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Evaluation of EPA TSCA Screening Level Approach

American Chemistry Council
1,3-Butadiene TSCA Risk Evaluation Consortium

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Prepared for:

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Executive Summary

Under the Toxic Substances Control Act (TSCA), the United States Environmental Protection Agency (US EPA) has a process for ensuring safety of existing TSCA chemicals which involves three stages (Prioritization, Risk Evaluation, and Risk Management). As part of the TSCA Risk Evaluation stage, the EPA published a draft of a proposed screening level methodology to evaluate potential chemical exposures and associated risks to fenceline communities in January 2022 ("Draft Screening Level Approach for Assessing Ambient Air and Water Exposures to Fenceline Communities", EPA Document# EPA-744-D-22-001, hereinafter referred to as the TSCA Screening Level Approach).

In this report, we assess EPA's proposed approach for making risk determination decisions and informing risk management actions for 1,3-butadiene, and propose refinements to the EPA's approach. Currently, the proposed TSCA Screening Level Approach involves a tiered methodology including a Pre-Screening stage (using EPA's Integrated Indoor-Outdoor Air Calculator – IIOAC), a Full-Screening stage (using EPA's air dispersion model AERMOD), and a Co-resident Screening stage (using EPA's Indoor Environment Concentration in Buildings with Conditioned and Unconditioned Zones model – IECCU). This report only examines the first two stages of the Screening Level Approach as they address outdoor air quality. To evaluate the TSCA Screening Level Approach, a case study facility with reported 1,3-butadiene emissions was chosen. The chosen facility was previously evaluated by the EPA as part of the Office of Air's Residual Risk Assessment for the Miscellaneous Organic Chemical Manufacturing National Emission Standards for Hazardous Air Pollutants (MON) in support of the 2020 Risk and Technology Review (RTR) (Docket EPA-HQ-OAR-2018-0746). Since 1,3-butadiene is a hazardous air pollutant, under the Clean Air Act, it was evaluated in the Residual Risk Assessment.

To assess the TSCA Screening Level approach, we compare the first two stages (Pre-Screening and Full-Screening) to an air dispersion model that is set up following the example provided in the 2020 MON RTR (referred to as facility-specific modeling in this work). This modeling study (i.e. where "modeling study" refers to the Pre-Screening, Full-Screening, and facility-specific AERMOD model) is repeated for the years 2019 and 2021. The modeled maximum concentrations for both years showed similar trends where TSCA Pre-screening (IIOAC) outputs consistently had the highest values (10.75 $\mu g/m^3$ and 9.69 $\mu g/m^3$ for years 2019 and 2021 respectively), followed by the TSCA Full-Screening AERMOD (1.04 $\mu g/m^3$ at the north fenceline receptor or 1200 m from facility's central source and 0.74 $\mu g/m^3$ also slightly north of the fenceline receptor or 1200 m from facility's central source), with the facility-specific AERMOD run producing the lowest output concentrations (0.44 $\mu g/m^3$ at the west fenceline receptor or 1200 m from the facility's central source and 0.46 $\mu g/m^3$ at the east fenceline receptor or 1300 m from the facility's central source).

The modeling studies highlight conservative results from the TSCA Screening Level Approach methodologies, where the concentrations from the Pre-screening stage are an order of magnitude greater than the Full-screening stage, and the Full-screening stage concentrations are almost twice as high as the facility-specific AERMOD run. Examining the modeled concentrations at various receptors extending from near-fenceline to ~5 miles away showed that **concentrations dropped considerably as distance from the facility increased for the TSCA Pre-screen, Full-screen, and the facility-specific models**. The facility-specific AERMOD following the EPA's 2020 MON RTR methodology, which is considered the best available science, produced the most predictive (albeit still conservative) concentrations of all three models, because it utilized the most specific multi-variable inputs.

Facilities that produce or use 1,3-butadiene are also regulated under the MON and Hazardous Organic NESHAP (HON) rules. Accordingly, this report highlights potential air quality impacts of emissions from the case study facility using predicted post-MON concentrations provided in the 2020 MON RTR docket. Additionally, there is a qualitative discussion of impacts on 1,3-butadiene concentrations after the final HON rule is promulgated in early 2024.

Since 1,3-butadiene has multiple sources and arises from various sources other than manufacturing and/or use, monitoring data can more accurately represent air concentrations at which communities are exposed. To put the air dispersion modeling studies into context, ambient air concentrations of 1,3-butadiene measured at various nationwide sites with automated gas chromatography (auto-GC) measurements from years 2017 to 2021 are analyzed. All average concentrations (with the exception of one Texas site in 2021) were found to be below 1 ppb.

This case study highlights the conservative results from the methodologies proposed in the TSCA Screening Level Approach. Using facility-specific data, a more refined air dispersion model run produces modeled concentrations that are more realistic and more closely match with ambient measurements.

1. Introduction/Background

1.1 EPA Toxic Substances Control Act

Under the Toxic Substances Control Act (TSCA), the United States Environmental Protection Agency (US EPA) has the authority to issue regulations which collect health/safety and exposure information, require testing, and control exposure to chemical substances and mixtures. Specifically, TSCA requires that the EPA maintain the TSCA Chemical Substances Inventory, require testing of chemical substances to evaluate health or environmental hazards, regulate the manufacture, processing, distribution, use, and/or disposal of any chemical that may present an unreasonable risk of injury to human health or the environment, and finally coordinate actions on TSCA-controlled substances with actions under other federal laws, including laws administered by other federal agencies or other laws administered by EPA.[1]

1.1.1 Risk Evaluation for Existing Chemicals

The three stages of the EPA's process for ensuring safety of existing TSCA chemicals are (1) Prioritization, (2) Risk Evaluation, and (3) Risk Management. The purpose of the Risk Evaluation step (which is addressed in this report) is to determine whether a chemical presents unreasonable risk to human health or the environment, including risk to a "potentially exposed or susceptible subpopulation"[2]. To inform Risk Evaluation, in January 2022, the EPA published a draft version of a proposed screening level methodology to evaluate potential chemical exposures and associated risks to fenceline communities ("Draft Screening Level Approach for Assessing Ambient Air and Water Exposures to Fenceline Communities", EPA Document# EPA-744-D-22-001).[3]

In this report, we examine the suitability of the TSCA Screening Level Approach for informing risk determination decisions and risk management actions for one of the TSCA chemicals that is also a hazardous air pollutant, namely 1,3-butadiene. Facilities that produce or use 1,3-butadiene are also regulated under two other EPA rules: (1) the national emission standards for hazardous air pollutants (NESHAP) for the miscellaneous organic chemical (MON) manufacturing industry, and (2) the NESHAP for synthetic organic chemical manufacturing industry (SOCMI), commonly known as the hazardous organic NESHAP rule (HON).

Currently, the EPA's TSCA Screening Level Approach involves a tiered screening methodology summarized in Figure 1.

Figure 1: Tiered screening adapted from EPA's TSCA Screening Level Approach for Assessing Ambient Air and Water Exposures to Fenceline Communities

This work aims to present a refinement of the proposed methodology in the TSCA Screening Level Approach, that is a more streamlined approach for the EPA to carry out the risk evaluation in a fit-for-purpose manner. The proposed refined approach is tiered, with increasing level of complexity and data requirements, only if the prior generic/conservative tier suggests unreasonable risk. Additional analysis with measured data would be conducted to further refine the predicted exposures. Figure 2 shows the proposed refinement of the TSCA Screening Level Approach for industrial facilities. Co-residential exposures are not considered in this work as they involve indoor air analysis whereas the scope of this work is ambient modeling and measurements.

[1] EPA TSCA webpage: https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/
[2] TSCA Risk Evaluation webpage: https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/risk-evaluations-existing-chemicals-under-tsca
[3] Draft TSCA Screening Level Approach document: https://www.epa.gov/system/files/documents/2022-01/draft-fenceline-report_sacc.pdf

This work aims to assess the feasibility of carrying out the refined tiered screening approach presented in Figure 2. To do so, we selected a case-study facility which is known to produce and/or use 1,3-butadiene and carried out the modeling and analysis presented in the refined methodology.

