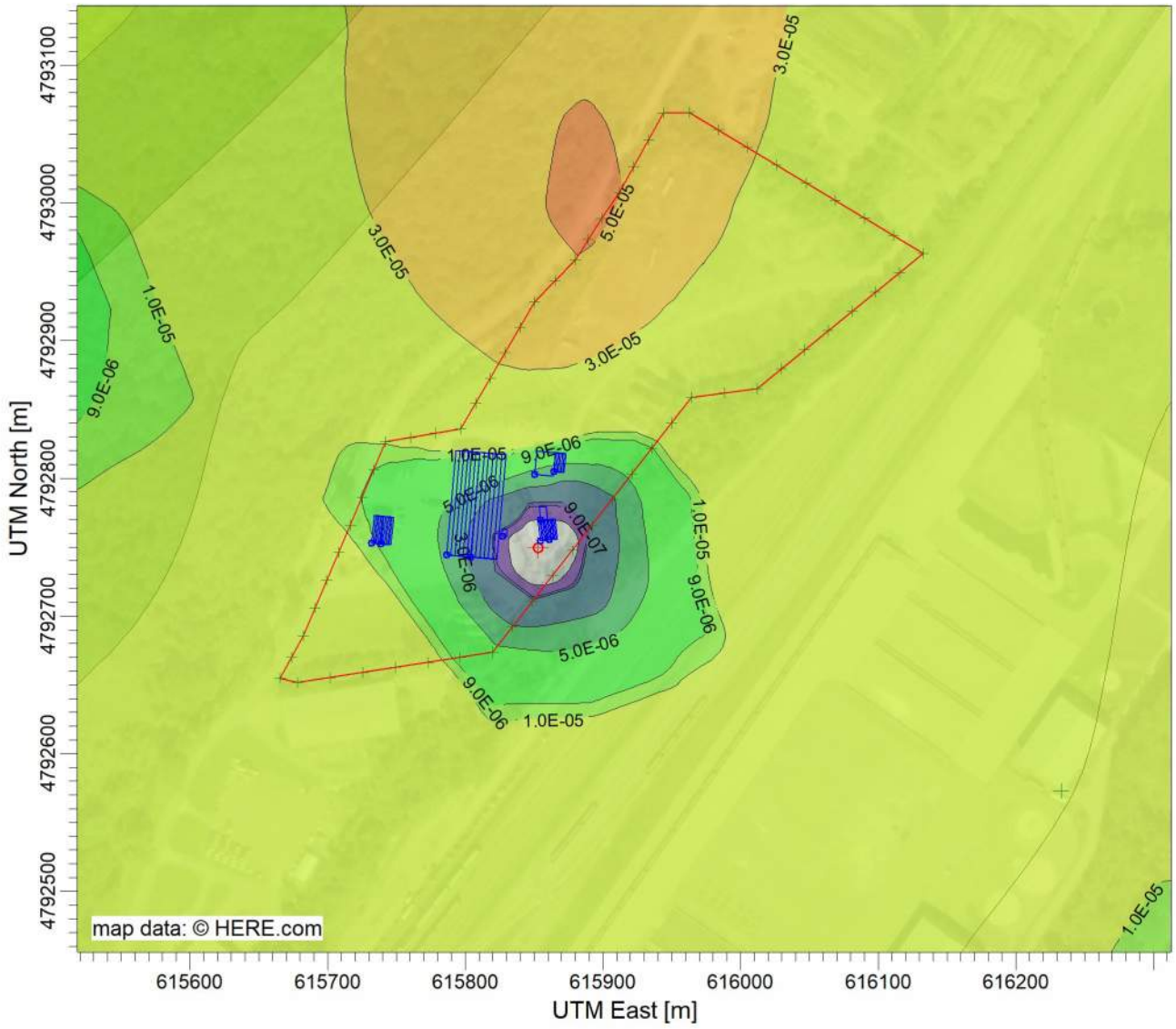
Max: 5.3E-03 [ug/m^3] at (615796.68, 4792835.91)

5.3E-05 9.0E-05 1.0E-04 3.0E-04 5.0E-04 9.0E-04 1.0E-03 3.0E-03 5.0E-03 5.3E-03

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Carbon Tetrafluoride (CAS No. 75-73-0) calculated emission rate based on literature (see reference in air modeling report) | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**5.3E-03 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

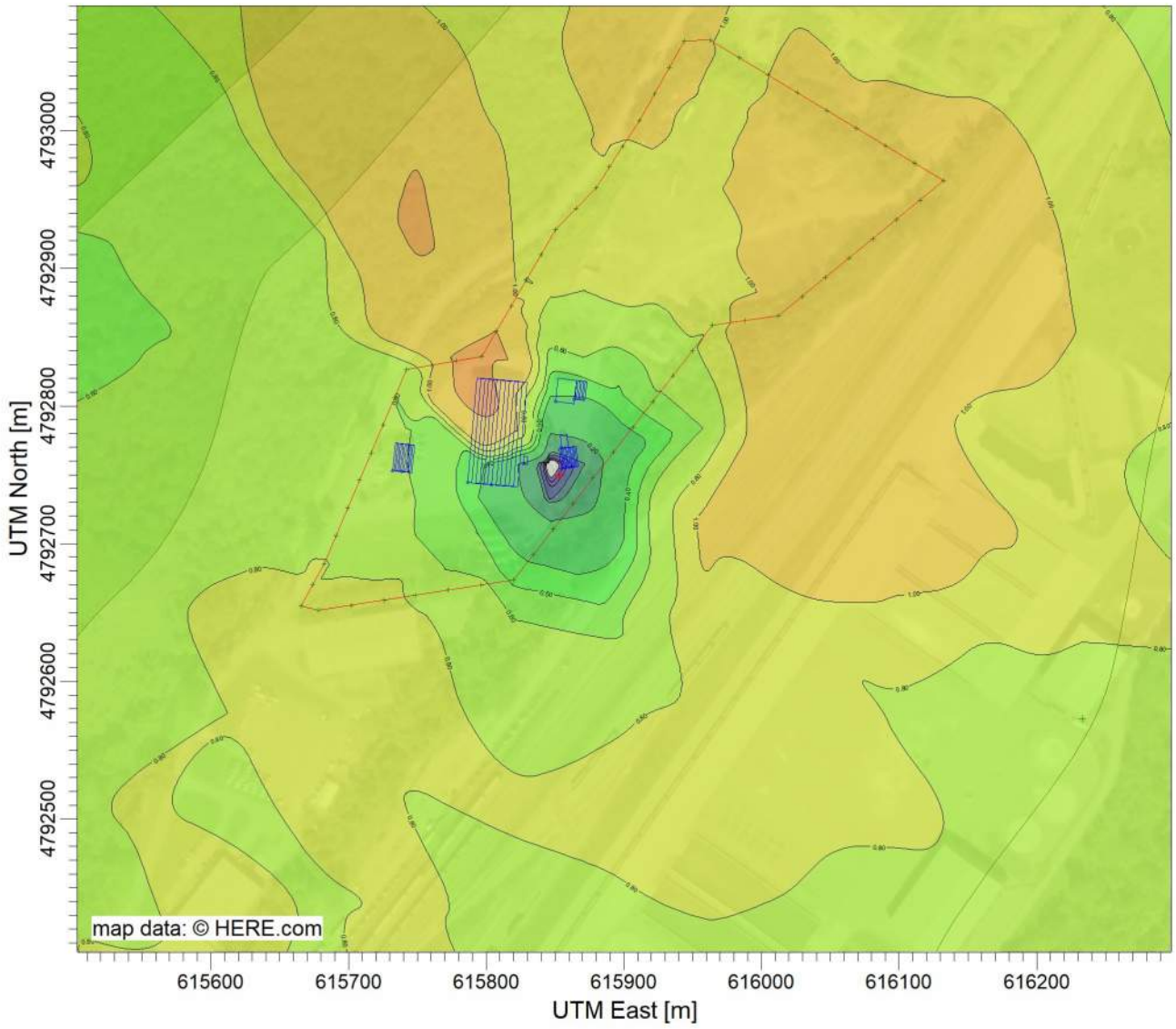
Max: 5.2E-05 [ug/m^3] at (615888.44, 4792991.00)

5.2E-07 9.0E-07 1.0E-06 3.0E-06 5.0E-06 9.0E-06 1.0E-05 3.0E-05 5.0E-05 5.2E-05

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Carbon Tetrafluoride (CAS No. 75-73-0) calculated emission rate based on literature (see reference in air modeling report) | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**5.2E-05 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

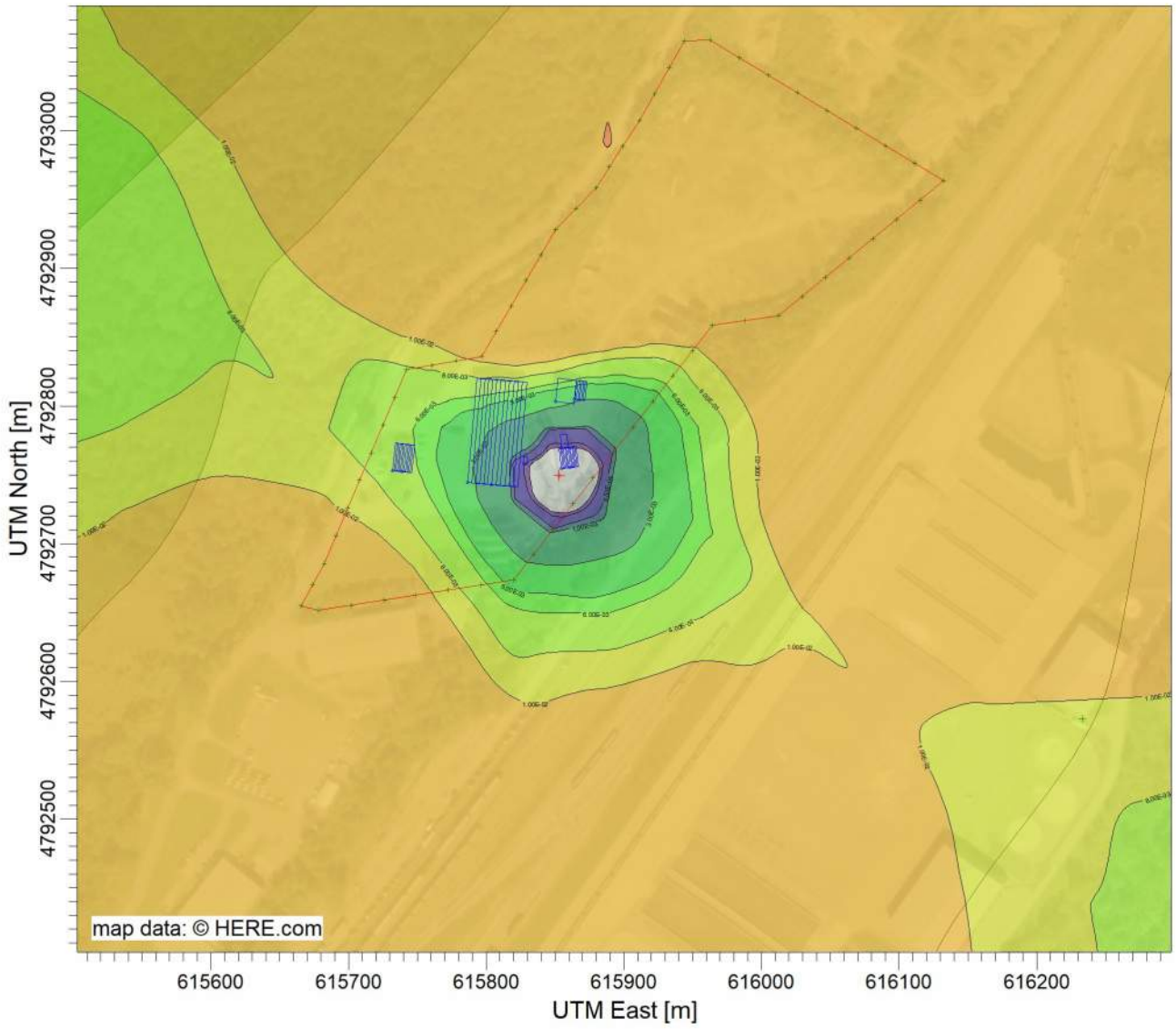
Max: 4.07 [ug/m^3] at (615796.68, 4792835.91)

0.04 0.05 0.06 0.08 0.10 0.20 0.40 0.50 0.60 0.80 1.00 2.00 4.00 4.07

| | | | |
|---|---|---|---|
| COMMENTS: | SOURCES: | COMPANY NAME: | |
| Air Dispersion Results | **1** | **C.T. MALE ASSOCIATES** | |
| "Representative" PFAS at 0.1 g/s | RECEPTORS: | MODELER: | |
| | **4001** | **C.T. MALE STAFF** | |
| | OUTPUT TYPE: | SCALE: 1:5,000 | |
| | **Concentration** | 0 0.1 km | |
| | MAX: | DATE: | PROJECT NO.: |
| | **4.07 ug/m^3** | **7/15/2024** | **22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

Max: 4.02E-02 [ug/m^3] at (615888.44, 4792991.00)

4.00E-04 5.00E-04 8.00E-04 1.00E-03 3.00E-03 5.00E-03 6.00E-03 8.00E-03 1.00E-02 4.00E-02 4.02E-02

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br>"Representative" PFAS at 0.1 g/s | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**4.02E-02 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

# Attachment B

## Summary of Dispersion Modeling Results and Graphical Representations of Output at 99.99% Destruction Efficiency

| Compound | CAS# | Soil Concentration (in ppb) | Emission Rate based on 99.99% DRE (in g/s) | Dispersion Results (in ug/m^3) | | File Name |
|---|---|---|---|---|---|---|
| | | | | Maximum Hourly | Maximum Annual | |
| **Perfluorobutane Sulfonate (PFBS)** | 375-73-5 | 0.085 | 6.42589E-11 | 2.61465E-09 | 2.58169E-11 | PFBS9999 |
| **Perfluorooctanoic acid (PFOA)** | 335-67-1 | 4.482 | 3.38833E-09 | 1.37869E-07 | 1.36131E-09 | PFOA9999 |
| **Perfluorononanoic acid (PFNA)** | 375-95-1 | 2.061 | 1.55809E-09 | 6.33975E-08 | 6.25984E-10 | PFNA9999 |
| **Perfluorohexanesulfonic acid (PFHxS)** | 335-46-4 | 0.220 | 1.66E-10 | 6.76733E-09 | 6.68202E-11 | PFHS9999 |
| **Perfluorooctanesulfonic acid (PFOS)** | 1763-23-1 | 58.793 | 4.44E-08 | 1.80851E-06 | 1.78571E-08 | PFOS9999 |
| **Sum of all PFAS Compounds[1]** | N/A | 89.485 | 6.76495E-08 | 2.75261E-06 | 2.71791E-08 | PFAS9999 |
| **Hydrogen Fluoride (HF)[2]** | 7664-39-3 | N/A | 3.08737E-02 | 1.25623 | 1.24039E-02 | HF |
| **Carbon Tetrafluoride ($CF_4$)[3]** | 75-73-0 | N/A | 1.29685E-04 | 5.27681E-03 | 5.21029E-05 | CF4 |
| **"Representative" PFAS at 0.1 g/s** | N/A | N/A | 0.1 | 4.06893 | 4.01764E-02 | CEFE2023 |

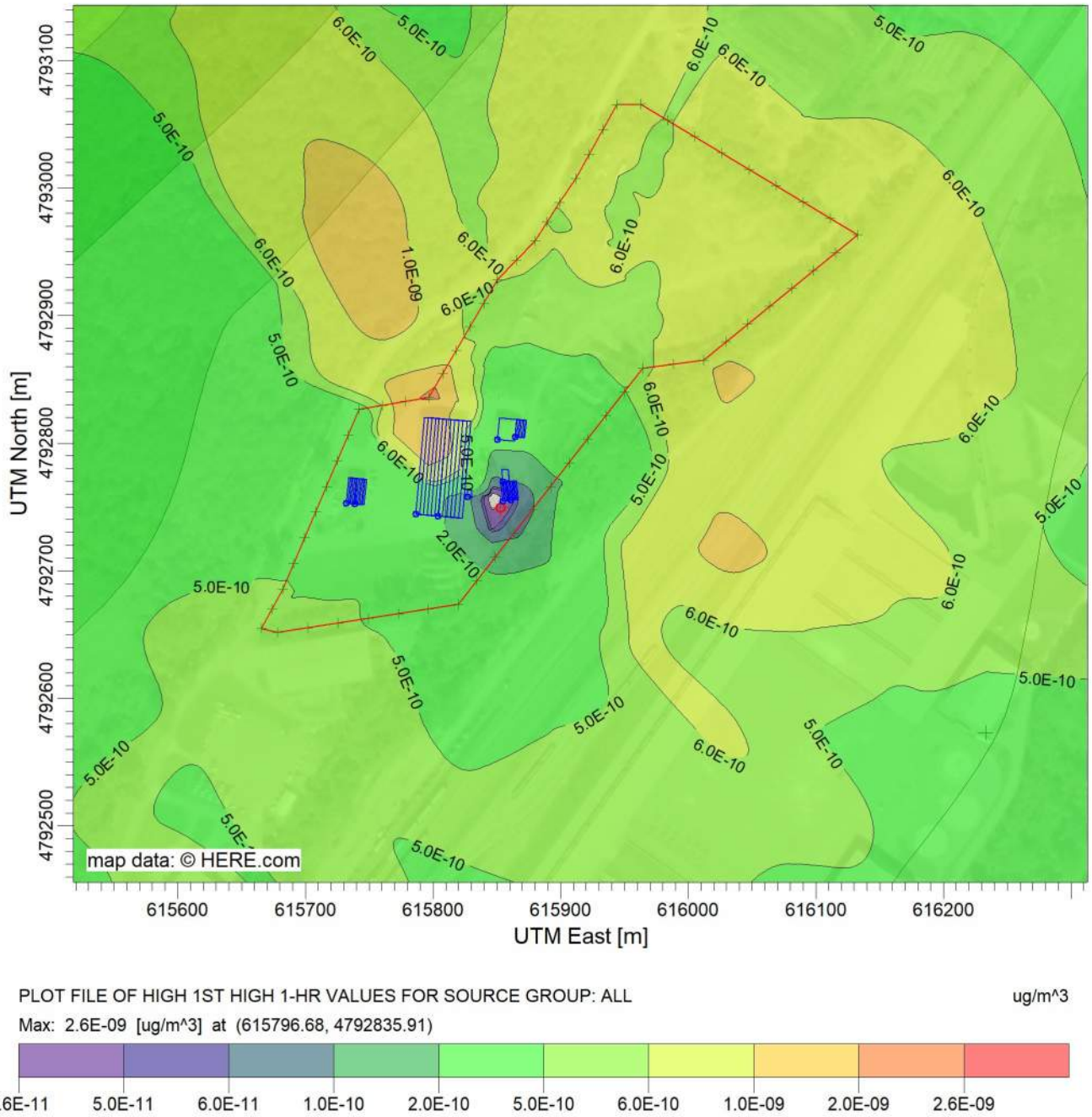
[1] - Sum of all sampled PFAS compounds.