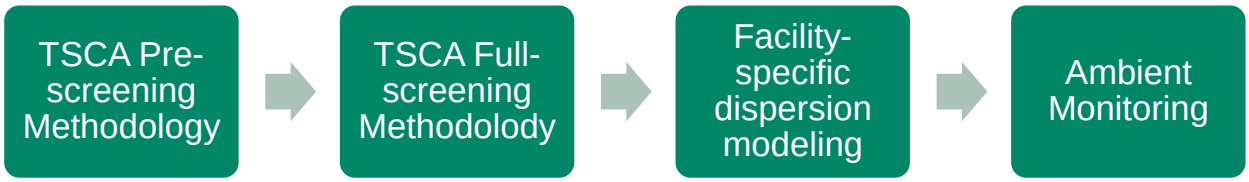


Figure 2: Proposed refinement of the tiered screening for industrial facilities (not for co-residential exposures)

1.1.2 Selection of Case Study facility

Consistent with EPA's commitment to leverage existing data, the selected case-study facility was previously evaluated as part of the EPA's Residual Risk Assessment for the MON in support of the 2020 Risk and Technology Review[4,5]. The chosen facility is a site in the Houston area which is known to have several neighboring industrial 1,3-butadiene sources and some non-industrial sources (such as traffic) given its location in an urban area. It is located near the Houston Ship Channel which is an area that has been the subject of several studies on air toxics including 1,3-butadiene[6,7,8] due to the presence of many oil refineries, chemical processing plants, and numerous major highways in proximity to residential areas. Additionally, the site is located near several air monitoring sites which record hourly 1,3-butadiene concentrations using automated gas chromatographs.

Figure 3 shows the locations of several 1,3-butadiene-emitting facilities (orange circles) and the nearest air monitoring sites (black kites) in the Harris County area. In the following sections of the report, a few key sites (shown on the map) will be discussed. The chosen facility is directly northwest of the HRM-16 air monitoring site. The Milby Park air monitoring site is located close to a number of 1,3-butadiene-emitting facilities, whereas the HRM-3 air monitoring site is at least 5 km away from the nearest 1,3-butadiene emitting facility. The chosen facility fenceline (shown in Figure 4) represents the location where the maximum emissions are measured, HRM-16 represents the location where slightly lower but still "high-end" concentrations may be detected, and the HRM-3 location represents an off-site location that should be minimally impacted by 1,3-butadiene emissions from neighboring facilities. Information on the Houston Regional Monitoring (HRM) network of air monitoring sites can be found through their website.[9]

[4] https://www.regulations.gov/document/EPA-HQ-OAR-2018-0746-0189
[5] MON Final Rule: https://www.federalregister.gov/documents/2020/08/12/2020-12776/national-emission-standards-for-hazardous-air-pollutants-miscellaneous-organic-chemical
[6] Air Pollutant Mapping with a Mobile Laboratory During the BEE-TEX Field Study: https://journals.sagepub.com/doi/pdf/10.4137/EHI.S15660
[7] Modeling of 1,3-butadiene in urban and industrial areas: https://www.sciencedirect.com/science/article/abs/pii/S1352231014009042
[8] Uncertainties in Air Toxics Calculated by the Dispersion Models AERMOD and ISCST3 in the Houston Ship Channel Area: https://journals.ametsoc.org/view/journals/apme/46/9/jam2540.1.xml
[9] HRM Houston Regional Monitoring - https://hrm.aecom.com/sitemap.htm

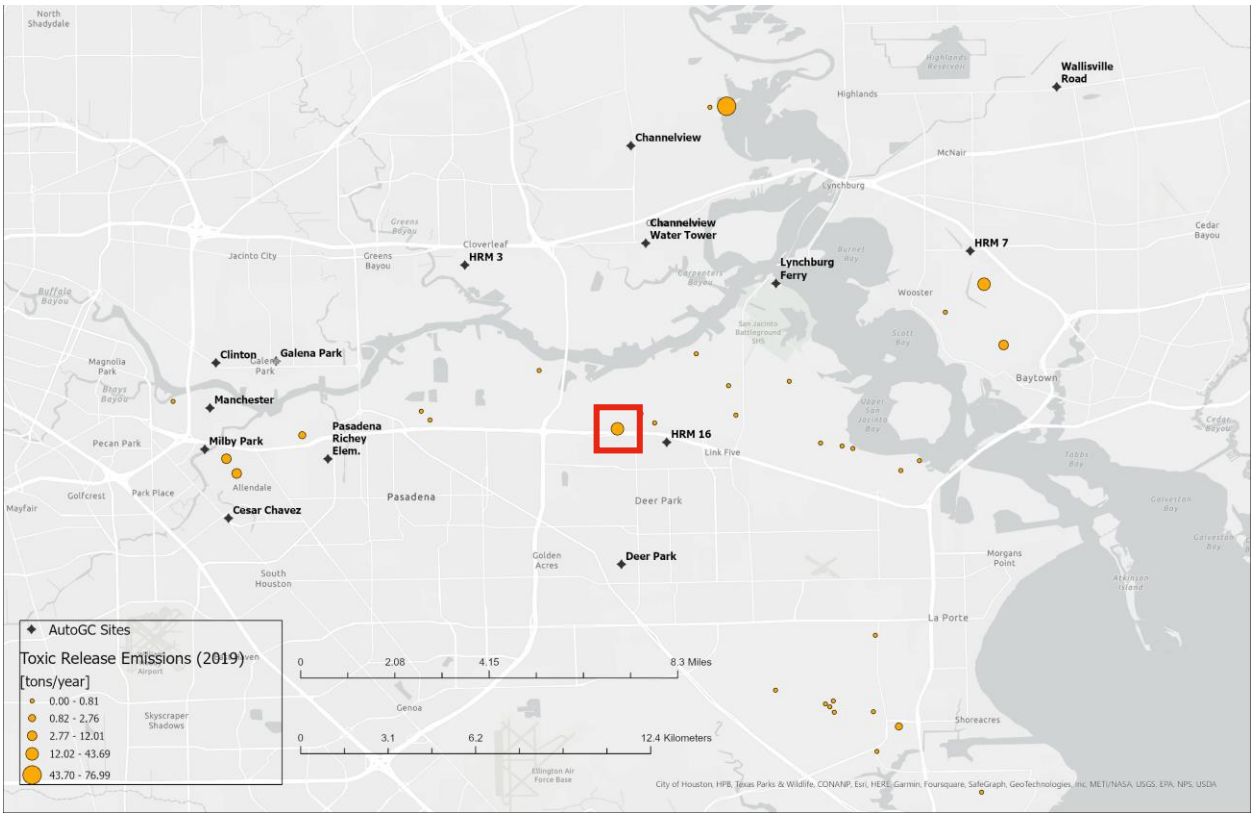


Figure 3: Map showing locations of Milby Park and HRM-3 sites in Houston, relative to neighboring TRI facilities with reported 1,3-butadiene emissions

This work presents the modeling study of this facility for the years 2019 and 2021, as well as for year 2019 data with predicted post-MON reductions based on the 2020 MON final rule[5]. The "modeling study" refers to the models described in Boxes 1, 2, and 3 shown in Figure 2. This work also provides a qualitative summary of potential emissions reductions based on the 2023 proposed HON rule, which is anticipated to be finalized by March 29, 2024[10]. Details on each of the models used in this work, as well as ambient air monitoring (Box 4) results, are presented in the following sections of the report.

Note that this work builds on previous verbal and written comments[11,12] submitted by the American Chemistry Council addressing the suitability of the TSCA Screening Level Approach.

2. TSCA Screening Level Approach

The TSCA Screening Level Approach describes tiered methodologies that are used to estimate ambient air concentrations and exposures for members of the public that are located between 5 to 10,000 meters from emission sources. Two of the three methodologies are the Ambient Air Pre-screening Methodology and the Ambient Air Full-screening Methodology. The third tier which is the Ambient Air Co-resident Screening Methodology is used to determine indoor air exposures for receptors living above or adjacent to a releasing facility. This report will focus on the outdoor air concentrations/exposures only; the third methodology is beyond the scope of this work. Additionally, the case-study facility is not located in a building with residents.

[10] https://www.federalregister.gov/documents/2023/04/25/2023-07188/new-source-performance-standards-for-the-synthetic-organic-chemical-manufacturing-industry-and
[11] Previous comments from ACC: https://www.regulations.gov/comment/EPA-HQ-OPPT-2021-0415-0066
[12] Previous comments from ACC: https://www.regulations.gov/comment/EPA-HQ-OPPT-2021-0415-0086

1.2 Pre-screening Integrated Indoor-Outdoor Air Calculator

The first methodology which is known as the Ambient Air Pre-screening Methodology is used to estimate ambient air concentrations and associated exposures based on maximum and mean releases of emitted chemicals. This methodology is independent of facility and use classifications, and results from this methodology are intended to inform the need for a full-screening level analysis. The pre-screening methodology utilizes EPA's Integrated Indoor/Outdoor Air Calculator (IIOAC) model[13] to estimate high-end (95th percentile) and central-tendency (mean) exposures to select receptors at pre-defined distances from a releasing facility (100, 1000 meters). The IIOAC estimates indoor and outdoor concentrations using pre-run results from a dataset of air dispersion scenarios that were run in a variety of meteorological and land-use settings within AERMOD. To run this Excel-based tool, several input parameters are required as discussed in the following section.

1.2.1 IIOAC Inputs

The following table presents parameters that are potential inputs for the IIOAC tool. Note that the parameters required/used for the modeling study in this report are in bold font.

Table 1: Input parameters for TSCA Pre-screening Methodology (IIOAC)

Emission Parameters • Source Type (e.g. **Point**, **Fugitive**, Area Water, Area Soil) • Duration of release (e.g. 1, 4, 8, **24 hours/day**) • **Mass Released per day (kg/day)** • **Release days per year**
System-specific Parameters • **Surface Area (m^2)** • Depth of water (m) • Flowrate (m^3/day)
Chemical-specific Parameters • **Chemical Name** • **CAS Number** • Vapor pressure (Torr) • Solubility (mg/L) • Organic carbon sorption coefficient (mL/g) • Volatilization half-life (1/day) • Molecular weight (g/mol)
Urban or rural setting
Particle size or **vapor** (only required for Point and Fugitive source types)
Climate Region (Specified in Guidance) • IIOAC uses one of fourteen conservatively developed meteorological datasets (e.g. Lake Charles, LA for South (Coastal) region) • Data sets are from years 2011 to 2015
Receptors pre-set by IIOAC (Specified in Guidance) Two groups: Inner ring "fenceline" receptors (~100 m from source), near-facility "community" receptors (~1000 m from source)

The TSCA Screening Level Approach calls for the use of EPA's Toxic Release Inventory (TRI)[14] data for the year of interest when finding emission rate values. The two years that were chosen for the modeling analyses in this report are 2019 and 2021. Year 2019 was chosen as a recent year that is representative of a period with regular weather conditions and industrial/vehicular activity patterns, and Year 2021 was chosen as an example of a year with a force majeure event (i.e. Winter storm Uri in Texas). For this report, 2019 and 2021 TRI data was extracted for facilities releasing 1,3-

[13] IIOAC webpage: https://www.epa.gov/tsca-screening-tools/iioac-integrated-indoor-outdoor-air-calculator
[14] TRI webpage: https://www.epa.gov/toxics-release-inventory-tri-program

butadiene. The particular case-study facility that was chosen for this report is a facility in the Houston area that emits 1,3-butadiene and is surrounded by a number of industrial and non-industrial 1,3-butadiene sources. The site is also located near several air monitoring stations which record 1,3-butadiene concentrations using automated gas chromatographs. This particular site exists within a single property boundary where four different companies operate. Of these four operators, two have reported 1,3-butadiene emission rates to the EPA's TRI. For the facilities of interest (TRIFD 77536SHLLLHIGHW and 77536DRPRK5900H) within the single property boundary, values for the FUGTIVE-AIR category (in pounds per year) were added and converted to the required IIOAC input units of kg/day assuming continuous year-long operation (24 hours/day, 7 days/week). The same was done for the STACK-AIR category. The FUGITIVE-AIR emission rates were used as inputs for the IIOAC run with Fugitive source type, and the STACK-AIR emission rates were used as inputs for the IIOAC run with the Point source type.

1.3 Full-screening Dispersion Model

The second methodology described by the TSCA Screening Level Approach document is known as the ambient air full-screening methodology. This methodology utilizes AERMOD to estimate concentrations at user-defined distances from a facility releasing a chemical that is undergoing risk evaluation, i.e. 1,3-butadiene in this report. AERMOD (American Meteorological Society/Environmental Protection Agency Regulatory Model) is an air dispersion model developed by the American Meteorological Society and the EPA's Regulatory Model Improvement Committee that is used for assessing air quality impacts near industrial sources of air pollution. The EPA requires the use of this refined dispersion model for State Implementation Plan (SIP) revisions for existing sources and for New Source Review (NSR) and Prevention of Significant Deterioration (PSD) programs.[15]

The TSCA Full-Screen methodology can be utilized after the pre-screening IIOAC tool, or independent of it, and is meant to provide a more thorough analysis than the pre-screening methodology to allow EPA to fully characterize identified risks for chemicals undergoing risk evaluation.[16]

1.3.1 TSCA Full-screening AERMOD ("Simplified AERMOD") Inputs

The following table presents the parameters that were used to set up the AERMOD run for the Full-screening methodology, following the guidance provided in the TSCA Screening Level Approach[17].

Figure 4 shows a screenshot of the AERMOD GUI software used for this analysis (BEEST) and captures the facility fenceline (blue border), single point and single area sources at the center of the facility, and a polar receptor grid extending from within the facility boundary up to 10 km beyond the fenceline. Discrete receptor points were added at coordinates corresponding to HRM-3 and HRM-16 air monitoring sites to investigate modeled concentrations at a near-source or near-fenceline location (HRM-16), and an off-site location downwind of the modeled facility (HRM-3), and to allow for comparison of modeled concentrations with ambient air monitoring data at both sites.

Note that the TSCA Full-screening approach is referred to as a "Simplified AERMOD" run throughout this report due to its consolidation of emission rates from all sources into one point source and one area source, and its use of preset source physical characteristics, as discussed in Table 2.

Table 2: Input parameters for TSCA Full-screening (Simplified AERMOD)

Emission Rates/Locations • Rates for Point and Area sources obtained from 2019 and 2021 TRI datasets (Facility TRIFD 77536SHLLLHIGHW and 77536DRPRK5900H) • Facility emissions centered on one location assigned coordinate of (0,0) (not based on actual release point locations of singular sources) • (0,0) coordinate represents latitude/longitude information reported to TRI
Source physical characteristics 1 POINT (Stack) source with: • Stack Height = 10 m

[15] https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models
[16] Section 2.1.2.2 (page 30) of TSCA Screening Level Approach guidance (EPA Document# EPA-744-D-22-001)
[17] Page 58 of TSCA Screening Level Approach guidance (EPA Document# EPA-744-D-22-001)

- Stack Diameter = 2 m
- Exit Temperature = 300 Kelvin
- Exit velocity of 5 m/s

1 AREA (Fugitive) source with:

- 10x10 m ground-level area source per facility
- Release height = 3.05 m
- Point and fugitive source are co-located
- Above assumptions are made since TRI data does NOT include source-specific physical characteristics, but facility-level emissions only

Meteorological Data

- Use meteorological dataset from closest meteorological station within EPA database of 824 stations
- Closest station to chosen facility with William P. Hobby Airport (HOU), which had pre-processed data available from TCEQ website[18]
- 2021 and 2019 HOU meteorological data with *low* surface roughness was used based on AERSURFACE run at facility site

Receptors

- Receptor distance up to 10 km from facility boundary
- Option of polar- or centroid-based receptor grid
- For (default) polar grids, set receptor grid as 16 radials (every 22.5°), and 13 rings
- Discrete receptor points added at HRM-3 and HRM-16 sites
- Flagpole height for all receptors = 1.8 m
- Flat terrain assumed

Urban setting

[18] TCEQ pre-processed meteorological datasets: https://www.tceq.texas.gov/permitting/air/modeling/aermod-datasets.html