[2] - Calculated emission rate based on conversion of all fluorine within PFAS compounds to hydrofluoric acid.

[3] - Calculated emission rate based on the following article:
Jonathan D. Krug, Paul M. Lemieux, Chun-Wai Lee, Jeffrey V. Ryan, Peter H. Kariher, Erin P. Shields, Lindsay C. Wickersham, Martin K. Denison, Kevin A. Davis, David A. Swensen, R. Preston Burnette, Jost O.L. Wendt & William P. Linak (2022) Combustion of C1 and C2 PFAS: Kinetic modeling and experiments, Journal of the Air & Waste Management Association, 72:3, 256-270, DOI: 10.1080/10962247.2021.2021317

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

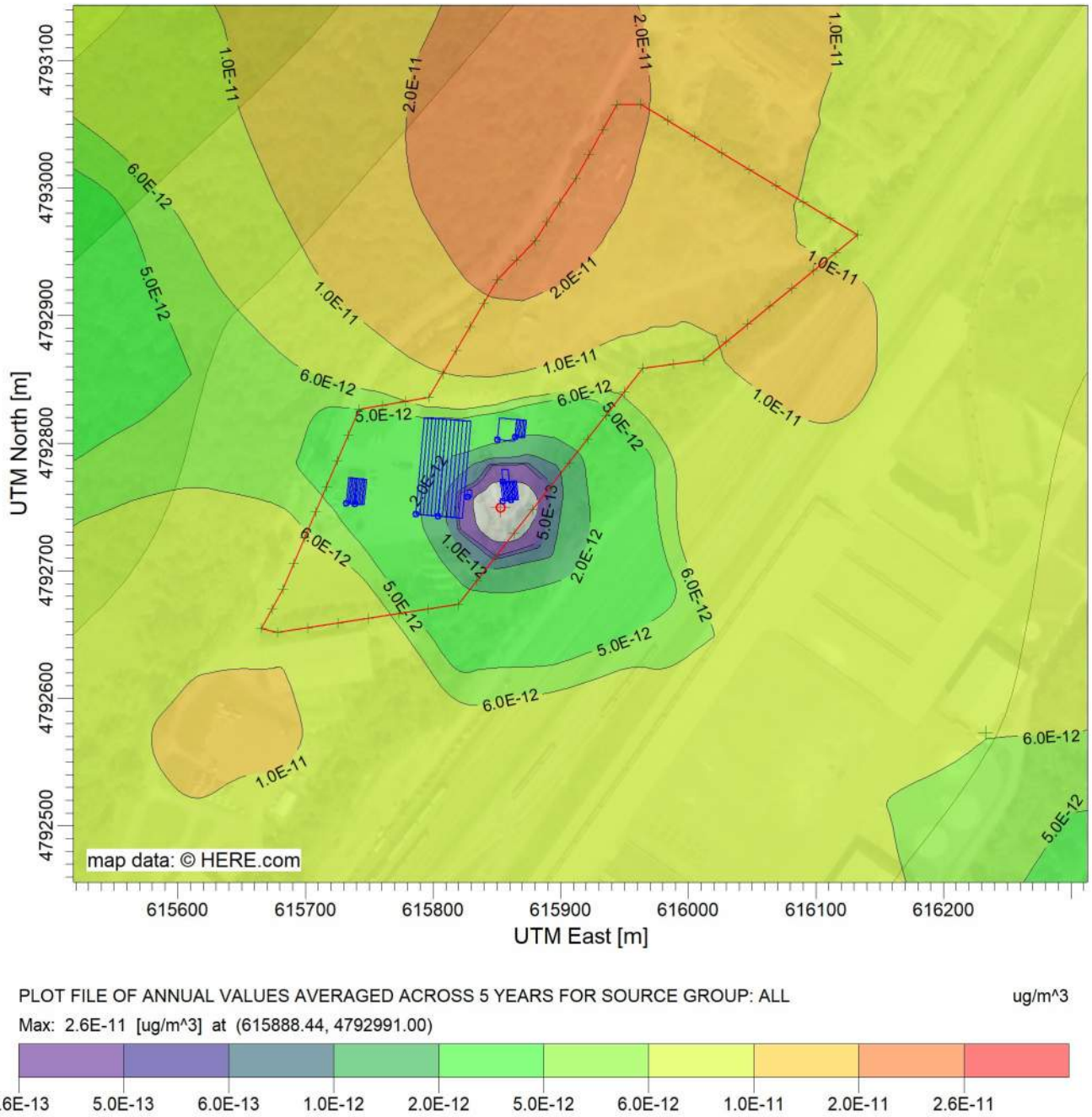
Max: 2.6E-09 [ug/m^3] at (615796.68, 4792835.91)

2.6E-11 5.0E-11 6.0E-11 1.0E-10 2.0E-10 5.0E-10 6.0E-10 1.0E-09 2.0E-09 2.6E-09

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorobutane Sulfonate (CAS No. 375-73-5) with Incoming Soil Concentration to Facility at 0.085 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**2.6E-09 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

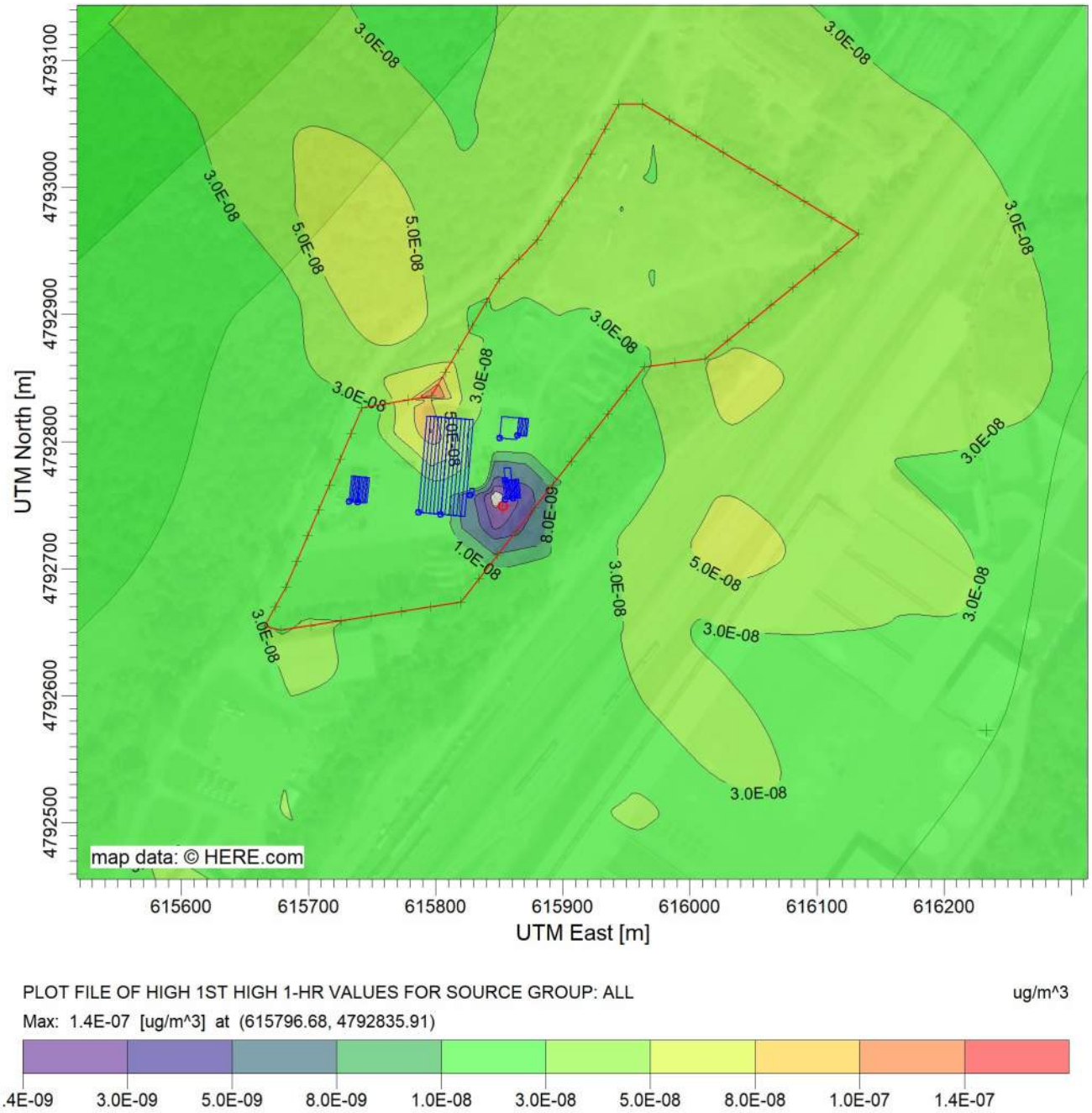
Max: 2.6E-11 [ug/m^3] at (615888.44, 4792991.00)

2.6E-13 5.0E-13 6.0E-13 1.0E-12 2.0E-12 5.0E-12 6.0E-12 1.0E-11 2.0E-11 2.6E-11

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorobutane Sulfonate (CAS No. 375-73-5) with Incoming Soil Concentration to Facility at 0.085 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**2.6E-11 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

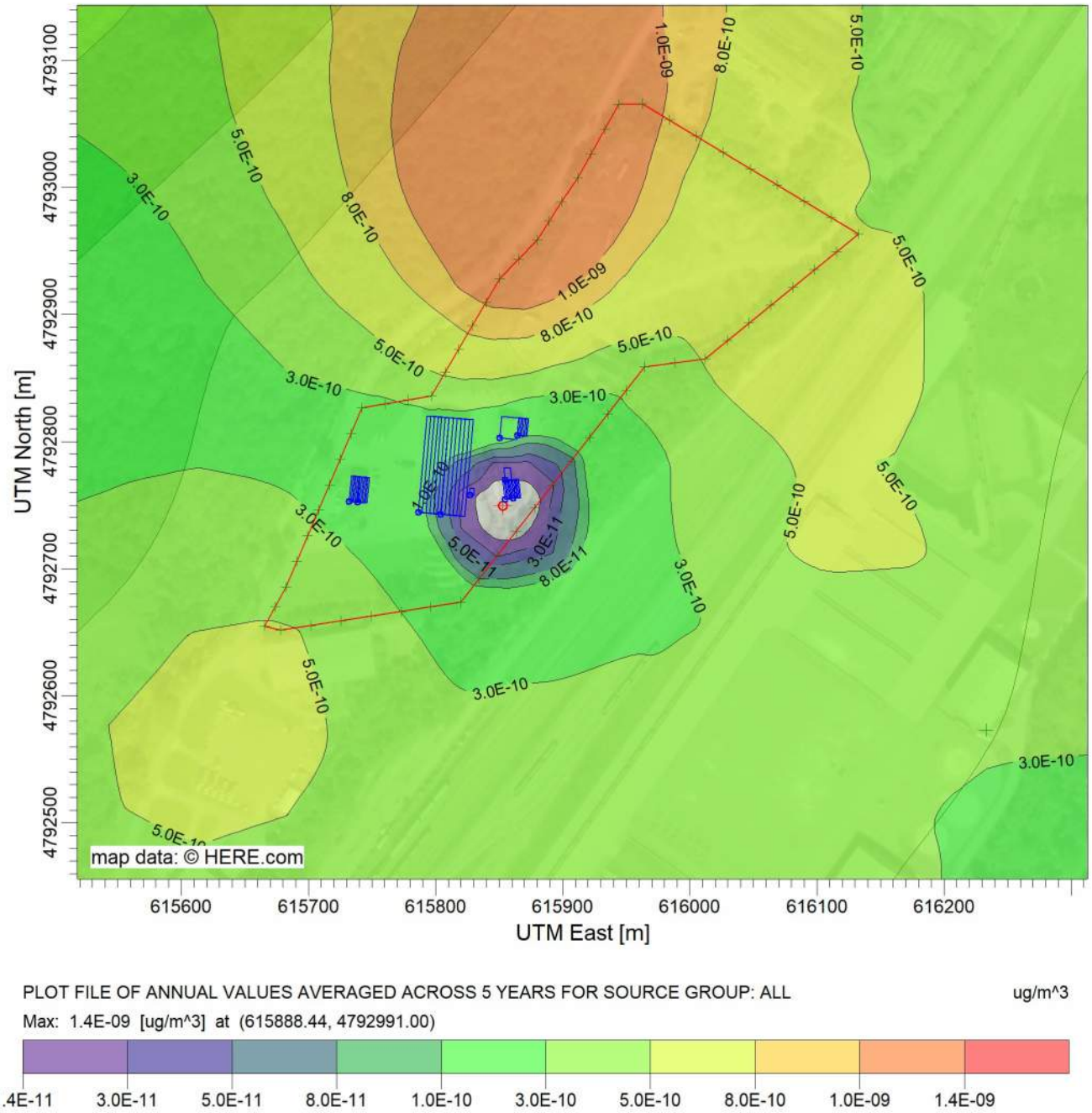
Max: 1.4E-07 [ug/m^3] at (615796.68, 4792835.91)

1.4E-09 3.0E-09 5.0E-09 8.0E-09 1.0E-08 3.0E-08 5.0E-08 8.0E-08 1.0E-07 1.4E-07

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorooctanoic Acid (CAS No. 335-67-1) with Incoming Soil Concentration to Facility at 4.482 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.4E-07 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

Max: 1.4E-09 [ug/m^3] at (615888.44, 4792991.00)

1.4E-11 | 3.0E-11 | 5.0E-11 | 8.0E-11 | 1.0E-10 | 3.0E-10 | 5.0E-10 | 8.0E-10 | 1.0E-09 | 1.4E-09

| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Perfluorooctanoic Acid (CAS No. 335-67-1) with Incoming Soil Concentration to Facility at 4.482 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.4E-09 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dipersion Concentration Based on 99.99% PFAS DRE**


PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

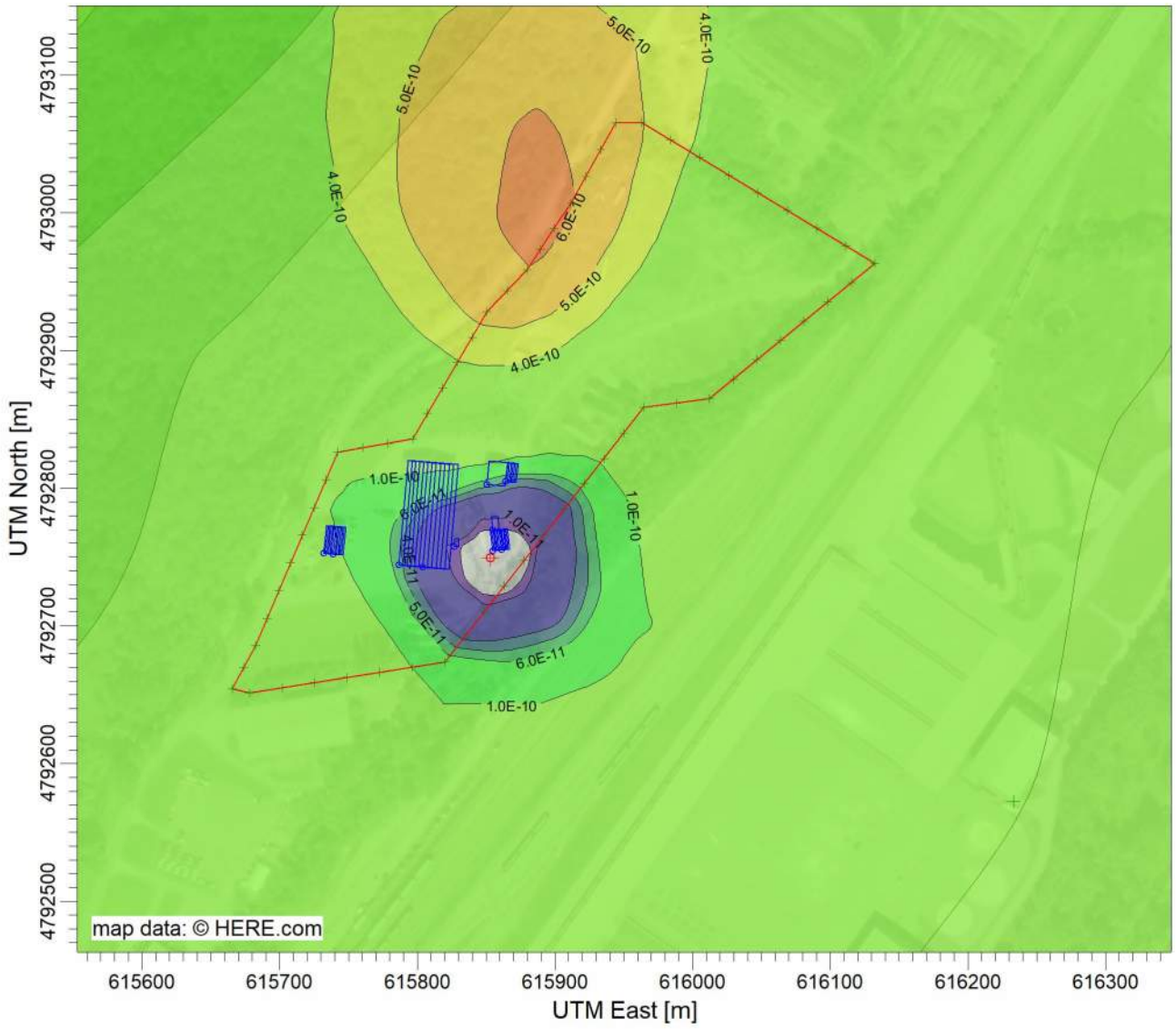
Max: 6.3E-08 [ug/m^3] at (615796.68, 4792835.91)

6.3E-10 1.0E-09 4.0E-09 5.0E-09 6.0E-09 1.0E-08 4.0E-08 5.0E-08 6.0E-08 6.3E-08

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorononanoic Acid (CAS No. 375-95-1) with Incoming Soil Concentration to Facility at 2.061 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**6.3E-08 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dipersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

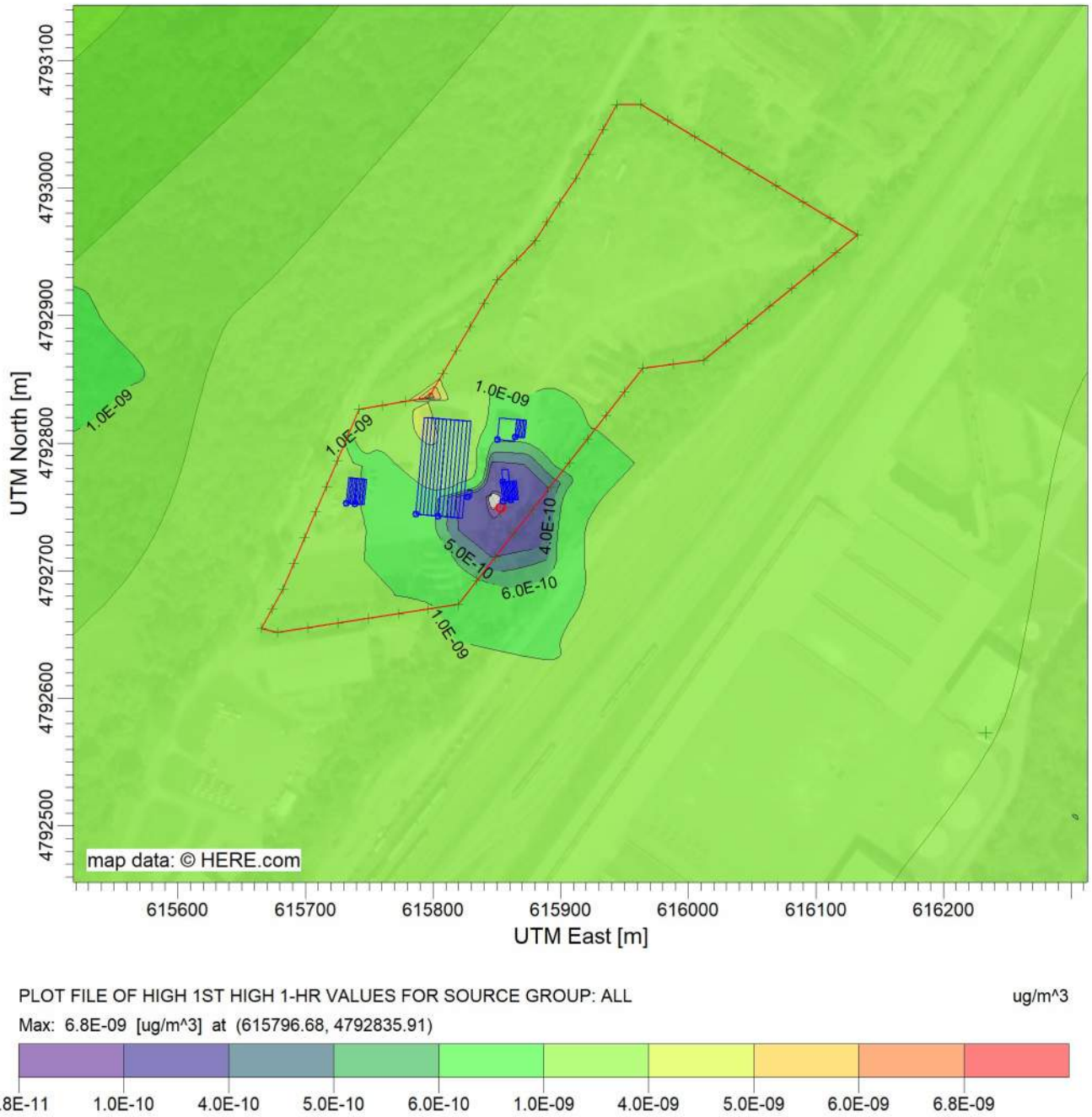
Max: 6.3E-10 [ug/m^3] at (615888.44, 4792991.00)

6.3E-12 1.0E-11 4.0E-11 5.0E-11 6.0E-11 1.0E-10 4.0E-10 5.0E-10 6.0E-10 6.3E-10

| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Perfluorononanoic Acid (CAS No. 375-95-1) with Incoming Soil Concentration to Facility at 2.061 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**6.3E-10 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

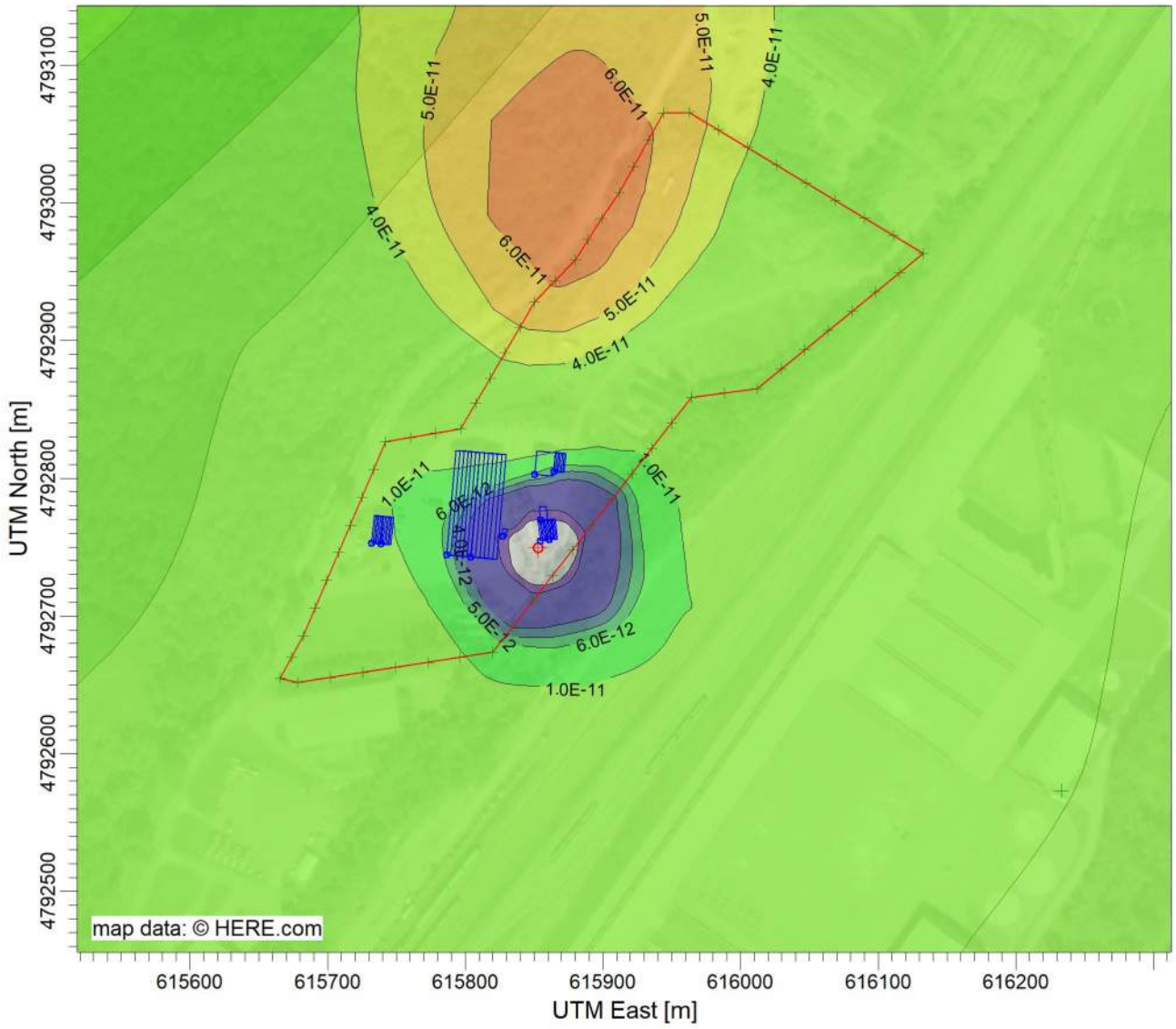
Max: 6.8E-09 [ug/m^3] at (615796.68, 4792835.91)

6.8E-11 1.0E-10 4.0E-10 5.0E-10 6.0E-10 1.0E-09 4.0E-09 5.0E-09 6.0E-09 6.8E-09

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Perfluorohexanesulfonic Acid (CAS No. 335-46-4) with Incoming Soil Concentration to Facility at 0.220 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**6.8E-09 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

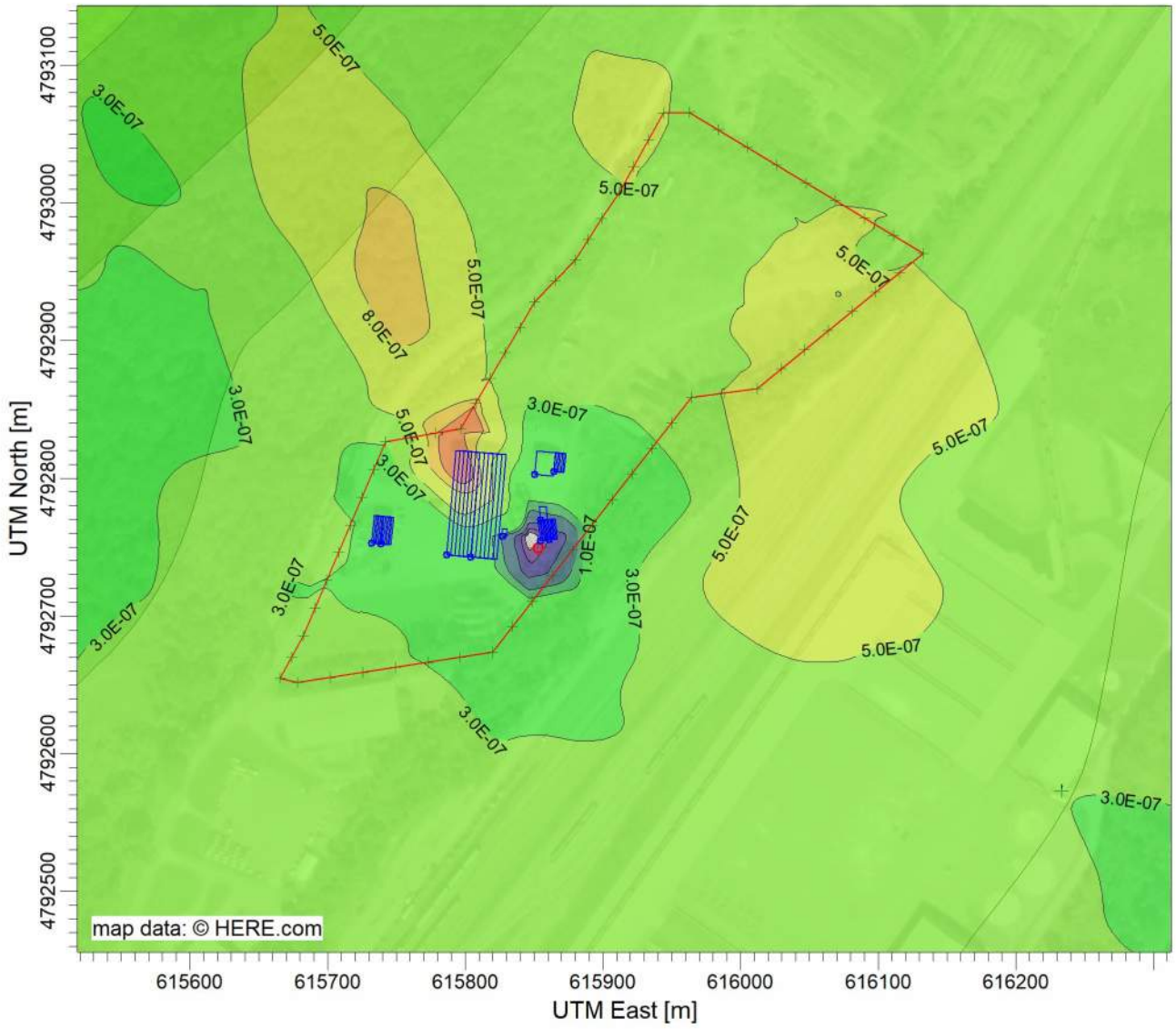
Max: 6.7E-11 [ug/m^3] at (615888.44, 4792991.00)

6.7E-13 1.0E-12 4.0E-12 5.0E-12 6.0E-12 1.0E-11 4.0E-11 5.0E-11 6.0E-11 6.7E-11

| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Perfluorohexanesulfonic Acid (CAS No. 335-46-4) with Incoming Soil Concentration to Facility at 0.220 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**6.7E-11 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

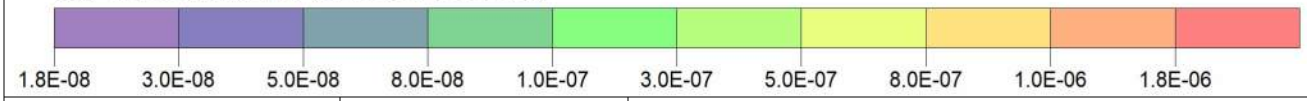
PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

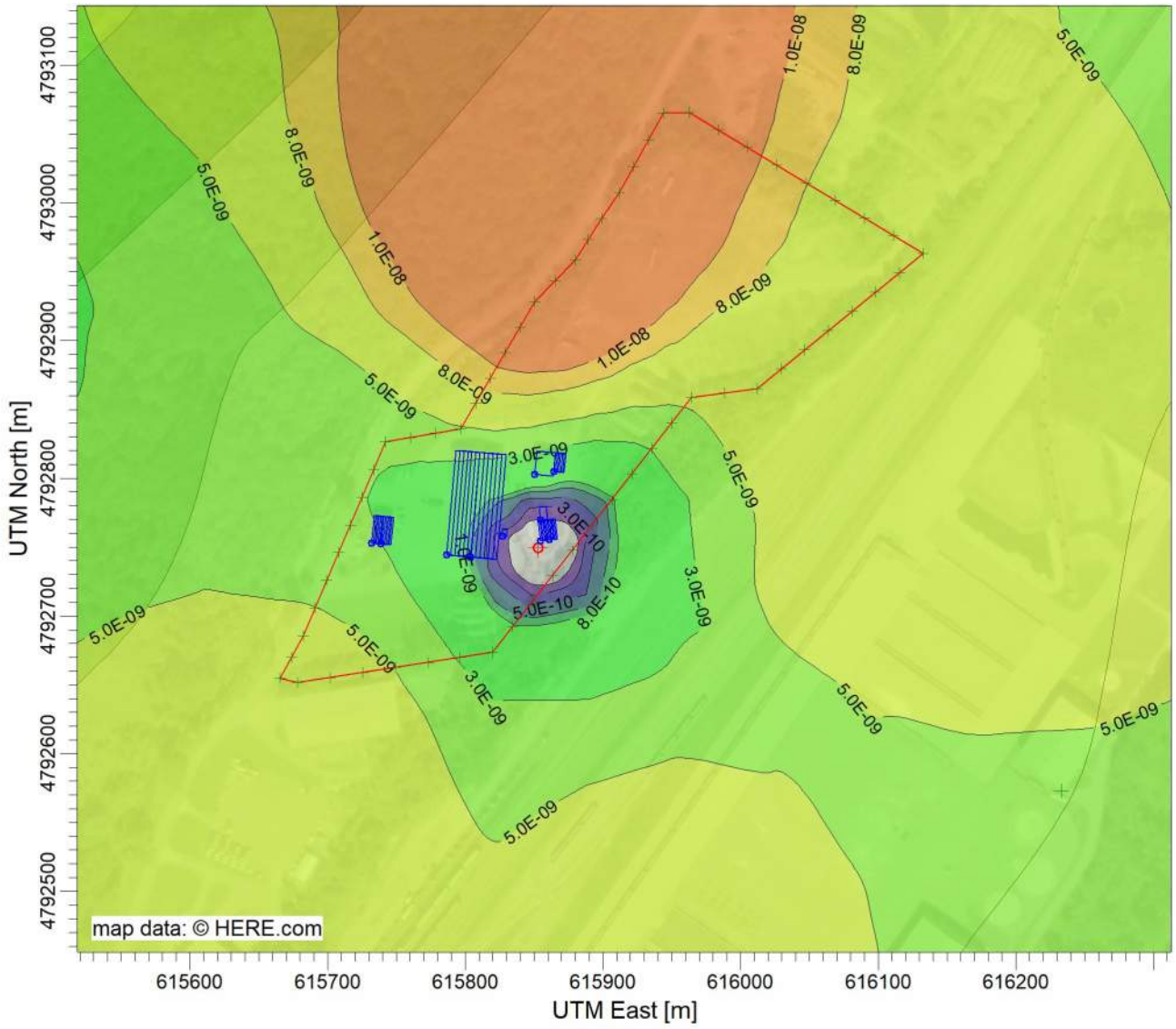
Max: 1.8E-06 [ug/m^3] at (615796.68, 4792835.91)




| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Perfluorooctanesulfonic Acid (CAS No. 1763-23-1) with Incoming Soil Concentration to Facility at 58.793 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.8E-06 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

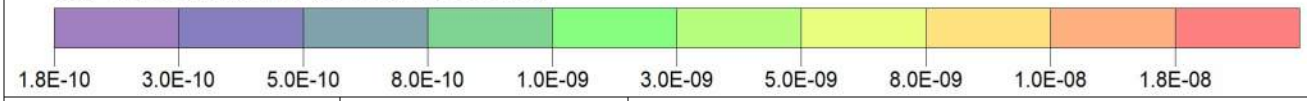
PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

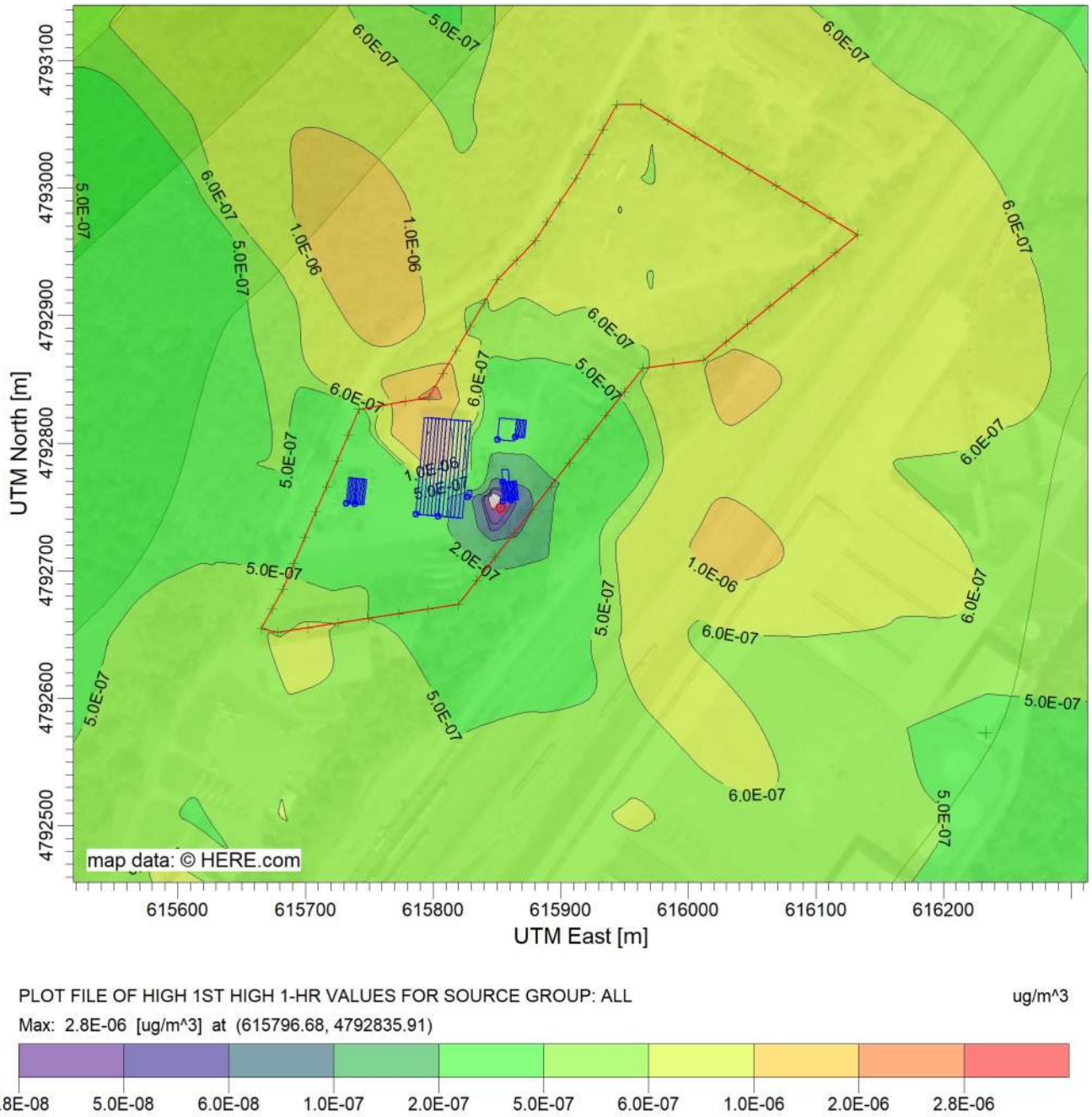
Max: 1.8E-08 [ug/m^3] at (615888.44, 4792991.00)




| COMMENTS: | SOURCES: | COMPANY NAME: | |
|---|---|---|---|
| Air Dispersion Results<br><br>Perfluorooctanesulfonic Acid (CAS No. 1763-23-1) with Incoming Soil Concentration to Facility at 58.793 ug/kg | **1** | **C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**1.8E-08 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Hourly Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF HIGH 1ST HIGH 1-HR VALUES FOR SOURCE GROUP: ALL ug/m^3

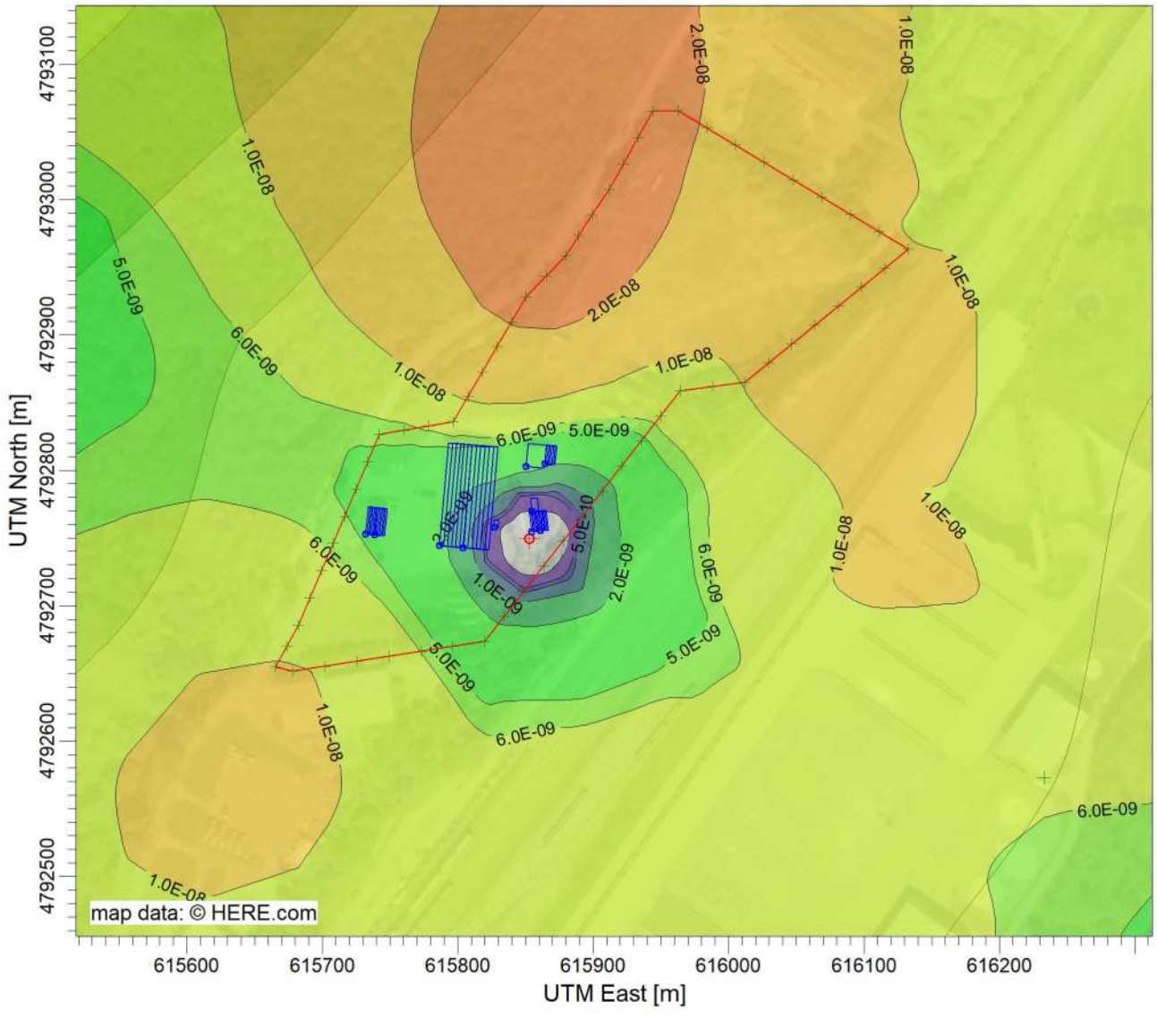
Max: 2.8E-06 [ug/m^3] at (615796.68, 4792835.91)

2.8E-08 5.0E-08 6.0E-08 1.0E-07 2.0E-07 5.0E-07 6.0E-07 1.0E-06 2.0E-06 2.8E-06

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Sum of All PFAS Compounds with Incoming Soil Concentration to Facility at 89.485 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**2.8E-06 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

PROJECT TITLE:

**Air Dispersion Modeling - Clean Earth Fort Edward, NY Site**
**Maximum Annual Dispersion Concentration Based on 99.99% PFAS DRE**




PLOT FILE OF ANNUAL VALUES AVERAGED ACROSS 5 YEARS FOR SOURCE GROUP: ALL ug/m^3

Max: 2.7E-08 [ug/m^3] at (615888.44, 4792991.00)

2.7E-10 5.0E-10 6.0E-10 1.0E-09 2.0E-09 5.0E-09 6.0E-09 1.0E-08 2.0E-08 2.7E-08

| | | | |
|---|---|---|---|
| COMMENTS:<br>Air Dispersion Results<br><br>Sum of All PFAS Compounds with Incoming Soil Concentration to Facility at 89.485 ug/kg | SOURCES:<br>**1** | COMPANY NAME:<br>**C.T. MALE ASSOCIATES** | |
| | RECEPTORS:<br>**4001** | MODELER:<br>**C.T. MALE STAFF** | |
| | OUTPUT TYPE:<br>**Concentration** | SCALE: 1:5,000<br>0 0.1 km | |
| | MAX:<br>**2.7E-08 ug/m^3** | DATE:<br>**7/15/2024** | PROJECT NO.:<br>**22.2756** |

# Attachment C

## NYSDOH Prepared "Summary of Toxicological Assessment for Carbon Tetrafluoride in Support of the Development of an AGC and SGC for the NYSDEC"

**Bureau of Toxic Substance Assessment**
**Division of Environmental Health Assessment**
**Center for Environmental Health**
**October 2023**

# Summary of the Toxicological Assessment of Carbon Tetrafluoride in Support of the Development of an Annual Guideline Concentration (AGC) and Short-term Guideline Concentration (SGC) for the NYS Department of Environmental Conservation (NYS DEC)

## 1. Executive Summary of Recommended Annual Guideline Concentration

At the request of the NYS DEC's Division of Air Resources, the New York State Department of Health's (NYS DOH) Bureau of Toxic Substance Assessment (BTSA) evaluated the toxicity of carbon tetrafluoride in support of the development of an AGC. As described in the bulleted summaries below, the NYS DOH searched for acute, subchronic and chronic toxicity information from authoritative bodies and the scientific literature. The toxicological database for carbon tetrafluoride was found to be very limited and inadequate to derive an AGC. Chemical-specific toxicity data sufficient to evaluate the potential for portal-of-entry effects (including irritation at the site of contact) and/or systemic effects from acute, subchronic or chronic exposures (via oral and inhalation routes of exposure) were not available for carbon tetrafluoride. Thus, NYS DOH evaluated the toxicity of structurally similar chemicals to derive an AGC for carbon tetrafluoride by inference to structurally similar chemicals for which toxicity information is available. This approach is permitted under the NYS DEC (2021) guidelines for the derivation of AGCs, which states: "if information about a chemical is limited, structure activity relationships for chemicals of close or similar structure will be used to calculate an interim AGC." Therefore, the NYS DOH recommends an AGC for carbon tetrafluoride of 0.33 milligrams per cubic meter ($mg/m^3$) based upon the toxicity of two structurally similar analogues (i.e., trichlorofluoromethane and dichlorodifluoromethane). Since chemical-specific toxicity information on carbon tetrafluoride was found to be insufficient to inform whether the health effects of carbon tetrafluoride are likely to be portal-of-entry, systemic or both, carbon tetrafluoride is being treated as a Category 3 gas based on toxicity studies for the two selected analogues (trichlorofluoromethane and dichlorodifluoromethane), which demonstrate that the predominant toxicological effects from inhalation exposure to these two chemicals are systemic effects. Inhalation toxicity values from authoritative bodies are available for these two chemicals and are based on noncancer health effects from inhalation exposures in animals and humans. The NYS DOH used these inhalation toxicity values, along with the application of uncertainty factors to account for less than lifetime exposures in the critical studies to derive the recommended AGC for carbon tetrafluoride. Based on the uncertainties and limitations presented by the absence of chemical-specific toxicity information for carbon tetrafluoride, the NYS DOH supports the adoption of 0.33 $mg/m^3$ as an interim AGC value, which could change if new and adequate chemical-specific toxicity data become available.