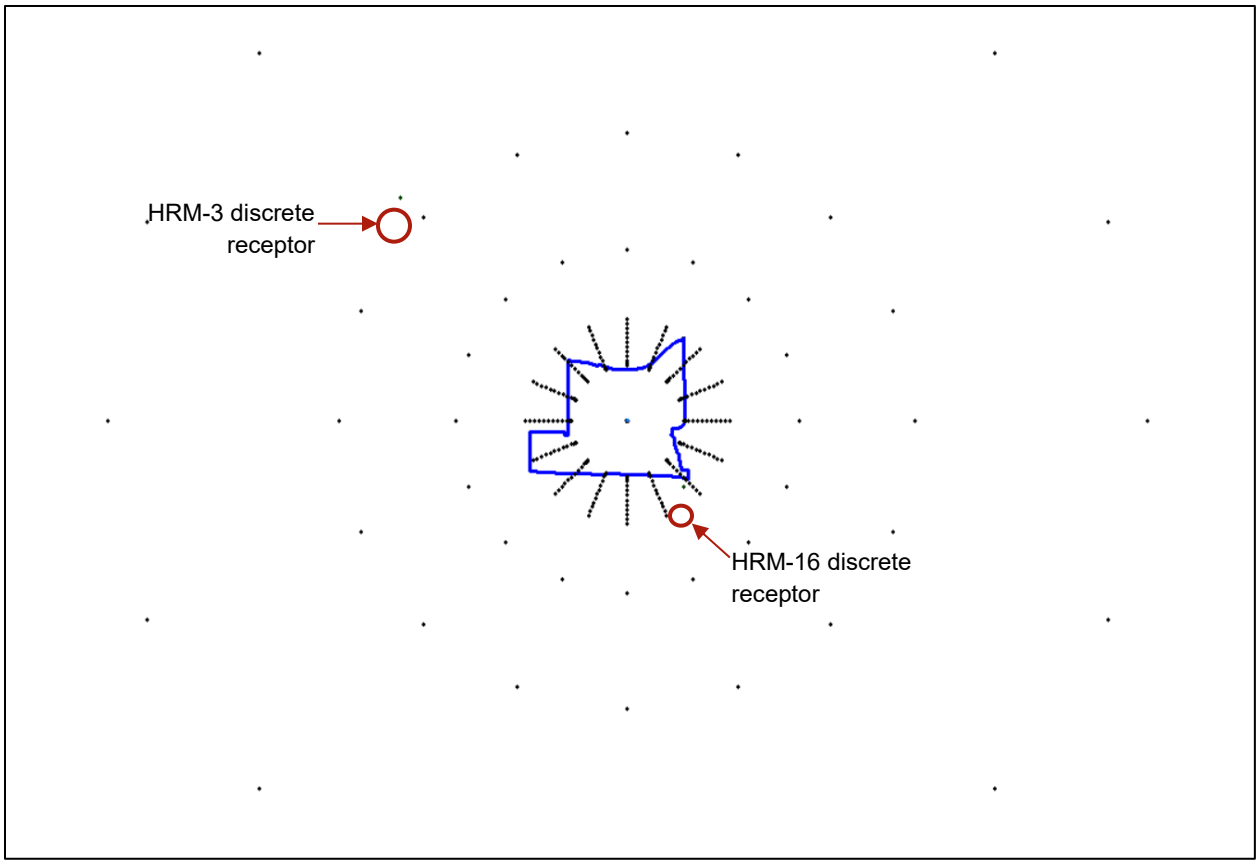


Figure 4: Snippet of BEEST input setup for TSCA full-screening methodology (sources at central point, blue fenceline, polar receptor grid)

3. Facility-Specific Dispersion Modeling

1.4 Permit-style Dispersion Modeling

Modeled output concentrations from the TSCA full-screening methodology (simplified AERMOD) can be compared to AERMOD runs following the EPA's method of AERMOD setup used in the Residual Risk Assessment review for the 2020 MON RTR final rule[4]. The EPA's AERMOD setup used in the MON RTR is similar to the dispersion model setup suggested by the TCEQ's Air Permits Division Air Quality Modeling Guidelines (APDG 6232, November 2019)[19]. The following section of this report discusses the required inputs for an air dispersion model setup following the EPA's MON RTR approach and TCEQ guidance (also referred to as "permit-style" dispersion model in this work).[19] Later sections of this report compare model outputs from the TSCA Full-screening methodology (simplified AERMOD) and the "permit-style" (facility-specific AERMOD) run. It is useful to note here that the permit-style AERMOD run is considered the best available science as it utilizes the EPA's preferred dispersion model for modeling steady-state plumes, and incorporates a necessary level of detail when dealing with model inputs, as seen in the 2020 MON RTR.

1.4.1 Permit-style (Facility-specific AERMOD) Inputs

The following table presents the parameters that were used to set up the AERMOD run for the permit-style model run, following the guidance provided in the TCEQ Air Permits Division Air Quality Modeling Guidelines[19] and the latest MON RTR. Figure 5 shows a screenshot of model setup in the BEEST software and captures all point (red dots) and area (blue boxes) sources, and the receptor grid modeled after TCEQ guidelines as discussed in detail in Table 3. Discrete

[19] TCEQ Air Quality Modeling Guidelines: https://www.tceq.texas.gov/assets/public/permitting/air/Modeling/guidance/airquality-mod-guidelines6232.pdf

receptor points were added at coordinates corresponding to HRM-3 and HRM-16 air monitoring sites to investigate modeled concentrations at a near-source location (HRM-16, not shown in Figure 5), and an off-site location downwind of the modeled facility (HRM-3), and to allow for comparison of modeled concentrations with ambient air monitoring data at both sites.

Table 3: Input parameters for permit-style model (Facility-specific AERMOD)

Emission Rates/Locations

- Rates for Point and Area sources obtained from 2020 National Emission Inventory (NEI)[20] for the 2021 model study, and from EPA 2019 modeling files[21] for the 2019 model study (Facility ID 4168511, corresponding to Facility TRIFD 77536SHLLLHIGHW and 77536DRPRK5900H)
- Coordinates for point and area sources provided in 2020 NEI and 2019 modeling file (based on actual release points)
- Total site emissions from multiple owners/operators

Source physical characteristics

72 point sources with the following source-specific parameters entered based on 2020 NEI or 2019 EPA modeling data:

- Stack Height
- Stack Diameter
- Exit Temperature
- Exit velocity

26 area sources with the following source-specific parameters entered based on 2020 NEI or 2019 EPA modeling data:

- Release area
- Release height
- Fugitive Easterly/Northerly length

Meteorological Data

- On-site meteorological data used from TCEQ site (HRM-16) near the facility (0.82 miles southeast of facility)
- Closest station to chosen facility with William P. Hobby Airport (HOU), which had pre-processed data available from TCEQ website[22]
- Upper Air data from Lake Charles, Louisiana (closest site with data availability)[23]
- Surface data, 1-minute, and 5-minute Automated Surface Observing Systems (ASOS) from William P. Hobby (KHOU) airport[24]
- AERMINUTE run using KHOU 1-minute and 5-minute data (2019, 2021)
- AERSURFACE run for Primary location (HRM-16, i.e., onsite meteorological data site), and Secondary location (KHOU)
    - Land Cover/Impervious/Tree Canopy files for surface characterizations based on National Land Cover Database (NLCD)[25] data
- AERMET Stage 1 and Stage 2 runs completed successfully (separate for 2019 and 2021 data)
- Output profile (.pfl) and Surface file (.scf) generated for input into AERMOD