## 2. Search Criteria Used to Evaluate the Toxicity of Carbon Tetrafluoride

To evaluate whether an AGC and/or SGC could be derived based on chemical-specific toxicity information on carbon tetrafluoride, internet searches were performed for the following six key areas of information:

1) Physical-chemical properties
2) Basic information on chemical use and manufacturing

3) Chronic and subchronic toxicity values (including oral and inhalation cancer and noncancer toxicity values)
4) Toxicity studies from the scientific literature (acute, subchronic and chronic studies for oral and inhalation routes of exposure)
5) Other toxicity information (e.g., pharmacokinetics and mode-of-action (MOA) for toxicity)
6) Occupational exposure limits

## 3. Physical-Chemical Properties and Chemical Use of Carbon Tetrafluoride

Carbon tetrafluoride is a colorless, odorless, nonflammable gas that is used as a refrigerant (PubChem, 2023). Carbon tetrafluoride is also a stable combustion byproduct that can be emitted into air via the incineration of fluorine-containing waste (Lohmann et al., 2020). Carbon tetrafluoride can also be emitted into air through industrial activities, such as aluminum production (US EPA and IAI, 2008). Additional information on the physical-chemical properties of carbon tetrafluoride is provided in Appendix B (Table B – 1).

## 4. Toxicity Information on Carbon Tetrafluoride

The available information on the toxicity of carbon tetrafluoride is very limited. Chronic and subchronic toxicity values from authoritative bodies are not available. In addition, chronic or subchronic carbon tetrafluoride toxicity studies by the inhalation or oral routes of exposure were not found. The toxicological database on carbon tetrafluoride is inadequate to derive toxicity values[1] based on cancer or noncancer long term health effects, and thus, is inadequate to derive an AGC using chemical-specific information.

NYS DEC (2021) uses acute toxicity data (e.g., lethality data) for toxicity classification of air contaminants and uses occupational exposure limits to derive AGC/SGC values in the absence of chronic toxicity values. While BTSA has not derived health-based guidance values for evaluating acute occupational exposures in the past, in order to assess the overall completeness of the toxicological database for carbon tetrafluoride, acute toxicity studies (inhalation and oral routes of exposure) and occupational exposure limits were included in the search criteria.

Fluorine-based occupational exposure limits for carbon tetrafluoride from European countries (NIOSH, 2023) were found (Appendix B, Table B - 2). However, occupational exposure limits for carbon tetrafluoride are not available from the authoritative bodies that are preferred by NYS DEC (2021) for AGC/SGC development (e.g., American Conference of Governmental Industrial Hygienists (ACGIH)).

Information on the acute toxicity of carbon tetrafluoride is very limited. An acute exposure study is available in the scientific literature (Makowski et al., 2022). However, this study does not use a traditional study design for acute toxicity testing (US EPA, 1998). Rats were exposed via inhalation to normobaric air, hyperbaric air, or a hyperbaric mixture containing a high concentration of carbon tetrafluoride (i.e., 79% carbon tetrafluoride, 21% oxygen) for 30 minutes per day for 5 days. Statistically significant effects on bodyweight were reported in females exposed to hyperbaric carbon tetrafluoride, but the authors reported that these bodyweights were within the normal range reported in the scientific literature. The lowest published lethal concentration is 895,000 parts per million per 15 minutes in rats via inhalation exposure (NIOSH, 2023). The available

[1] Both inhalation and oral toxicity values were considered based on the potential use of route-to-route extrapolation for health effects that are systemic (i.e., not point-of-contact).

information, while limited, suggests low acute toxicity.[2] However, the available information on the acute toxicity of carbon tetrafluoride is limited and insufficient to derive a chemical-specific SGC.

## 5. Identification of Structurally Similar Carbon Tetrafluoride Analogues

Given that the available chemical-specific information on carbon tetrafluoride was insufficient to derive an AGC (which was the focus of this assessment), the next phase of the assessment was to identify possible carbon tetrafluoride analogues to evaluate the chronic and subchronic toxicity of structurally similar compounds. Use of toxicity data on structurally similar compounds for inference to the potential toxicity of carbon tetrafluoride, in the absence of chemical-specific information, is permitted under NYS DEC (2021) guidelines for the derivation of AGCs.

Online tools, including ChemIDPlus[3] (NLM, 2022), Integrated Chemical Environment (NTP, 2022) and the Comptox Dashboard (US EPA, 2022)[4], were used to identify structurally similar analogues to carbon tetrafluoride. Structurally similar analogues meeting criteria of greater than or equal to 80% similarity, 0.8 similarity threshold or 0.8 Tanimoto score are included in Appendix B (Table B – 3). While disparate similarity metrics cannot be directly compared, higher values (on scales of 0 to 100% or 0 to 1) generally indicate higher levels of structural similarity to carbon tetrafluoride. Table 1 includes structural similarity scores from Appendix B (Table B – 3) for a subset of structurally similar carbon tetrafluoride analogues for which inhalation toxicity values are available.

## 6. Method for Obtaining Toxicity Information on Structurally Similar Carbon Tetrafluoride Analogues

The online tools for quantitatively assessing structural similarity to carbon tetrafluoride provided approximately 20 structurally similar analogues for consideration (Appendix B, Table B - 3). For these chemicals, online searches were performed for the six key areas of information listed in Section 2 (e.g., physical chemical properties, acute, subchronic and chronic toxicity values, scientific literature on acute, subchronic and chronic toxicity).

To streamline the process for obtaining toxicity information on structurally similar analogues, initial searches were performed using the Comptox Dashboard (US EPA, 2022), which provided available toxicity values. Moreover, consistent with NYS DEC (2021) guidance, toxicity values derived by US EPA were prioritized in this

[2] Two additional studies were found that evaluate the health effects of exposure in mice to different pressures of gases and gas mixtures (Clarke et al, 1978; Daniels et al., 1979). However, these studies could not be used to assess acute inhalation toxicity as they do not utilize a traditional acute toxicity study design (US EPA, 1998), there were co-exposures to gas mixtures, and air concentrations of carbon tetrafluoride were not reported. Exposure metrics were reported as measures of pressure in these studies (i.e., in atmosphere (ATM) or pounds per square inch (PSI)).

[3] The ChemIDPlus (NLM, 2022) is no longer active as of 2023. The ChemIDPlus database is now part of PubChem. However, the chemical similarity tool in PubChem (NLM, 2023) differs from and provides a different suite of chemicals than ChemIDPlus. The PubChem tool provides less useful analogues than the original ChemIDPlus similarity results and were not considered in this assessment.

[4] Structurally similar compounds were retrieved from the Comptox Dashboard using the "Chemical Details" tab in the carbon tetrafluoride chemical profile. The Comptox Dashboard GenRA tool was also used to determine whether the ToxRef (*in vivo* data) and ToxCast (*in vitro* data) databases could provide suitable analogues for assessment using the automated read-across feature in the Comptox Dashboard GenRA tool. However, the chemicals retrieved via GenRA using *in vivo* data filters (i.e., ToxRef) generally had lower structural similarity based on toxprint and morgan fingerprints (e.g., < 0.5 jaccard similarity for most analogues). Thus, while GenRA was performed as part of this assessment, it ultimately was not used for surrogate selection given the emphasis on identifying chemicals with a high level of structural similarity to carbon tetrafluoride as a means of inferring and predicting toxicity.

assessment for screening of carbon tetrafluoride analogues. The Comptox Dashboard was also used to screen and identify toxicity studies on carbon tetrafluoride analogues via the PubMed Abstract Sifter (US EPA, 2022).

ChemIDPlus (NLM, 2022) and PubChem (NLM, 2023) chemical databases were used to obtain general information on chemical structure, use, physical chemical properties, and acute toxicity information on structurally similar analogues. While additional internet searches were performed, as needed, this hierarchal approach to sourcing and prioritizing toxicity information was implemented given the large number of chemicals that were screened and evaluated in this assessment.

## 7. Toxicity Information on Structurally Similar Carbon Tetrafluoride Analogues

There was limited toxicity information available on most of the identified surrogates. Only three of the approximately 20 structurally similar chemicals (i.e., trichlorofluoromethane, dichlorodifluoromethane and carbon tetrachloride) had available toxicity values that could be used to derive an AGC. Table 1 shows the available cancer and noncancer inhalation toxicity that were found on the three surrogates. However, as described in previous sections, chemical-specific toxicity information on carbon tetrafluoride is insufficient to evaluate carcinogenicity or to support a biological rationale for assessing carbon tetrafluoride carcinogenicity using chemical correlation. Therefore, while searches were performed for information on both cancer and noncancer toxicity of carbon tetrafluoride analogues, noncancer toxicity was prioritized for consideration in the development of a potential AGC.

Of the three analogues, carbon tetrachloride had the most extensive toxicity database. For example, US EPA Integrated Risk Information System (IRIS) derived cancer and noncancer toxicity values for carbon tetrachloride based on oral and inhalation exposure (US EPA IRIS, 2010). Additional inhalation toxicity values were also identified via the Comptox Dashboard (US EPA, 2022) from authoritative bodies such as the Agency for Toxic Substances and Disease Registry (ATSDR, 2005, 2023) and California Office of Environmental Health Hazard Assessment (CA OEHHA, 2008, 2023). By comparison, the toxicity databases were limited for trichlorofluoromethane and dichlorodifluoromethane. For example, oral reference doses for each chemical were derived by US EPA IRIS. However, inhalation toxicity and the potential for carcinogenicity were not assessed under the IRIS program. US EPA derived subchronic reference concentrations (RfCs) under US EPA's Superfund program (i.e., provisional peer-reviewed toxicity values (PPRTV)). However, US EPA did not derive chronic RfCs for trichlorofluoromethane and dichlorodifluoromethane, and determined that there was "inadequate information to assess the carcinogenic potential" of these chemicals.

Table 1 below includes summaries of available inhalation toxicity values for trichlorofluoromethane, dichlorodifluoromethane and carbon tetrachloride from US EPA and other authoritative bodies (e.g., CA OEHHA, Danish Ministry of the Environment (DME), ATSDR and the Michigan Department of Environmental Quality (DEQ)). The toxicity values derived by US EPA, CA OEHHA, ATSDR and the Michigan DEQ are based on extra-respiratory (systemic) effects in animals or humans, and involve application of physiologically based pharmacokinetic (PBPK) modeling or dosimetric adjustment factors for Category 3 gases to calculate human equivalent concentrations (HECs). These methods are consistent with currently accepted risk assessment practices for deriving RfCs.[5] However, the DME did not calculate HECs to derive RfCs and instead used

[5]US EPA guidance for deriving RfCs (US EPA, 1994, 2012) recommends inhalation dosimetry to extrapolate from inhalation exposure levels in animals to inhalation exposures in humans. In the absence of physiologically based pharmacokinetic (PBPK) models for

uncertainty factors to account for pharmacokinetic and pharmacodynamic differences between animals and humans.

extrapolating between animals and humans, the default recommended approach for application of inhalation dosimetry considers physical-chemical properties as determinants of chemical uptake into the respiratory system (US EPA, 1994, 2012). Category 1 gas characteristics include high solubility in water and/or rapid irreversible reactivity. Category 1 gases do not accumulate in blood and elicit site of contact effects at the portal of entry. Category 2 gases have moderate solubility in water, may be rapidly reversibly reactive or moderately to slowly irreversibly metabolized in the respiratory tract. Category 2 gases have the potential for accumulation in blood and effects may be systemic or at the portal of entry. Category 3 gases have low water solubility, are relatively unreactive in surface liquid and tissue, can accumulate in blood, and have systemic toxicity.

**Table 1. Available Inhalation Toxicity Values for Structurally Similar Carbon Tetrafluoride Analogues Identified via Quantitative Structural Similarity Assessment Tools[A,B]**

| Chemical Name/ CAS Number | Toxicity Value | Source | Study Details | POD/DAF | Toxicity Endpoint | Uncertainty Factors |
|---|---|---|---|---|---|---|
| **Analogues (listed in the order of most to least structurally similar to carbon tetrafluoride)** | | | | | | |
| Trichlorofluoromethane (Freon 11)<br>75-69-4<br><br>*95% structural similarity to carbon tetrafluoride | 1 mg/m$^3$ Subchronic p-RfC | US EPA, 2009; provisional peer-reviewed toxicity Value (PPRTV) | Single exposure concentration study; 5620 mg/m$^3$ in humans exposed via inhalation 8 hour/day, 5 days/week, for 2 to 4 weeks | $LOEL_{ADJ}$ = 1338 mg/m$^3$ | Small decrements in cognitive performance in humans | 1000<br>$UF_L$ = 10<br>$UF_H$ = 10<br>$UF_D$ = 10 |
| | 570 mg/m$^3$ Health-based quality criterion in air | DME, 2014 | Single exposure concentration study; Guinea pigs, rats and dogs exposed continuously to 57,000 mg/m$^3$ for 90 days. | NOEL = 57,000 mg/m$^3$<br>An HEC was not calculated; Applied UF approach[C] | No adverse effects reported | 100<br>$UF_A$ = 10<br>$UF_H$ = 10 |
| | 0.13 mg/m$^3$ Initial Threshold Screening Level (ITSL) | Michigan DEQ, 2019a | Adopted US EPA (2009) PPRTV (See above) with application of additional uncertainty factor | | | 10,000<br>$UF_L$ = 10<br>$UF_H$ = 10<br>$UF_D$ = 10<br>UFs = 10 |
| Dichlorodifluoromethane (Freon 12)<br>75-71-8<br><br>*95% structural similarity to carbon tetrafluoride | 1 mg/m$^3$ Subchronic p-RfC;<br>Chronic screening level[D] | US EPA, 2010; PPRTV | Single exposure concentration study; 0 or 4,136 mg/m$^3$ for 8 hours/day, 5 days/week for 6 weeks in guinea pigs, rabbits, dogs, and monkeys | $LOEL_{ADJ[HEC]}$ = 985 mg/m$^3$<br>DAF = 1 (Category 3 Gas) | Decreased bodyweight gain in guinea pigs, rabbits, dogs, and monkeys | 1000<br>$UF_A$ = 3<br>$UF_H$ = 10<br>$UF_L$ = 10<br>$UF_D$ = 3 |
| | 14 mg/m$^3$ Health-based quality criterion in air | DME, 2014 | 90 day continuous exposure in guinea-pigs showed to single concentration of 4,100 mg/m$^3$ | LOEL = 4,100 mg/m$^3$<br>An HEC was not calculated; Applied UF approach[C] | Fatty infiltration and necrosis in the liver | 100<br>$UF_A$ = 10<br>$UF_H$ = 10 |
| | 0.33 mg/m$^3$ ITSL | Michigan DEQ, 2019b | Adopted US EPA (2010) PPRTV (See above) with application of additional uncertainty factor[E] | | | 3000<br>$UF_A$ = 3<br>$UF_H$ = 10<br>$UF_L$ = 10<br>$UF_S$ = 10 |
| Carbon tetrachloride (Freon 10)<br>56-23-5<br><br>*88% structural similarity to carbon tetrafluoride | 0.1 mg/m$^3$ RfC | US EPA IRIS, 2010 | Whole body exposure in rats to 0, 31.5, 157, or 786 mg/m$^3$ (99.8% pure) vapor for 6 hours/day, 5 days/ week for 104 weeks | $BMCL_{10[HEC]}$ = 14.3 mg/m$^3$<br>*A human PBPK model was used to obtain HEC (Category 3 gas) | Fatty changes in the liver | 100<br>$UF_A$ = 3<br>$UF_H$ = 10<br>$UF_D$ = 3 |

| Chemical Name/ CAS Number | Toxicity Value | Source | Study Details | POD/DAF | Toxicity Endpoint | Uncertainty Factors |
|---|---|---|---|---|---|---|
| | $6 \times 10^{-6}$ per mcg/$m^3$ Unit Risk[F] | | BDF1 mice exposed to carbon tetrachloride vapor for 104 weeks (6 hours/ day, 5 days/week) | $LEC_{10}$, lower 95% bound on exposure at 10% extra risk - $1.78 \times 10^4$ mcg/$m^3$ | Increased incidence in adrenal gland tumors | Not applicable |
| | 0.04 mg/$m^3$ Chronic Reference Exposure Level | CA OEHHA (2008, 2023) | Guinea pigs exposed to 0, 5, 10, 25, 50, 100, 200 and 400 ppm (0, 37, 74, 186, 372, 744, 1487, 2974 mg/$m^3$) carbon tetrachloride for varying duration. At the LOEL (37 p mg/$m^3$) exposure was for 7 hours/day, 5 days/week for 7.3 months. | $LOEL_{ADJ[HEC]}$ = 10.7 mg/$m^3$<br><br>RGDR = 1.7 (Category 3 gas) | Increase in liver weight and liver lipid content | 300<br>$UF_A$ = 3<br>$UF_H$ = 10<br>$UF_L$ = 3<br>$UF_S$ = 3 |
| | $4.2 \times 10^{-5}$ per mcg/$m^3$ Unit Risk | CA OEHHA (2011, 2023) | Based on cross-route extrapolation from an oral cancer potency factor derived by US EPA in 1984. | | Increased incidence in liver tumors in mice | Not applicable |
| | 0.19 mg/$m^3$ (0.03 ppm) Inhalation Minimal Risk Level | ATSDR, 2005 | Whole body exposure to e (>99% pure) to 0, 5, 25, or 125 ppm (0, 37, 186, 930 mg/$m^3$) carbon tetrachloride for 6 hours/day,<br>5 days/week for 104 weeks.<br>LOEL = 186 mg/$m^3$ | $NOEL_{ADJ[HEC]}$ = 0.9 ppm (6.7 mg/$m^3$)<br><br>DAF = 1 (Category 3 gas) | increased liver weight, serum enzymes, and liver histopathology (fatty change, granulation, foci, deposition of ceroid, fibrosis, and cirrhosis) | 30<br>$UF_A$ = 3<br>$UF_H$ = 10 |

[A]Table Definitions: ADJ (adjusted for continuous exposure), BMCL (benchmark concentration lower bound), DAF (dosimetric adjustment factor), HEC (human equivalent concentration), LOEL (lowest-observed-effect-level), NOEL (no-observed-effect-level), POD (point-of-departure), p-RfC (provisional reference concentrations), RfC (reference concentration), RGDR (Regional Gas Dose Ratio), $UF_A$ (interspecies uncertainty factor), $UF_D$ (database uncertainty factor), $UF_H$ (intraspecies uncertainty factor) $UF_L$ (LOEL-to-NOEL uncertainty factor), $UF_S$ (uncertainty factor for less than lifetime exposure).