Receptors

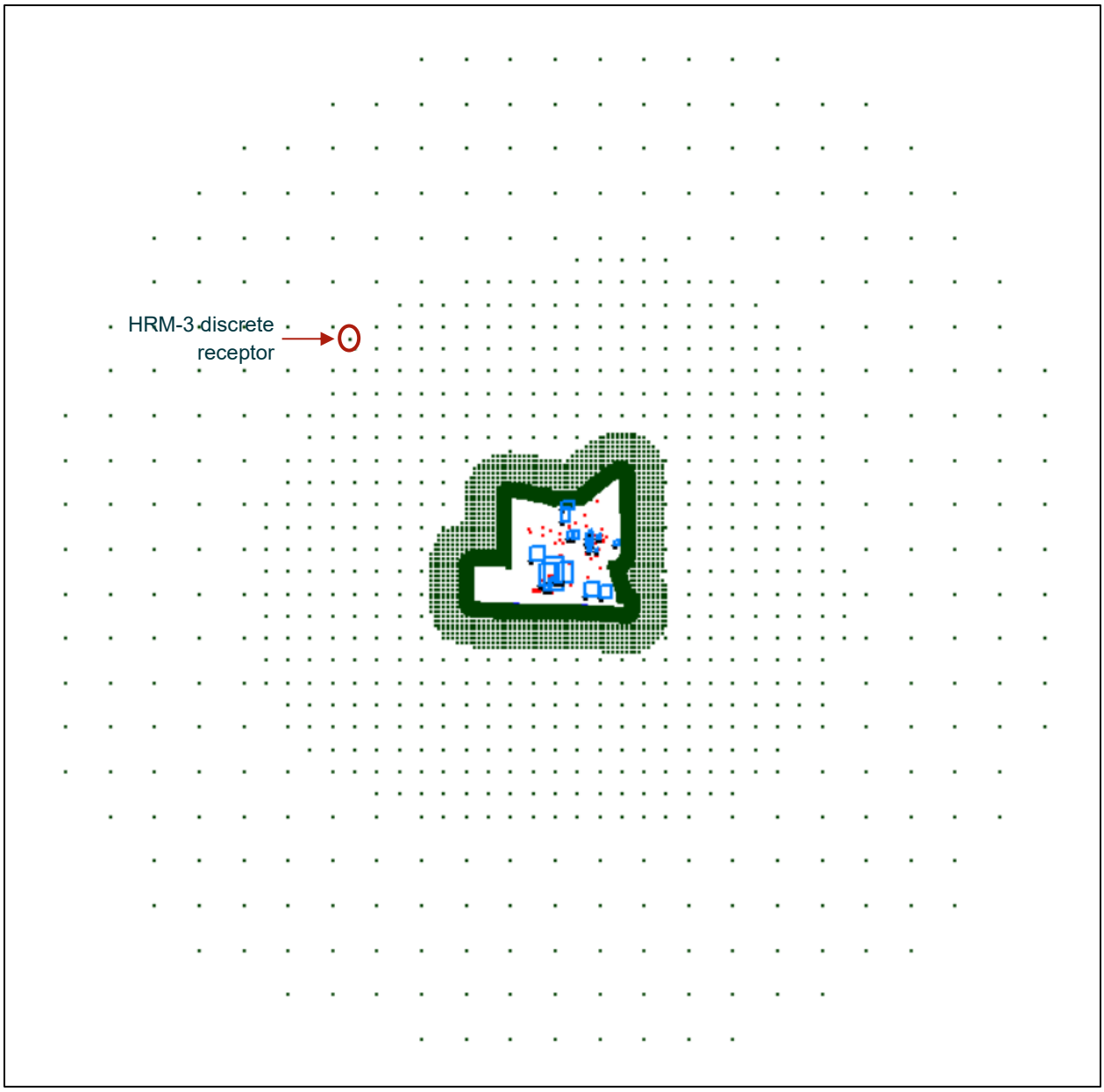
- Fenceline determined by examination of facility aerial imagery
- Receptor grid designed based on TCEQ Air Quality Modeling Guidelines (APDG 6232)
- Tight receptors spaced 25 meters apart; extending up to 300 m from facility
- Fine receptors spaced 100 meters apart; extending up to 1 km from facility
- Medium receptors spaced 500 meters apart; extending up to 5 km from facility
- Coarse receptors spaced 1 km apart; extending up to 50 km from facility
- Discrete receptor points added at HRM-3 and HRM-16 sites

Urban setting

To provide additional context to the meteorological dataset synthesis for the permit-style AERMOD run, on-site meteorological data from the TCEQ monitoring site neighboring the chosen facility – HRM-16 – was used. One year (2019 and 2021) hourly data from HRM-16 which included wind speed (mph), wind direction (degrees), temperature

[20] EPA 2020 NEI data webpage: https://www.epa.gov/air-emissions-inventories/2020-national-emissions-inventory-nei-data
[21] EPA 2019 Emissions Modeling webpage: https://www.epa.gov/air-emissions-modeling/2019-emissions-modeling-platform
[22] TCEQ pre-processed meteorological datasets: https://www.tceq.texas.gov/permitting/air/modeling/aermod-datasets.html
[23] Data accessed from NOAA/ESRL Radiosonde Database: https://ruc.noaa.gov/raobs/
[24] Data access: https://www.ncei.noaa.gov/pub/data/noaa/ and https://www.ncei.noaa.gov/pub/data/asos-onemin/
[25] NLCD Land Cover/ Impervious/Tree canopy files obtained from https://www.mrlc.gov/viewer/

(°F), pressure (inHg) was downloaded from the TCEQ's TAMISWeb database.[26] Gaps in data of 4 hours or less were supplemented with interpolated data from the HRM-16 site. Gaps in data greater than 4 hours were supplemented with meteorological data from the TCEQ's Houston Deer Park site (5.02 km away from Hexion Deer Park facility).



[26] TAMISWeb webpage: https://www17.tceq.texas.gov/tamis/index.cfm

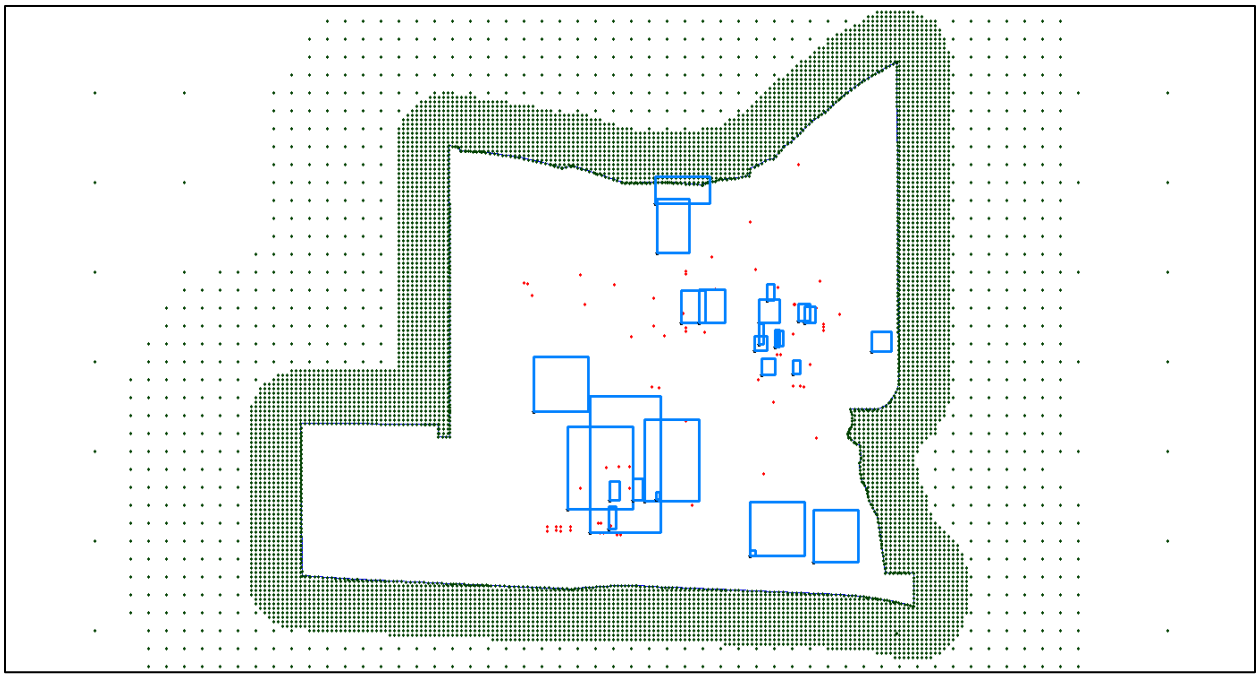


Figure 5: Snippets of BEEST input setup for permit-style model (including full receptor grid, and zoomed in to show sources)

It is important to note here the difference between the sources for emission rates used in the TSCA Full-Screen model, i.e. facility-wide emission rates reported to the TRI, compared to the Facility-Specific AERMOD, i.e. source-specific emissions rates reported to the NEI. To provide context on the difference between the two EPA-managed databases, the NEI is a comprehensive emissions inventory that tracks air pollutants from various sources including stationary sources (such as industrial facilities), mobile sources (such as traffic), and other nonpoint and area sources. TRI is a publicly available databased containing information on the release and transfer of toxic chemicals only from industrial facilities across the United States. Not all industrial facilities are required to report to TRI; only those that meet specific criteria outlined by the Environmental Protection Agency (EPA) must report their toxic releases and waste management activities. The same is true for facilities reporting to the NEI; only those facilities that exceed certain emission rates in a year are required to report a yearly emissions inventory to their state environmental agency.

A joint report published by the EPA and several state, local, and tribal environmental agencies (SLTs) [27] explored the difference between the two EPA-managed databases in more depth. Some of the overarching findings indicate that:

1. The NEI includes more facilities (88,000 facilities) than the TRI (22,000 facilities)
2. ~50% of facilities that report to the TRI also report to the NEI (10,238 out of 20,258 facilities)
3. When summed across all facilities, roughly half of pollutant emission rates agree within 10% (and three quarters of pollutants agree within 20%)
4. When comparing the emissions of pollutants by individual facilities, roughly half of the TRI and NEI rates are within 10% of each other
5. Out of a total of 4,797 records where TRI and NEI emissions were comparable (i.e. within 2% of one another), approximately 27% had noticeable differences in how emissions were allocated to stack and fugitive releases.

For the refined modeling tier, TRI data can be used to verify the quality of the NEI data or gap-fill NEI data, as recommended in the joint EPA and SLT report[27]. The reason for recommending the use of NEI data for the refined tier (Facility-specific AERMOD) is that TRI data lacks necessary detail on release parameters for stack and fugitive sources (e.g. stack height, stack temperature, exit velocity, area release height, etc.). The EPA is aware that stack height has the greatest impact on predicted air pollutant concentrations, where a 40-meter median stack height compared to a 10-meter median stack height reduces peak concentration by a factor of 20 and the peak occurs 4 times further downwind[28,29]. Using the more granular or source-characterized data from the NEI provides improved inputs for a more

[27] https://www.epa.gov/sites/default/files/2019-02/documents/final-report-phase2-tri-nei-slt.pdf
[28] Comment in EPA docket: https://www.regulations.gov/comment/EPA-HQ-OPPT-2021-0415-0086
[29] https://www.epa.gov/rsei/estimate-stack-heights-and-exit-gas-velocities-tri-facilities-oppts-risk-screening

accurate risk evaluation. In addition, the NEI has been rated as a high-quality data source according to the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances*[30], making it a reliable source of inputs for the proposed Facility-specific AERMOD.

1.4.1.1 Choice of AERMOD Graphical User Interface

For this modeling exercise, AERMOD was run using BEEST which is a graphical user interface (GUI) for AERMOD, sold and maintained by Providence Oris[31]. The regulatory default option was selected when running AERMOD using BEEST and no "BETA" options were used. Other commonly used GUIs used to run AERMOD include Lakes Environmental Software AERMOD View[32] and Trinity Consultants' BREEZE AERMOD GUI[33]. The use of a graphical user interface to facilitate setting up model inputs and analyzing model results does not affect model concentrations, especially when the AERMOD model code is not altered. Recent guidance from the EPA highlights that if changes are made to a preferred model (such as AERMOD) without affecting modeled concentrations, the preferred status of the model is unchanged. In this case, the use of a GUI is an example of a modification that does not affect model concentrations.[34]

Another model that is used primarily for performing risk assessments for sources emitting air toxics to ambient air is the EPA's Human Exposure Model (HEM)[35]. HEM only addresses the inhalation exposure pathway and is designed to predict the risk associated with chemicals emitted into the ambient air, which is defined as the vicinity of a facility but beyond its property boundary. The current version of HEM (HEM 4.2) includes (1) AERMOD as the atmospheric dispersion model, with included pre-processed meteorological data, (2) US Census Bureau population data at the Census block level (currently using 2020 data). The AERMOD code included in HEM-4 is the same as that used in the aforementioned GUIs, so output concentrations from HEM (estimated in micrograms per cubic meter) should be unchanged across these softwares. The main difference is that HEM-4 extends the exposure estimates by combining them with pollutant health reference values to estimate cancer risks and noncancer hazards, among other risk measures.

[30] https://www.regulations.gov/document/EPA-HQ-OPPT-2021-0414-0005
[31] https://www.providenceoris.com/product/beest-suite/
[32] https://www.weblakes.com/software/air-dispersion/aermod-view/
[33] https://www.trinityconsultants.com/software/dispersion/aermod
[34] https://www.federalregister.gov/documents/2023/10/23/2023-22876/guideline-on-air-quality-models-enhancements-to-the-aermod-dispersion-modeling-system
[35] https://www.epa.gov/fera/risk-assessment-and-modeling-human-exposure-model-hem

1.4.2 Results

Table 4 shows the input values to the IIOAC and TSCA Full Screening Model which are based on reported emission rates to the 2019 and 2021 Toxic Release Inventory. Table 5 and Table 6 show results of the TSCA Pre-screening (Box 1 shown in Figure 2) and Full-screening (Box 2 shown in Figure 2) models (IIAOC and "Simplified AERMOD") compared to a permit-style AERMOD run (Box 3 shown in Figure 2) (i.e. a dispersion model run following the example provided in the EPA's RTR for the 2020 MON final rule (Docket EPA-HQ-OAR-2018-0746)[36] for the years 2019 and 2021. Note that within the IIOAC tool, high-end values are defined as the 95th percentile result, whereas AERMOD results are the "maximum" which is defined as the maximum annual result averaged over one year for the given receptor points (extending from fenceline to 10 km out).[37] Note that in Table 5 and Table 6, the concentrations are provided in μg m^{-3} with corresponding ppb values provided in parentheses. Contour plots showing output concentrations for Box 2 and Box 3 models for Years 2019 and 2021 are available in Appendix A.

Table 4: Toxic Release Inventory (TRI) emission rates, used as inputs to AERMOD (IIOAC and TSCA Full Screen model)

TRI Reporting Year	"AIR-STACK" Category Emission Rate (lbs/year)	"AIR-FUGITIVE" Category Emission Rate (lbs/year)
2019	49,000	5720
2021	42,000	5330

Table 5: Box 1 to Box 3 Model Study Results for Year 2019

Unit: μg/m^3 (ppb)	TSCA Pre-screening IIOAC Point | Area		TSCA Full-screening (Simplified AERMOD)	Permit-style (Facility-specific AERMOD)
Fenceline concentration (high-end)	4.37 (1.97)	6.38 (2.87)		
Community concentration (high-end)	1.22 (0.55)	0.44 (0.20)		
Model Maximum concentration			1.04 (0.47)	0.44 (0.20)
HRM-3 Receptor concentration			0.06 (0.03)	0.04 (0.02)
HRM-16 Receptor concentration			0.12 (0.05)	0.05 (0.02)

Table 6: Box 1 to Box 3 Model Study Results for Year 2021

Unit: μg/m^3 (ppb)	TSCA Pre-screening IIOAC Point | Area		TSCA Full-screening (Simplified AERMOD)	Permit-style (Facility-specific AERMOD)
Fenceline concentration (high-end)	3.75 (1.69)	5.94 (2.67)		
Community concentration (high-end)	1.04 (0.47)	0.41 (0.18)		
Model Maximum concentration			0.74 (0.33)	0.46 (0.21)

[36] EPA MON RTR Supporting documents: https://www.regulations.gov/document/EPA-HQ-OAR-2018-0746-0189
[37] IIOAC 1.0 users guide: https://www.epa.gov/sites/default/files/2019-06/documents/iioac_1.0_users_guide_may_2019.pdf

HRM-3 Receptor concentration		0.04 (0.02)	0.03 (0.01)
HRM-16 Receptor concentration		0.11 (0.05)	0.04 (0.02)

Building on the discussion on TSCA screening model inputs in sections 1.2.1 and 1.3.1, the 2019 TRI data for the chosen facility had a total emission rate of 49,000 lbs/year for point ("stack") sources, and 5720 lbs/year for fugitive sources. The 2021 TRI data for the facility showed a total emission rate of 42,000 lbs/year for point sources, and 5330 lbs/year for fugitive sources. The IIOAC fenceline and community output concentrations are accordingly similar for years 2019 and 2021, with slightly higher output concentrations for 2019 corresponding to the higher reported TRI emissions for that year. Focusing on year 2019 (the year with higher emission rates), adding IIOAC output concentrations from point (4.37 µg m^{-3}) and area (6.38 µg m^{-3}) sources result in a high-end fenceline concentration of 10.75 µg/m^3 (4.84 ppb) and a high-end community concentration of 1.66 µg/m^3 (0.75 ppb). Additionally, as detailed in the forthcoming section of this report, the measured annual average concentration of 1,3-butadiene for the year 2019 at the HRM-16 (near-fenceline) site was 0.393 µg/m^3 or 0.18 ppb. This is considerably lower (<4%) than the predicted-IIOAC fenceline value, which highlights the overly conservative results of this prescreening tool. A similar analysis for the year 2021 IIOAC output concentrations shows that the measured annual average concentration (0.389 µg/m^3 or 0.18 ppb) at HRM-16 (near-fenceline) is less than 5% of the IIOAC-predicted high-end fenceline concentration of 9.69 µg/m^3 or 4.36 ppb(which is based on the sum of the point – 3.75 µg m^{-3} – and area – 5.94 µg m^{-3} – source output concentrations).