[B] As described in Section 5, structural similarity scores for carbon tetrafluoride analogues come from online tools, including ChemIDPlus[6] (NLM, 2022), Integrated Chemical Environment (NTP, 2022) and the Comptox Dashboard (US EPA, 2022). Higher structural similarity scores (on scales of 0 to 100% or 0 to 1) generally indicate higher levels of structural similarity to carbon tetrafluoride. Table 1 includes the subset of carbon tetrafluoride analogues for which inhalation toxicity values were found. The full list of structurally similar analogues meeting criteria of greater than or equal to 80% similarity, 0.8 similarity threshold or 0.8 Tanimoto score can be found in Appendix B (Table B – 3).

[C]Current US EPA guidance for deriving RfCs (US EPA, 1994) recommends the use of mathematical models (i.e., physiologically based pharmacokinetic modeling (PBPK)) or dosimetric adjustment factors (DAFs) to extrapolate from inhalation exposure levels in animals to inhalation exposures to humans. In the absence of available PBPK models for extrapolating between animals and humans, the default recommended approach for application of DAFs considers the physical-chemical properties of chemicals (i.e., whether chemicals are particles or gases) and pharmacokinetics (i.e., whether chemicals are reactive at the site of contact (Category 1 gases), absorbed and distributed systemically and elicit systemic effects (Category 3 gases), or both (Category 2 gases)) in order to calculate human equivalent concentrations (HECs) from inhalation exposure levels in animals. US EPA used a DAF to calculate an HEC for dichlorodifluoromethane from animal inhalation exposure levels and did not use a DAF for trichlorofluoromethane as the POD was based on human health effects. However, DME (2014) used the uncertainty factor approach to account for both pharmacokinetic and pharmacodynamic differences between animals and humans (i.e., applied a total uncertainty factor of 10 for interspecies extrapolation) in toxicity value derivations.

[6] The ChemIDPlus (NLM, 2022) is no longer active as of 2023. The ChemIDPlus database is now part of PubChem. However, the chemical similarity tool in PubChem (NLM, 2023) differs from and provides a different suite of chemicals than ChemIDPlus. The PubChem tool provides less useful analogues than the original ChemIDPlus similarity results and were not considered in this assessment.

[D]US EPA (2010) did not derive a chronic RfC for dichlorodifluoromethane. However, US EPA indicated that a "screening level" chronic RfC of 0.1 mg/$m^3$ could be derived by using an additional UF of 10 for chronic-to-subchronic extrapolation, which would result in a total UF 10,000. According to current risk assessment practices for deriving an RfC, total uncertainty factors (i.e., for extrapolation from a LOEL to a NOEL, from a subchronic to lifetime study, and for intra- and interspecies extrapolation) are typically limited to a maximum of 3000, even when there are four areas of uncertainty being addressed through application of uncertainty factors.

[E]Michigan DEQ (2019b) also calculated a screening chronic provisional value of 0.1 mg/$m^3$ using a total UF of 10,000.

[F]$10^{-6}$ Cancer Risk Level = 0.17 mcg/$m^3$ (0.00017 mg/$m^3$)

## 8. Comparison of Carbon Tetrafluoride Analogues

### 8.1. Comparison of Toxicity Values

Of the three structurally similar analogues for which toxicity values were found (Table 1), trichlorofluoromethane and dichlorodifluoromethane had the highest structural similarity to carbon tetrafluoride (both with about 95% structural similarity). The structural similarity between carbon tetrachloride and carbon tetrafluoride was lower (about 88%). However, the toxicity of carbon tetrachloride is well characterized compared to the other two analogues, and carbon tetrachloride has the lowest inhalation toxicity value from US EPA[7] (Table 1) of the three analogues. In addition, the US EPA IRIS (2010) RfC derivation for carbon tetrachloride (0.1 mg/m$^3$) includes several favorable attributes, such as use of a lifetime-exposure toxicity study in rodents, benchmark dose modeling to estimate a point-of-departure (POD), and pharmacokinetic modeling to obtain a human equivalent concentration (instead of use of default dosimetry calculations). US EPA IRIS (2010) assigned a medium overall confidence in their RfC assessment, high confidence in the selected key study, and medium confidence in the toxicity database for carbon tetrachloride.

By contrast, the US EPA derivations for trichlorofluoromethane and dichlorodifluoromethane (subchronic provisional RfCs of 1 mg/m$^3$ for each chemical) are limited in that they are both subchronic toxicity values and are based on lowest-observed-effect levels (LOELs) from short-term, single exposure studies (Table 1). The RfC for trichlorofluoromethane is based on health effects in humans (i.e., cognitive effects in humans exposed via inhalation to 5620 mg/m$^3$ trichlorofluoromethane for 8 hours per day, 5 days per week, for up to 4 weeks (Stewart et al., 1975, 1978, reviewed in US EPA, 2009)). PODs based on health effects in humans are generally preferred to use of health effects in animals for derivation of inhalation toxicity values. However, US EPA (2009) also applied a database uncertainty factor of 10 due to the limited availability of inhalation toxicity studies on trichlorofluoromethane (e.g., lack of reproductive, developmental, and comprehensive neurobehavioral toxicity studies). US EPA (2009) assigned a low overall confidence in the provisional subchronic RfC for trichlorofluoromethane, medium-to-low confidence in the selected key study, and low confidence in the toxicity database.

The provisional RfC for dichlorodifluoromethane is based on short-term health effects in laboratory animals. The LOEL selected as the POD based on toxicity in animals is lower than the no-observed-effect level (NOEL) of 1,179 mg/m$^3$) reported in a study of humans exposed via inhalation to a single concentration for 8 hours per day, 5 days per week for up to 4 weeks (Stewart et al., 1978, reviewed in US EPA, 2010). The US EPA provisional RfC for dichlorodifluoromethane includes a database uncertainty factor of 3 for lack of reproductive and developmental toxicity. US EPA did not apply a full database uncertainty factor of 10, in part, due to the presence of one chronic duration inhalation study of dichlorodifluoromethane in rodents (Maltoni et al., 1988). This study examined the carcinogenicity of dichlorodifluoromethane and reported no treatment related differences in tumor incidence in the organs and systems of rats and mice examined in the study (e.g., brain, mammary glands, blood). However, this study reported limited information on noncancer toxicity (US EPA, 2010). The only noncancer findings reported in the study were that effects on bodyweight were not observed in rats and mice. Thus, the US EPA (2010) considered the highest exposure concentration tested in this study to be a NOEL (2,976 mg/m$^3$). It should be noted that the NOEL from the Maltoni et al. (1988) study is

[7] Consistent with NYS DEC (2021) guidance, toxicity values derived by US EPA were prioritized in this assessment for screening of carbon tetrafluoride analogues.

much higher than the POD of 985 mg/m$^3$ selected as the basis of US EPA's subchronic provisional RfC for dichlorodifluoromethane. US EPA (2010) assigned a low overall confidence in the provisional subchronic RfC, low confidence in the selected key study, and low-to-medium confidence in the toxicity database.

With respect to the two fluorinated structurally similar analogues, the US EPA provisional RfC derivations for trichlorofluoromethane and dichlorofluoromethane are of similar quality, with similar strengths and weaknesses. Thus, for trichlorofluoromethane and dichlorofluoromethane a strong rationale for choosing one chemical and corresponding toxicity value over the other as a potential basis of an AGC for carbon tetrafluoride was not apparent. Therefore, it was concluded at this stage in the assessment that additional information was needed on the three analogues (carbon tetrachloride, trichlorofluoromethane and dichlorodifluoromethane) in order to determine whether a biological rationale could be formulated to inform surrogate selection based on factors such as pharmacokinetics and modes-of-action for toxicity. Surrogate selection for use in deriving an AGC for carbon tetrafluoride is covered in subsequent sections of this document (Sections 8.2, 9.1, 9.2, 10, 11.1 and 11.2). These sections consider additional supporting information and provide a scientific rationale for recommending an approach to deriving an AGC for carbon tetrafluoride.

### 8.2. Chemical Property Considerations

In comparing the toxicity of carbon tetrachloride, trichlorofluoromethane and dichlorodifluoromethane, physical-chemical properties (Appendix B, Table B - 1), including chemical makeup, were also considered. For example, the low boiling points of the three analogues (Appendix B, Table B - 1) indicate that they are volatile organic chemicals. In terms of chemical makeup, while the analogues are all fully halogenated methanes, carbon tetrachloride and carbon tetrafluoride differ in chemical composition given that the former is fully chlorinated and the latter is a fully fluorinated. Toxicity comparisons between groups of chemicals with similar halogen makeup is a common practice in human health risk assessment (e.g., per- and polyfluoroalkyl substances (PFAS), polychlorinated dibenzo-*p*-dioxins, polybrominated diphenyl ethers, polychlorinated biphenyls). However, evidence to support a rationale for assuming similar toxicity between chemicals with dissimilar halogen makeup, such as fully chlorinated and fully fluorinated chemicals, was not found. The presence or absence of fluorine could also play an important role in chemical attributes. For example, the carbon-fluorine covalent bond is considered the strongest in organic chemistry, and has a low reactivity due to factors such as the electronegativity of fluorine, the polarity of the bond, and poor accessibility to the bonded fluorine atom's valence electrons (Chan et al., 2011). In addition, information on fully fluorinated chemicals, such as PFAS, indicates that some fluorinated chemicals have high thermal and chemical stability, are persistent in the environment, and do not readily undergo biological transformation (Langenbach and Wilson, 2021). Thus, the dissimilarities in halogen makeup between carbon tetrachloride and carbon tetrafluoride reduced the confidence in the use of a precautionary principal approach at this stage of the assessment (i.e., selection of carbon tetrachloride, the chemical with the lowest RfC and most robust toxicity database, as the basis of an AGC for carbon tetrafluoride).

## 9. Structurally Related Fluorinated Chemicals

### 9.1. Identification of Related Fluorinated Chemicals

Since there was limited toxicity information on the approximately 20 chemical analogues initially identified by the structural similarity tools, the assessment of potential carbon tetrafluoride analogues was widened to include additional fluorinated compounds (e.g., partially halogenated methanes and haloalkanes identified in

authoritative body documents on chlorofluorocarbons, chemicals identified in other online structural assessment tools (e.g., the free ChemMine tool (Backman et al., 2022) and through professional judgement). This additional screening was performed to address important limitations in the assessment due to compounding uncertainties presented by both the absence of chemical-specific toxicity data on carbon tetrafluoride and the limited toxicity databases on the inhalation toxicity of structurally similar compounds as a whole and for trichlorofluoromethane and dichlorodifluoromethane, specifically. While the additional screening of fluorinated chemicals was not exhaustive, it provided additional related chemicals for consideration (e.g., 20 to 30 additional chemicals).

Any chemicals that had carbon chains of greater than 2 carbons or that had carbon-to-carbon double bonds were excluded from screening as the focus of this part of the assessment was to find chemicals with potential structural and functional similarities to carbon tetrafluoride. The remaining related fluorinated chemicals were screened for chronic or subchronic toxicity values, with an emphasis on inhalation toxicity values (Section 9.2). If other relevant toxicity information were readily available (e.g., pharmacokinetics or MOA), the information was captured in the assessment.

### 9.2. Toxicity Screening of Related Fluorinated Chemicals

The same search method for obtaining toxicity information described in Section 6 was used to identify toxicity values for screening of related chemicals. These searches of more than 20 related chemicals yielded 10 additional chronic and subchronic inhalation toxicity values for eight fluorinated chemicals (halomethanes and haloalkanes) for consideration. The available toxicity values for these additional compounds (Table 2) were generally higher than the ones found for the three structurally similar analogues evaluated in this assessment (Table 1). While the toxicity databases for the additional chemicals were limited, the additional data on fluorinated halomethanes and haloalkanes were not suggestive of high noncancer toxicity. Had the available toxicity data for these compounds demonstrated higher toxicity than the initial three analogues identified by structural similarity, application of the precautionary principal to select carbon tetrachloride as the surrogate chemical for use in deriving an AGC could have been reconsidered at this stage in the assessment. However, since this was not the case, the two fluorinated analogues from the initial structural similarity assessment (i.e., trichlorofluoromethane and dichlorodifluoromethane) remained options for deriving an AGC for carbon tetrafluoride. Thus, the screening of these additional related fluorinated compounds served to increase the confidence in the selection of the two partially fluorinated structurally similar carbon tetrafluoride analogues.

**Table 2. Available Inhalation Toxicity Values for Chemicals that are Structurally Related to Carbon Tetrafluoride[A,B]**

| Chemical Name/ CAS Number | Toxicity Value | Source | Study Details | POD/DAF | Toxicity Endpoint | Uncertainty Factors |
|---|---|---|---|---|---|---|
| Dichlorofluoromethane (Freon 21) 75-43-4 | 0.13 $mg/m^3$ Health-based quality criterion in air | DME, 2014 | Rats exposed via inhalation to 213, 640 or 2130 $mg/m^3$ (6 hours/day, 5 days/week, for 90 days). LOEL = 213 $mg/m^3$ | $LOEL_{ADJ}$= 38 $mg/m^3$<br>An HEC was not calculated; Applied UF approach[C] | Histopathological changes in the liver | 300<br>$UF_A$ = 10<br>$UF_H$ = 10<br>$UF_L$ = 3 |
| Chlorodifluoromethane (Freon 22) 75-45-6 | 50 $mg/m^3$ RfC | US EPA IRIS, 1993 | Whole-body exposure to 0, 3540, 35,370, or 176,800 $mg/m^3$ for 5 hours/day, 5 days/week, for up to 118 weeks (females) or 131 weeks (males). LOEL = 176,800 $mg/m^3$ | $NOEL_{ADJ[HEC]}$ = 5260 $mg/m^3$<br>DAF = 1 | Increased kidney, adrenal and pituitary weights in rats. | 100<br>$UF_A$ = 3<br>$UF_H$ = 10<br>$UF_D$ = 3 |
| 2-Chloro-1,1,1-trifluoroethane (Freon 133a) 75-88-7 | 2.1 $mg/m^3$ Health-based quality criterion in air | DME, 2014 | Inhalation exposure to rat dams (2,500 $mg/m^3$ for 6 hours/day on gestation days 6 to 15), which corresponds to 625 $mg/m^3$ after adjusting for continuous exposure. Documentation of study details is limited. | $LOEL_{ADJ}$ = 625 $mg/m^3$<br>An HEC was not calculated; Applied UF approach[C]. | Developmental toxicity at concentrations that did not cause maternal toxicity | 300<br>$UF_A$ = 10<br>$UF_H$ = 10<br>$UF_L$ = 3 |
| 1,1,1,2-Tetrafluoroethane (Freon 134a) 811-97-2 | 80 $mg/m^3$ RfC | US EPA IRIS, 1995a | Rats whole-body exposed 0, 10,400, 41,700, and 208,600 $mg/m^3$ for 6 hours/day, 5 days/week. Duration adjusted concentrations = 1860, 7450, or 37,250 $mg/m^3$<br>LOEL = 37,250 $mg/m^3$ | $BMC_{10[ADJ]}$ = 8200 $mg/m^3$<br>DAF = 1 (Category 3 Gas) | Leydig cell hyperplasia | 100<br>$UF_A$ = 3<br>$UF_H$ = 10<br>$UF_D$ = 3 |
| 1,1,2-Trichloro-1,2,2-trifluoroethane (Freon 113) 76-13-1 | 5 $mg/m^3$ Chronic p-RfC | US EPA, 2016; PPRTV | cross-sectional study of workers exposed via inhalation for an average of 2.77 years. LOEL = 19,160 $mg/m^3$ | $NOEL_{ADJ}$ = 1440 $mg/m^3$ | Slight impairment of psychomotor performance reported in two male volunteers for 1.5 hours | 300<br>$UF_H$ = 10<br>$UF_S$= 10<br>$UF_D$ = 3 |
| | 50 $mg/m^3$ Subchronic p-RfC | | | | | 30<br>$UF_H$ = 10<br>$UF_D$ = 3 |
| | 109 $mg/m^3$ Health-based quality criterion in air | DME, 2014 | 2-year inhalation study in rats exposed 5 days/week to 15,300 $mg/m^3$ and 76,600 $mg/^3$. LOEL = 76,600 $mg/m^3$ | $NOEL_{ADJ}$= 10,900 $mg/m^3$<br>An HEC was not calculated; Applied UF approach[C] | Decreased body weight | 100<br>$UF_A$ = 10<br>$UF_H$ = 10 |
| 1,1,1-Trifluoroethane (Freon 143a) 420-46-2 | 20 $mg/m^3$ Chronic p-RfC | US EPA 2015; PPRTV | 3−8-weeks-old rats exposed via inhalation (whole-body) to 0, 2,000, 10,000, or 40,000 ppm (0, 6,874, 34,370, and 137,500 $mg/m^3$) 6 hours/day, 5 days/week, for 90 days. | $NOEL_{ADJ[HEC]}$ = 24,550 $mg/m^3$<br>DAF = 1 (Category 3 Gas) | No effects reported at highest concentration | 1000<br>$UF_A$ = 3<br>$UF_H$ = 10<br>$UF_D$ = 3<br>$UF_S$ = 10 |
| | 200 $mg/m^3$ | | | $NOEL_{ADJ[HEC]}$ = 24,550 $mg/m^3$ | | 100<br>$UF_A$ = 3 |