Expanding on the locations of the modeled maximum concentrations, the 2019 TSCA Full-Screening AERMOD gave an output maximum concentration of 1.04 µg/m^3 at the north fenceline receptor (1200 m from facility's central source). The 2021 TSCA Full-Screening AERMOD gave an output maximum concentration of 0.74 µg/m^3 also north of the fenceline receptor (1200 m from facility's central source). The 2019 facility-specific AERMOD run produced the lowest output concentrations of all three models (0.44 µg/m^3 at the west fenceline receptor or 1200 m from the facility's central source). The 2021 facility-specific AERMOD concentration was also the lowest of all three models with an output concentration of 0.46 µg/m^3 at the east fenceline receptor or 1300 m from the facility's central source. All maximum concentrations were observed directly at the fenceline receptors, however the 2019 and 2021 maximum concentrations for the facility-specific AERMOD run were observed at different locations of the receptors (west versus east respectively). This is likely due to the use of different meteorological datasets for the different years, as presented in the EPA MON RTR and TCEQ dispersion modeling guidelines. This difference in location was not observed in the TSCA Full-Screen model, likely because the meteorological dataset was based on Houston Hobby Airport data, which is considerably farther from the modeled facility than the nearby HRM-16 site.
Further highlighting the overly conservative output concentrations estimated by the proposed TSCA pre-screening methodology (IIOAC), a comparison with the TSCA full-screening methodology (simplified AERMOD) shows that the IIOAC-predicted output concentrations are about an order of magnitude greater than those predicted by a simplified AERMOD run (e.g. 10.75 µg/m^3 vs. 1.04 µg/m^3 for the 2019 TRI dataset). Although the IIOAC tool is built based on pre-run AERMOD scenarios, it is apparent that certain changes incorporated in the TSCA full-screen approach help make the model outputs more realistic and considerably less conservative, even though the input emission rates are the same (2019 TRI or 2021 TRI datasets). The major difference between both methods was the ability to choose a more representative meteorological dataset for the facility of choice (William P. Hobby airport (TX) instead of the pre-set IIOAC choice of Lake Charles, LA).

When comparing the TSCA full-screen methodology (simplified AERMOD) to the permit-style AERMOD run, it is important to note that major differences include the use of emission inventory rates (2020 NEI and NEI-off-year 2019 EPA modeling file emission rates), placement of source coordinates at actual emission points, use of a "denser" receptor grid, and the use of on-site meteorological data. With these differences in mind, the permit-style AERMOD runs for 2019 and 2021 provide output concentrations that are ~50% less than the TSCA full-screening approach. This applies for both modeling years, and for the various receptor points (maximum receptor point, HRM-16 or near-fenceline point, HRM-3, or offsite receptor point). While a true permit-style AERMOD run would also include building downwash from neighboring facilities, the setup in this report follows the dispersion modeling methodology used in the MON RTR (2020) docket[36] which excludes downwash effects.

1.4.3 Modeling study using predicted post-MON concentrations

On August 12th 2020, the EPA published its final rule on "National Emission Standards for Hazardous Air Pollutants: Miscellaneous Organic Chemical Manufacturing Residual Risk and Technology Review" in which the preamble mentions significant emission reduction of HAPs[38] including 1,3-butadiene. The preamble states the "sources of HAP emissions regulated by the MON include the following: process vents, storage tanks, transfer racks, equipment leaks, wastewater streams, and heat exchange systems." Furthermore, the EPA included supplemental attachments[39] in the docket that provide predicted post-control emission rates for all evaluated sources. The reductions were based on the facility location, type of source (process vent, storage tank, etc.), and the MON chemical in question. For the facility used in this modeling study, the EPA's predicted post-control emission rates were 3.9% less than the actual emission rates for fugitive/area sources. Thus, the modeling study (Boxes 1, 2, and 3 in Figure 2) was conducted again modifying the 2019 emission rates by the emission reductions predicted in the MON rule (3.9% for fugitive sources), while keeping all other parameters constant.

Table 7 provides the model study results for year 2019 data with predicted post-MON reductions applied. Note that the compliance dates for several changes (e.g. ethylene oxide provisions) in the 2020 MON Final Rule were effective upon publication of the final rule (August 12th 2020), while the compliance date for some changes (including replacement of maintenance startup and shutdown exemptions with the obligation to "comply at all times"; new requirements for multi-point flares, etc.) was 3 years from the publication of the final rule (i.e. August 12th 2023).

Note that in Table 7, the concentrations are provided in µg m^{-3} with corresponding ppb values provided in parentheses.

Table 7: Box 1 to Box 3 Model Study Results for Year 2019 (post-MON reduction)

Unit: µg/m³ (ppb)	TSCA Pre-screening IIOAC Point | Area		TSCA Full-screening (Simplified AERMOD)	Permit-style (Facility-specific AERMOD)
Fenceline concentration (high-end)	4.37 (1.97)	6.13 (2.76)		
Community concentration (high-end)	1.22 (0.55)	0.42 (0.19)		
Model Maximum concentration			1.03 (0.46)	0.43 (0.19)
HRM-3 Receptor concentration			0.06 (0.03)	0.04 (0.02)
HRM-16 Receptor concentration			0.12 (0.05)	0.05 (0.02)

Given the small percentage difference in predicted emission rates for this facility's sources (3.9% for fugitive sources), the model study outputs are unsurprisingly like the 2019 model study results with no post-MON reductions applied. The same conclusions from the 2019 and 2021 model studies apply: the IIOAC tool provides the most conservative results, followed by the simplified AERMOD run, and the facility-specific AERMOD run.

1.4.4 Comments on predicted post-HON conditions

On April 25th 2023, the EPA published a proposed rule titled "New Source Performance Standards for the Synthetic Organic Chemical Manufacturing Industry and National Emission Standards for Hazardous Air Pollutants for the Synthetic Organic Chemical Manufacturing Industry (SOCMI) and Group I & II Polymers and Resins Industry (P&R)", hereby referred to as the proposed HON rule.[40] The preamble of the rule claims that there will be reduced emissions of various HAPs from improvements to flares, process vents, heat exchange systems, equipment leaks, wastewater systems, maintenance vents, storage tanks, and pressure relief devices (PRDs). Additionally, the proposed HON rule

[38] RTR for 2020 MON final rule preamble: https://www.federalregister.gov/d/2020-12776/p-456
[39] Attachment within rule docket documentation: https://downloads.regulations.gov/EPA-HQ-OAR-2018-0746-0189/attachment_1.xlsx
[40] Proposed HON rule webpage: https://www.federalregister.gov/documents/2023/04/25/2023-07188/new-source-performance-standards-for-the-synthetic-organic-chemical-manufacturing-industry-and

will include fenceline monitoring for facilities in the SOCMI and P&R I source categories that use, produce, store, or emit benzene, 1,3-butadiene, chloroprene, ethylene oxide, ethylene dichloride, or vinyl chloride.

Notably, while the TSCA pre-screening and full-screening outputs for the 2019, 2021, and post-MON 2019 studies result in concentrations greater than or close to the proposed HON rule action level (3 µg/m^3 for 1,3-butadiene), the permit-style (facility-specific) AERMOD simulations predict maximum concentrations that are lower (maximum annual average of 0.46 µg/m^3 for Year 2021).

The following table (Table 8) summarizes information on HON impacts from an operational perspective. For the facility that was modelled in the present analysis, the post-HON emission reductions of 1,3-butadiene are expected to be minor. This is since the test facility already meets TCEQ's HRVOC requirements for controls, monitoring/testing, recordkeeping, and reporting. Furthermore, all the flares on this site are already covered by other EPA regulations (i.e., refinery flare rule and ethylene MACT).

If another test facility is considered, one not already subject to HRVOC requirements, then an estimate of 1,3-butadiene emission reductions can be assumed from TCEQ documents[41]. The design of the HRVOC program was to achieve a 36% reduction in HRVOCs, specifically ethylene, propylene, 1,3-butadiene and butenes. This level of emission reduction can be reasonably assumed for each individual HRVOC.

Depending on the starting status for another test facility and the types of emission sources at the facility, 1,3-butadiene emission reductions could be up to 36%. However, for most facilities, existing MON and EMACT requirements likely would result in significantly smaller emission reductions.