| Chemical Name/ CAS Number | Toxicity Value | Source | Study Details | POD/DAF | Toxicity Endpoint | Uncertainty Factors |
|---|---|---|---|---|---|---|
| | Subchronic p-RfC | | | DAF = 1 (Category 3 Gas) | | $UF_H$ = 10<br>$UF_D$ = 3 |
| 1-Chloro-1,1-difluoroethane (Freon 142b)<br>75-68-3 | 50 mg/m$^3$ RfC | US EPA IRIS, 1995b | Rats were exposed via whole-body inhalation exposure for 6 hours/day, 5 days/week for 104 weeks to 0, 1000, 10,000, or 20,000 ppm (4110, 41,100, or 82,200 mg/m$^3$). NOEL corresponds to the highest concentration tested. | $NOEL_{ADJ[HEC]}$ = 14,710 mg/m$^3$<br>DAF = 1 (Category 3 Gas) | No effects reported at the highest concentration | 300<br>$UF_A$ = 3<br>$UF_H$ = 10<br>$UF_D$ = 10 |

[A]Per the search methodology of this assessment, this Table provides inhalation toxicity values derived by US EPA, if available, or toxicity values from other authoritative bodies when toxicity values from US EPA were not found.

[B]Table Definitions: ADJ (adjusted), BMC (benchmark concentration), DAF (dosimetric adjustment factor), HEC (human equivalent concentration), LOEL (lowest-observed-effect-level), NOEL (no-observed-effect-level), POD (point-of-departure), p-RfC (provisional reference concentrations), RfC (reference concentration), $UF_A$ (interspecies uncertainty factor), $UF_D$ (database uncertainty factor), $UF_H$ (intraspecies uncertainty factor) $UF_L$ (LOEL-to-NOEL uncertainty factor), $UF_S$ (uncertainty factor for less than lifetime exposure)

[C]Current US EPA guidance for deriving RfCs (US EPA, 1994) recommends the use of mathematical models (i.e., physiologically based pharmacokinetic modeling (PBPK) or dosimetric adjustment factors (DAFs) to extrapolate from inhalation exposure levels in animals to inhalation exposures to humans. In the absence of available PBPK models for extrapolating between animals and humans, the default recommended approach for application of DAFs considers the physical-chemical properties of chemicals (i.e., whether chemicals are particles or gases) and pharmacokinetics (i.e., whether chemicals are reactive at the site of contact (Category 1 gases), absorbed and distributed systemically and elicit systemic effects (Category 3 gases), or both (Category 2 gases)). in order to calculate human equivalent concentrations (HECs) from inhalation exposure levels in animals. US EPA used a DAF to calculate an HEC for dichlorodifluoromethane from animal inhalation exposure levels and did not use a DAF for trichlorofluoromethane as the POD was based on human health effects. However, DME (2014) used the uncertainty factor approach to account for both pharmacokinetic and pharmacodynamic differences between animals and humans (i.e., applied a total uncertainty factor of 10 for interspecies extrapolation) in toxicity value derivations.

[D]ECETOC (2008) summarized a gestational study with a lower LOEL in rats (1,400 mg/m$^3$). Female Sprague-Dawley rats were exposed to 280, 1,400, 2,800 mg/m$^3$ for 6 hours/day, 5 days/week on gestation days 6 through 15. Slight increases in extra ribs were reported at 1,400 and 2,800 mg/m$^3$ (Coate, 1977). ECETOC (2008) also summarized additional findings from Coate et al. (1977), which reported an even lower LOEL for effects in male Sprague-Dawley rats exposed for 6 hours/day 5 days/week to 0, 280, 1,400 or 2,800 mg/m$^3$ chlorofluoromethane for 13 weeks. Relative spleen weights were significantly lower than the control in all exposed groups (i.e., LOEL of 280 mg/m$^3$) and reproductive effects (i.e., decreased relative testis weight and hypospermatogenesis) occurred at the highest level of exposure.

## 10. Summary of Information on MOA for Noncancer Toxicity of Carbon Tetrafluoride and Analogues

Since chemical correlation analyses can be informed by both structural and functional similarities, the final phase of the assessment included consideration of available information on the MOA for noncancer toxicity as well as pharmacokinetics (i.e., absorption, distribution, metabolism, excretion) of carbon tetrafluoride and the three structurally similar analogues (trichlorofluoromethane, dichlorodifluoromethane and carbon tetrachloride). The assessment was also informed by any relevant information found for the related fluorinated compounds identified for screening. The purpose of this was to explore potential biological rationales for structurally similar analogue selection. The following bullets summarize the key findings of this phase of the assessment.

- There are no studies available on the pharmacokinetics or chronic and subchronic toxicity of carbon tetrafluoride. While it is unknown whether carbon tetrafluoride is metabolized following inhalation exposure, a study of energetic parameters associated with carbon tetrafluoride molecular bonds and information on other related chemicals, suggests that carbon-fluorine bonds may be less prone to biological transformation than carbon bonds with other halogens (Koski et al., 1997; Yin et al., 1995).
- The hypothesized MOA for the noncancer liver effects of carbon tetrachloride involves the production of highly reactive chlorinated metabolites, which occurs through reductive dehalogenation via cytochrome P-450.[8] However, since carbon tetrafluoride is fully fluorinated, even if metabolized by reductive dehalogenation via cytochrome P-450, it would be unlikely for the metabolites to be chlorinated free radicals like those produced during the metabolism of carbon tetrachloride. As noted in the bullet above, studies on carbon tetrafluoride metabolism were not found. However, a study of chemical properties (energetic parameters such as bond strength and vertical electron affinity) suggests that metabolism of carbon tetrafluoride and free radical production may be unlikely (Koski et al., 1997).
- According to US EPA (2009), available data suggest little or no metabolism of inhaled trichlorofluoromethane. Most of the compound is rapidly eliminated unchanged via exhaled air and only traces of radioactivity are recovered in the urine or feces (from exposure to radiolabeled trichlorofluoromethane). An *in vitro* study suggests that rat liver microsomes could dechlorinate trichlorofluoromethane to a fluorinated metabolite (dichlorofluoromethane). However, there are currently no *in vivo* data to support this finding. Studies on dichlorodifluoromethane also suggest little to no metabolism following inhalation exposures (WHO, 1990).

[8] Carbon tetrachloride is metabolized via a cytochrome P-450 pathway, which includes reductive dehalogenation (reductive cleavage of one carbon-chloride bond) and formation of the trichloromethyl radical. The trichloromethyl radical can undergo anaerobic or aerobic transformation to other chlorine containing intermediates. Regarding the potential MOA for noncancer effects, US EPA IRIS[11] stated the following: "liver metabolism rate was selected as the primary dose metric for liver effects, based on evidence that metabolism of carbon tetrachloride via CYP2E1 to highly reactive free radical metabolites plays a crucial role in its MOA in producing liver toxicity (described in Section 4.5). The primary reactive metabolites that are thought to participate in carbon tetrachloride toxicity are the trichloromethyl radical ($\cdot CCl_3$) and the trichloromethyl peroxy radical ($O\text{-}OCCl_3$), although other reactive species may also contribute to a lesser extent (e.g., dichlorocarbene, $:CCl_2$)."

## 11. Derivation of an AGC for Carbon Tetrafluoride

### 11.1. Uncertainties and Limitations of the Assessment

Traditional toxicological assessments rely heavily on chemical-specific toxicity studies on the chemical of interest. However, when such data are not available, a risk assessment can be performed using structural activity relationships and read-across to infer the toxicity of a chemical lacking toxicity data by drawing comparisons to a structurally similar chemical with a more robust toxicological database (Health Canada, 2022; OECD, 2023). While this approach fulfills data needs when chemical-specific toxicity data are lacking, assessing and outlining of uncertainties is a key step in the selection of analogues and the implementation of a weight-of-evidence approach (Health Canada, 2022; Schultz et al., 2015).

The assessment of the toxicity of carbon tetrafluoride and structurally similar analogues has three main areas of uncertainty.

1) As described in Section 4, there was no information available on the chronic or subchronic toxicity of carbon tetrafluoride in an online search of the toxicological literature. Given that toxicity data were lacking, there was insufficient information to evaluate MOA or to assess whether the effects of carbon tetrafluoride are likely to be systemic or point-of-contact based on chemical specific information. Appendix A provides additional information on the potential for carbon tetrafluoride to elicit point-of-contact and/or systemic effects based on toxicity information for structurally similar analogues.
2) Carbon tetrachloride and its toxicologically active metabolites do not contain any fluorines. Thus, while the toxicity database for carbon tetrachloride is more robust than other analogues considered in this assessment, there is no strong biological rationale to suggest similar toxicity or similar toxicity pathways for carbon tetrafluoride and carbon tetrachloride, despite the chemicals having similar structures, since they don't share similar chemical makeup (i.e., the chemicals do not contain any common halogens). Therefore, carbon tetrachloride was not selected as the basis of an AGC due to uncertainties related to chemical properties and considerations related to MOA.
3) With respect to the two fluorinated structurally similar analogues (trichlorofluoromethane and dichlorodifluoromethane), the overall databases on inhalation toxicity as well as the critical studies used to derive provisional RfCs are limited. The provisional RfC derivation corresponding to the lowest LOEL for dichlorodifluoromethane (i.e., the US EPA (2010) subchronic RfC of 1 $mg/m^3$) is based on short-term exposure in animals (6 weeks) and a total uncertainty factor of 1000 across four areas of uncertainty (Table 1). The provisional RfC derivation corresponding to the lowest LOEL for trichlorofluoromethane (i.e., the US EPA (2009) subchronic RfC of 1 $mg/m^3$) is based on a short-term exposure in humans (2 to 4 weeks) and has a total uncertainty factor of 1000 based on three areas of uncertainty (Table 1).

With respect to the third point, some of the uncertainties associated with the limited inhalation toxicity databases on trichlorofluoromethane and dichlorodifluoromethane were reduced through the additional screening of structurally related fluorinated chemicals (e.g., partially fluorinated halomethanes and haloalkanes). These structurally related fluorinated chemicals were not captured in the structural similarity assessment. However, some of these chemicals, in addition to being structurally related to carbon tetrafluoride, have similar industrial use as refrigerants. As a whole, the available inhalation toxicity values for

these chemicals did not demonstrate a high level of toxicity. With the exception of dichlorofluoromethane, all seven of the other structurally related chemicals had inhalation toxicity values that are higher than the RfCs derived by US EPA for trichlorofluoromethane and dichlorodifluoromethane. The DME (2014) derived an inhalation toxicity value of 0.13 mg/m$^3$ for dichlorofluoromethane based on histopathological effects in the liver of rats following repeated inhalation exposure (i.e., 213, 640 or 2130 mg/m$^3$ dichlorofluoromethane for 6 hours per day, 5 days per week, for 90 days). Effects were reported at the lowest level of exposure, which corresponds to 38 mg/m$^3$ when adjusted for continuous exposure. The DME applied a total uncertainty factor of 300 (i.e., 10 for interspecies extrapolation, 10 for intraspecies extrapolation and 3 for use of a LOEL). The LOEL in the DME derivation for dichlorofluoromethane is lower than the LOELs selected as the POD for trichlorofluoromethane and dichlorodifluoromethane in the US EPA derivations of provisional subchronic RfCs (i.e., LOELs of 1338 and 985 mg/m$^3$, respectively). However, US EPA applied total uncertainty factors of 1000 in the derivations for both trichlorofluoromethane and dichlorodifluoromethane (Table 1). Therefore, the provisional subchronic RfCs for trichlorofluoromethane and dichlorodifluoromethane (1 mg/m$^3$ for both chemicals) are 38-fold lower than the LOEL of 38 mg/m$^3$ for dichlorofluoromethane. Therefore, screening of additional fluorinated chemicals (described in Section 9 and Table 2), increased overall confidence in the assessment of structurally similar carbon tetrafluoride analogues and the potential selection of trichlorofluoromethane and/or dichlorodifluoromethane as the basis of an AGC for carbon tetrafluoride.

### 11.2. Surrogate Selection and AGC Recommendations

Both trichlorofluoromethane and dichlorodifluoromethane are selected as surrogates for evaluating the toxicity of carbon tetrafluoride given that a biological rationale for selecting one analogue over the other was not apparent based on an assessment of the toxicity and pharmacokinetics of the chemicals (See Sections 7, 8 and 10). In addition, the strengths and weaknesses of the respective US EPA provisional subchronic RfC derivations for trichlorofluoromethane and dichlorodifluoromethane were similar. Therefore, the approach for derivation of an AGC based on structural activity relationships is to use the subchronic RfCs for the two fluorinated analogues (1 mg/m$^3$ each for trichlorofluoromethane and dichlorodifluoromethane, Table 1) and increase the total uncertainty factor from 1000 to 3000, which is typically the maximum total uncertainty factor that can be applied to a derivation of an RfC across 4 areas of uncertainty.[9] The increase in total uncertainty factors addresses the use of subchronic toxicity endpoints in the derivation and would yield an AGC of 0.33 mg/m$^3$ for carbon tetrafluoride. Given the selection of trichlorofluoromethane and dichlorodifluoromethane as surrogates, carbon tetrafluoride is being treated as a Category 3 gas based on the systemic effects of the surrogates in the absence of chemical-specific toxicity data on carbon tetrafluoride (see Appendix A for additional details). The PODs used in the US EPA provisional RfC derivations for trichlorofluoromethane and dichlorodifluoromethane are based on extrarespiratory effects (e.g., cognitive effects in humans and effects on bodyweight gain in laboratory animals, respectively). In addition, for both analogues, the most reliable evidence of toxicity from inhalation exposure correspond to systemic effects.

Evidence to support the derivation of an AGC of 0.33 mg/m$^3$ for carbon tetrafluoride also comes from the screening of several structurally related fluorinated chemicals. The results of the screening collectively suggest that an AGC of 0.33 mg/m$^3$ for carbon tetrafluoride would be adequately protective of noncancer health effects if the toxicity of carbon tetrafluoride is similar to that of other fluorinated halomethanes or fluorinated

[9]According to current risk assessment practices for deriving an RfC, total uncertainty factors are typically limited to a maximum of 3000, even when there are four areas of uncertainty being addressed through application of uncertainty factors.

haloethanes (Tables 1 and 2). Of the inhalation toxicity value derivations for structurally related chemicals (Table 2), the POD corresponding to the lowest LOEL is 38 mg/m$^3$ for dichlorofluoromethane. The AGC of 0.33 mg/m$^3$ is about 115-fold lower than this effect level.

The recommended approach for deriving an AGC for carbon tetrafluoride of 0.33 mg/m$^3$ is also supported by mechanistic information, which suggests that trichlorofluoromethane and dichlorodifluoromethane are not metabolized or metabolized to a small degree. While the MOAs for these chemicals are not known, it seems possible that toxicity could be resulting from the parent compounds, which both contain fluorine atoms. However, given the technical limitations of the assessment presented by data gaps in the available toxicity information on carbon tetrafluoride and the selected surrogates, the AGC should be reconsidered by NYS DEC if studies on the toxicity of carbon tetrafluoride become available in the future and suggest a different degree of toxicity that is not addressed by the current assessment.

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## Appendix A: Supplemental Information

### A.1. Summary of Toxicity Information Relevant to the Assessment of Portal-of-Entry versus Systemic Effects of Carbon Tetrafluoride

The literature review on carbon tetrafluoride included a search for both oral and inhalation toxicity studies (acute, subchronic and chronic). However, chemical-specific toxicity data to evaluate the potential for portal-of-entry effects (including irritation at the site of contact), first pass liver effects, and systemic effects from acute oral or inhalation studies are not available for carbon tetrafluoride.

In the absence of chemical specific toxicity studies that provide evidence as to whether the toxicological effects of carbon tetrafluoride are portal-of-entry and/or systemic, carbon tetrafluoride is being treated as a Category 3 gas based on the available toxicity information on carbon tetrafluoride analogues (i.e., trichlorofluoromethane and dichlorodifluoromethane). The points-of-departure (PODs) used by US EPA (2009, 2010) to derive subchronic reference concentrations (RfCs) for trichlorofluoromethane and dichlorodifluoromethane correspond to extrarespiratory effects following inhalation exposures (e.g., cognitive effects in humans and effects on bodyweight gain in laboratory animals, respectively). In addition, for both compounds, the most reliable evidence of toxicity from inhalation exposure correspond to systemic effects (see Section A.3 below for more information).

### A.2. Odor Thresholds for Carbon Tetrafluoride and Selected Surrogates

Carbon tetrafluoride is a colorless, odorless gas. An odor threshold was not found in PubChem[3] or via online searches of authoritative body information.

Dichlorodifluoromethane, one of the selected carbon tetrafluoride surrogates, is a colorless gas with an ether-like odor at extremely high concentrations. An odor threshold was not listed for dichlorodifluoromethane in PubChem. However, a fact sheet from the Occupational Safety and Health Administration indicates that 1000 parts per million (ppm) is a "normal range of odor threshold" for halocarbons, including dichlorodifluoromethane (OSHA, 2015). Thus, for dichlorodifluoromethane, this corresponds to an air concentration of 4,950 mg/m$^3$.

Trichlorofluoromethane, the other selected surrogate, is a colorless to water-white, nearly odorless liquid or gas. It has an odor threshold of 200,000 ppm (1.1 x $10^6$ mg/m$^3$) in PubChem (NLM, 2023).

### A.3. Additional Details on Respiratory and Liver Effects for Dichlorodifluoromethane and Trichlorofluoromethane Reported in US EPA (2009, 2010)

#### A.3.1 Trichlorofluoromethane

The POD selected by US EPA (2009) for use in deriving a subchronic RfC for trichlorofluoromethane corresponds to a lowest-observed-effect-level (LOEL) for cognitive effects in humans. Thus, a dosimetric adjustment factor was not needed for the derivation. However, evidence of toxicity in laboratory animals suggests that trichlorofluoromethane is also a Category 3 gas.

The only other LOEL from inhalation exposure identified in the US EPA (2009) assessment comes from a 90-day study of continuous exposure (0 or 5620 mg/m$^3$) trichlorofluoromethane in several species of laboratory

animals (Jenkins et al., 1970; reviewed in US EPA, 2009). Nonspecific inflammatory changes in the lungs of all tested species and mild vacuolar changes in the liver of guinea pigs were reported. However, details on severity or incidence of effects were not provided. The study authors concluded that these findings were not related to exposure. US EPA (2009) did not include these effects in the selection of a LOEL for trichlorofluoromethane. US EPA (2009) identified renal effects in dogs as the LOEL corresponding to this study and considered the same exposure level (5620 mg/m$^3$) to be a NOEL for other animal species examined in this study.

The same authors (Jenkins et al., 1970; reviewed in US EPA, 2009) performed a subchronic study of intermittent inhalation exposure to trichlorofluoromethane (0 or 56,200 mg/m$^3$ for 8 hours/day, 5 days/week, for 6 weeks) and reported a variety of histopathological effects (e.g., mild discoloration, characterized as a darkening of the tissue, of the liver in rats and guinea pigs, and nonspecific inflammatory changes of the lungs in guinea pigs, rats, and monkeys (incidences not reported)). However, the authors did not consider any of these histopathological findings to be related to exposure.  whether there were study quality issues. However, even if these histopathological changes were considered to be related to exposure, the exposure concentration is much higher than the LOEL for systemic effects in dogs.

In a 90-day study of male and female rats exposed to trichlorofluoromethane (0 or 56,200 mg/m$^3$ for 6 hours/day, 7 days/week), a variety of toxicity endpoints were evaluated, including liver and lung toxicity (Leuschner et al., 1983; reviewed in US EPA, 2009)[1]. However, adverse health effects were not reported in this study.

Effects that could be consistent with site of contact toxicity (e.g., edema and emphysema in the lungs) were reported in a short-term inhalation study (Clayton, 1966; reviewed in US EPA, 2009). A variety of other effects from histological examination were also reported (e.g., vacuolation of cells in the liver). However, study limitations (e.g., there was only a single exposure concentration of 67,416 mg/m$^3$ tested in the study, the sample size was three, and there were no control animals used in the study) preclude use of these findings to evaluate the toxicity of trichlorofluoromethane or carbon tetrafluoride by proxy.

The US EPA Integrated Risk Information System (US EPA IRIS, 1987a) has a reference dose for trichlorofluoromethane that is based on mortality and histopathological effects on the heart and lungs of rats exposed via gavage for 78 weeks.

### A.3.2 Dichlorodifluoromethane

Subchronic inhalation studies on dichlorodifluoromethane reported histopathological effects in the lungs of both controls and treated animals (Leuschner et al., 1983; Prendergast et al., 1967; reviewed in US EPA, 2010), and thus, do not provide conclusive evidence of effects at the site of contact.

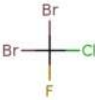
Focal necrosis and fatty infiltration of the liver were reported in a subchronic inhalation study of dichlorodifluoromethane in guinea pigs (Predergast et al., 1967; reviewed in US EPA, 2010). However, liver effects were not observed in any of the other animal species tested. In addition, a subchronic inhalation study of rats and dogs that included a detailed examination of liver toxicity showed no effects on the liver at exposures of up to 12,375 mg/m$^3$ (Leuschner et al., 1983; reviewed in US EPA, 2010)[2]. Due to potential

differences in species sensitivity to liver effects from inhalation exposure to dichlorodifluoromethane, US EPA (2010) did not consider liver toxicity to be a critical effect of inhalation exposure.

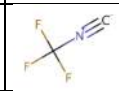
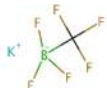
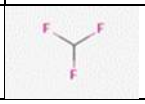
The POD used in the derivation of US EPA's (2010) subchronic RfC for dichlorodifluoromethane corresponds to reduced bodyweight gain in inhalation exposure studies in laboratory animals. The same critical effect was used as POD by US EPA (2010) and US EPA IRIS (1987b) to derive subchronic and chronic reference doses, respectively, for dichlorodifluoromethane based on oral exposure studies in laboratory animals.

## Appendix B: Supplemental Tables

### Table B - 1. Physical-Chemical Properties of Carbon Tetrafluoride and Analogues from ChemIDPlus[a]

| Analogue | Structure | Melting Point (°Celsius) | Boiling Point (°Celsius) | log P (octanol-water) | Water Solubility[b] (mg/L) | Vapor Pressure[b] (mm Hg) | Henry's Law Constant[b] (atm-$m^3$/mole) | Atmospheric OH Rate Constant[b] ($cm^3$/molecule-sec) |
|---|---|---|---|---|---|---|---|---|
| Carbon Tetrafluoride |  | -184 | -128.00 | 1.18 | -- | 18.80 | 5.15 | 4.00E-16 |
| Chlorotrifluoromethane (Freon-13) |  | -181 | -81.40 | 1.65 | 90.00 | 21400 | 1.38 | 7.00E-16 |
| Trichloromonofluoromethane (Freon-11) |  | -111 | 23.70 | 2.53 | 1100.00 | 803 | 0.10 | 5.00E-16 |
| Dichlorodifluoromethane (Freon-12 |  | -158 | -29.80 | 2.16 | 280.00 | 4850 | 0.34 | 4.00E-16 |
| Dibromodifluoromethane (Freon 12-B2) |  | -110 | 25.00 | 1.99 | 313.00 | 820 | 0.03 | 5.90E-16 |
| Bromotrifluoromethane (Freon 13-B1) |  | -172 | -57.80 | 1.86 | 320.00 | 12200 | 0.50 | 1.00E-16 |
| Tribromofluoromethane |  | -73.6 | 108 | 2.4 | -- | -- | -- | 0.0 |
| Dibromochlorofluoromethane |  | -- | 80.3 | 2.31 | -- | -- | -- | 2.31 |
| Bromochlorodifluoromethane (Freon 12B1) |  | -160 | -3.70 | 1.90 | 277.00 | 2070 | 0.09 | 1.00E-15 |
| Carbon tetrachloride (Freon 10) |  | -23 | 76.80 | 2.83 | 793.00 | 115 | 0.03 | 1.20E-16 |
| Bromodichlorofluoromethane |  | -106 | 52 | -- | -- | -- | -- | -- |
| Tetrabromomethane |  | 90.1 | 189.5 | 3.42 | 240.00 | -- | 4.91E-04 | 0.0 |
| Tribromochloromethane |  | 55 | 158.5 | 2.71 | -- | -- | -- | 0.0 |
| Bromotrichloromethane |  | -5.7 | 105 | 2.53 | 869 | 39 | 3.71E-04 | 0.0 |
| Dibromodichloromethane |  | 38.00 | 150.2 | 2.62 | -- | -- | -- | 0.0 |
| Trifluoroiodomethane (Freon 13T1) |  | -- | -22.5 | 2.01 | -- | -- | -- | 5.2E-14 |

## Appendix B: Supplemental Tables

| Analogue | Structure | Melting Point (°Celsius) | Boiling Point (°Celsius) | log P (octanol-water) | Water Solubility[b] (mg/L) | Vapor Pressure[b] (mm Hg) | Henry's Law Constant[b] (atm-$m^3$/mole) | Atmospheric OH Rate Constant[b] ($cm^3$/molecule-sec) |
|---|---|---|---|---|---|---|---|---|
| Trifluoromethylisocyanide |  | -- | -- | -- | -- | -- | -- | -- |
| (Trifluoromethyl)silane |  | -- | -- | -- | -- | -- | -- | -- |
| Potassium trifluoro(trifluoromethyl)borate(1-) |  | -- | -- | -- | -- | -- | -- | -- |
| Trifluoromethane[c] |  | -155.18 | -82.0 | 0.64 | 4.09E+03 | 3.53E+04 | -- | -- |

[a]Analogues are listed non-alphabetically based on structural similarity (see Supplementary Table 3).

[b]At 25 degrees Celsius.

[c]Values obtained from PubChem (NLM, 2023).

## Appendix B: Supplemental Tables

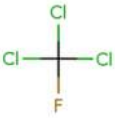
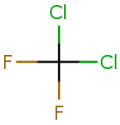
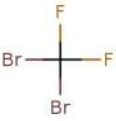
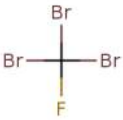
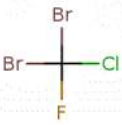
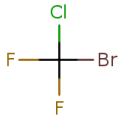
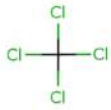
**Table B - 2. Available Occupational Exposure Limits for Structurally Similar Carbon Tetrafluoride Analogues**

| Chemical | Occupational Exposure Limit | Source/Reference |
|---|---|---|
| Carbon tetrafluoride* | time-weighted average 2.5 mg(F)/$m^3$ | Occupational Exposure Limits listed in a fact sheet from the National Institute of Occupational Safety and Health (NIOSH, 2022) for Australia, Belgium, and Hungary |
| | short term exposure limit 10 mg(F)/$m^3$ | |
| | 3000 mg/$m^3$ | Short-term Occupational Exposure Limits listed in NIOSH (2022) for Russia |
| Trichlorofluoromethane | 1,000 ppm (5,600 mg/$m^3$) | NIOSH Recommended Exposure Limit (REL) Ceiling, Occupational Safety and Health Administration (OSHA) Permissible Exposure Limit (PEL) Time-weighted Average (TWA) and ACGIH Threshold Limit Value (TLV) Ceiling (NIOSH, 1994b) |
| Dichlorodifluoromethane | 1,000 ppm (4,950 mg/$m^3$) | NIOSH REL TWA, OSHA PEL TWA and ACGIH TLV TWA (NIOSH, 1994a) |
| Carbon tetrachloride | ACGIH TLV TWA: 5 ppm (31 mg/$m^3$)<br>ACGIH Short-term Exposure Limit (STEL): 10 ppm (63 mg/$m^3$) NIOSH REL: 2 ppm (12.6 mg/$m^3$) 60-minute STEL;<br>OSHA PEL: 10 ppm (74.4 mg/$m^3$) TWA, 25 ppm (ceiling) (185.9 mg/$m^3$),<br>200 ppm (1487.3 mg/$m^3$) 5-min maximum peak in any 4 hours | (ACGIH, 2023; NIOSH, 1994c) |

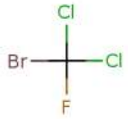
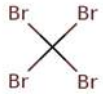
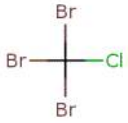
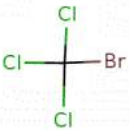
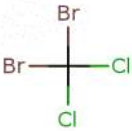
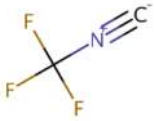
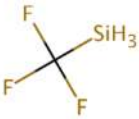
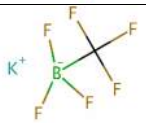
*The US Department of Energy (2022) and the US Department of Defense (US APHC, 2013) have short-term air guidelines for carbon tetrafluoride (i.e., Protective Action Criteria (PAC) and Military Exposure Guidelines (MEG), respectively). However, the derivation details for these values were not found online. In addition, NYS DEC (2021) guidance lists authoritative body sources for deriving AGCs and SGCs and does not include PACs or MEGs.

## Appendix B: Supplemental Tables

### Table B - 3. Carbon Tetrafluoride Analogues and Similarity Metrics

| Structural Analogues | RN | Structure | Molecular Weight | Similarity to Tetrafluoromethane (by % or Tanimoto Coefficient)[a] |
|---|---|---|---|---|
| Chemical of Interest: Carbon tetrafluoride | 75-73-0 |  | 88.003 | -- |
| **Analogues Identified via ChemIDPlus (NLM, 2022)** | | | | |
| Chlorotrifluoromethane (Freon-13) | 75-72-9 |  | 104.458 | 97.5309% similar |
| Trichlorofluoromethane (Freon-11) | 75-69-4 |  | 137.368 | 95.1807% similar |
| Dichlorodifluoromethane (Freon-12) | 75-71-8 |  | 120.913 | 95.1807% similar |
| Dibromodifluoromethane (Freon 12-B2) | 75-61-6 |  | 209.815 | 91.8605% similar |
| Bromotrifluoromethane (Freon 13B1) | 75-63-8 |  | 148.909 | 91.8605% similar |
| Tribromofluoromethane- | 353-54-8 |  | 270.721 | 91.8605% similar |
| Dibromochlorofluoromethane | 353-55-9 |  | 226.27 | 89.7727% similar |
| Bromochlorodifluoromethane (Freon 12B1) | 353-59-3 |  | 165.364 | 89.7727% similar |
| Carbon tetrachloride (Freon 10) | 56-23-5 |  | 181.819 | 87.7778% similar |

## Appendix B: Supplemental Tables

| Structural Analogues | RN | Structure | Molecular Weight | Similarity to Tetrafluoromethane (by % or Tanimoto Coefficient)[a] |
|---|---|---|---|---|
| Bromodichlorofluoromethane | 353-58-2 |  | 181.819 | 87.7778% similar |
| Tetrabromomethane | 558-13-4 |  | 331.627 | 84.8837% similar |
| Tribromochloromethane | 594-15-0 |  | 287.176 | 82.9545% similar |
| Bromotrichloromethane | 75-62-7 |  | 198.274 | 81.1111% similar |
| Dibromodichloromethane | 594-18-3 |  | 242.725 | 81.1111% similar |
| **Analogues Identified via Integrated Chemical Environment (NTP, 2022)** | | | | |
| Trifluoroiodomethane (Freon 13T1) | 2314-97-8 |  | 195.905 | 0.882353 (Tanimoto coefficient) |
| Trifluoromethylisocyanide | 105879-13-8 |  | 95.02 | 0.833333 (Tanimoto coefficient) |
| (Trifluoromethyl)silane | 10112-11-5 |  | 97.091 | 0.823529 (Tanimoto coefficient) |
| Potassium trifluoro(trifluoromethyl)borate(1-) | 42298-15-7 |  | 175.91 | 0.823529 (Tanimoto coefficient) |
| **Analogues Identified via the Comptox Dashboard (US EPA, 2022)** | | | | |
| Trifluoromethane | 75-46-7 |  | 70.014 | 0.833333313 (similarity threshold) |

[a]Structurally similar chemicals are characterized using online tools from ChemIDPlus, the Integrated Chemical Environment, and the Comptox Dashboard. Chemicals are grouped based on both similarity metric and online tool so that chemicals with common similarity metrics can be compared.