Table 8: Summary of HON impacts on facility operations

Source Type	Proposed Change
Heat Exchange Systems	• Monitoring must be conducted using the Modified El Paso Method with a leak definition of 6.2 parts per million by volume (ppmv). • Quarterly monitoring preceded by an initial 6-month period where monitoring is conducted monthly. • Establishes a delay of repair action level of 62 ppmv. If this value is exceeded, delay of repair cannot be used beyond 30 days.
Storage Vessels	• Group 1 storage tank characteristics will change from 75 m^3 -151 m^3 and 13.9 kPa to 38 m^3 – 151 m^3 and 6.9 kPa. • Internal floating roof (IFR) tanks must be equipped with deck covers for certain fittings and controls for guide poles. If a blanket, purge, or sweep is used between the floating and fixed roof, it must be routed to control.
Process Vents	• Group 1 process vent characteristics will change to any process vent that emits greater than or equal to 1.0 pounds/hour (lb/hr) of total organic hazardous air pollutants (HAP)
Fenceline Monitoring	• Fenceline monitors must be deployed to measure fenceline concentrations of benzene, 1,3-butadiene, chloroprene, ethylene dichloride, ethylene oxide, and vinyl chloride if the site uses, produces, stores, or emits any of these compounds. • Must initiate root cause analysis and take corrective actions to reduce fugitive emissions if measured concentrations exceed the action level for any monitored pollutants.
Flares	• Flares used to comply with the emissions standard are subject to the requirements in 40 CFR Part 63, Subpart CC (Refinery MACT), with certain clarifications and exemptions.
Pressure Relief Devices (PRDs)	• For PRDs not routed to a control device, process, fuel gas system, or drain system, the following requirements will be added: – Install monitoring system to alert when a PRD release occurs. – Three redundant prevention measures must be implemented. – Conduct a root cause analysis and initiate appropriate corrective action in response to any PRD releases. • Limit number of PRD releases to one, two, or three releases in a three-year period depending on the cause of the release.
Bypass Lines	• A monitoring system capable of detecting when stream is diverted through a bypass must be installed; or

[41] https://www3.epa.gov/ttnchie1/conference/ei17/session6/thomas.pdf

	– Bypass lines must be secured in a closed position with car-seal or lock and key type mechanism.
Maintenance Activities	• Work practice standards for storage vessel degassing, storage vessel maintenance, and equipment opening will be added. • Exemptions for startup, shutdown, and malfunction (SSM) will be removed.
Pressure Vessels	• Pressure vessels greater than 204.9 kPa and without emissions to atmosphere are no longer excluded from the definition of storage vessel. • A definition for pressure vessels has been added. • Must conduct leak detection and repair (LDAR) monitoring initially and annually, with a leak definition of 500 ppm.
Surge Control Vessels and Bottom Receivers	• Any equipment with total organic HAP greater than 1.0 lb/hr would require control to 98%, 20 ppmv, or emissions must be routed to a flare meeting the new flare requirements.
Transfer Operations	• The exemption for transfer operations at greater than 204.9 kPa has been removed.

The final rule is expected in Spring 2024.

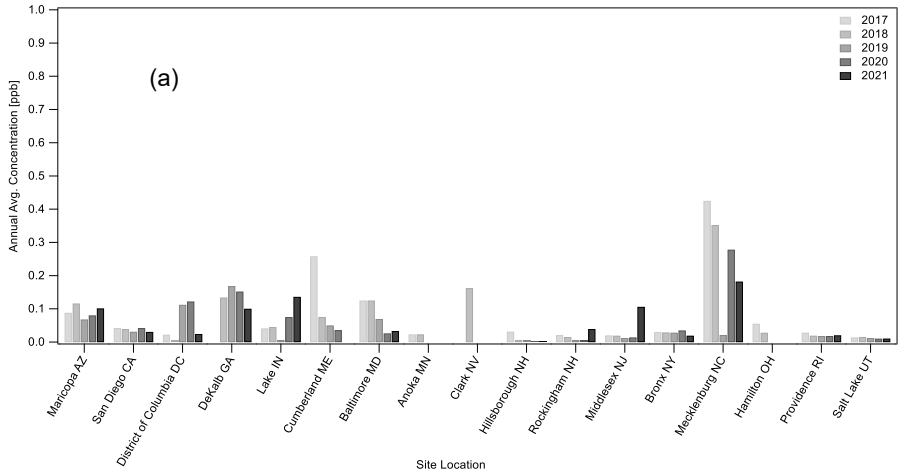
4. Ambient Air Monitoring

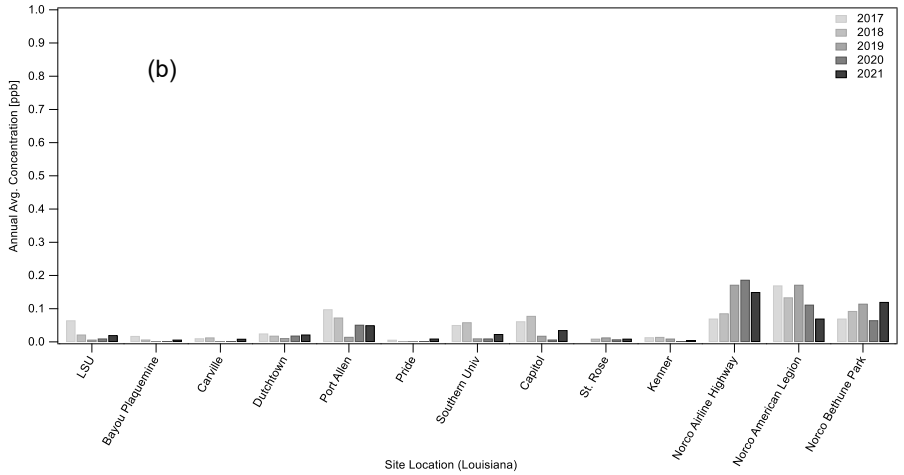
1.5 1,3-butadiene ambient air monitoring trends from 2017 to 2021

Since 1,3-butadiene has multiple sources and arises not only from manufacturing and/or use, monitoring data can more accurately represent air concentrations at which communities may be exposed. To put the air dispersion modeling study results from previous sections into context, ambient air concentrations of 1,3-butadiene measured at various sites with automated gas chromatography (auto-GC) measurements (owned/operated by EPA, LDEQ, and TCEQ) from years 2017 to 2021 were analyzed. Most sites that were selected for this data analysis are in the state of Texas. This data was chosen as the Texas air monitoring network is known to be one of the most extensive in the nation[42], with validated data that is available for public access[26].

Figure 6 provides annual average concentrations of 1,3-butadiene for (a) various nationwide sites, (b) sites in Louisiana, (c) sites in Texas (TCEQ Regions 4 and 12, i.e. Dallas/Fort Worth and Houston). The nationwide sites chosen are all air monitoring sites that collect autoGC data measuring various VOCs including 1,3-butadiene, and which have ambient air quality data publicly available through EPA's Air Quality System (AQS) website. The selected Texas and Louisiana sites are all air monitoring sites measuring 1,3-butadiene using an autoGC and which have publicly available air quality data available through the TCEQ website (TAMISweb) and LDEQ website[43] respectively. Since the TCEQ air monitoring network is one of the most expansive in the nation, we focus on air quality data from the cities of Houston and Dallas only. Site-to-site trends are generally consistent over the years of this analysis, and all annual average concentrations appear to be lower than 1 ppb (with the exception of one site in Texas in 2021, which experienced extreme weather conditions).

[42] TCEQ Ambient Air Monitoring webpage: https://www.tceq.texas.gov/airquality/monops
[43] https://www.deq.louisiana.gov/page/ambient-air-monitoring-data-reports


(a)
2017
2018
2019
2020
2021
Annual Avg. Concentration [ppb]
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Maricopa AZ
San Diego CA
District of Columbia DC
DeKalb GA
Lake IN
Cumberland ME
Baltimore MD
Anoka MN
Clark NV
Hillsborough NH
Rockingham NH
Middlesex NJ
Bronx NY
Mecklenburg NC
Hamilton OH
Providence RI
Salt Lake UT
Site Location


(b)
2017
2018
2019
2020
2021
Annual Avg. Concentration [ppb]
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
LSU
Bayou Plaquemine
Carville
Dutchtown
Port Allen
Pride
Southern Univ
Capitol
St. Rose
Kenner
Norco Airline Highway
Norco American Legion
Norco Bethune Park
Site Location (Louisiana)

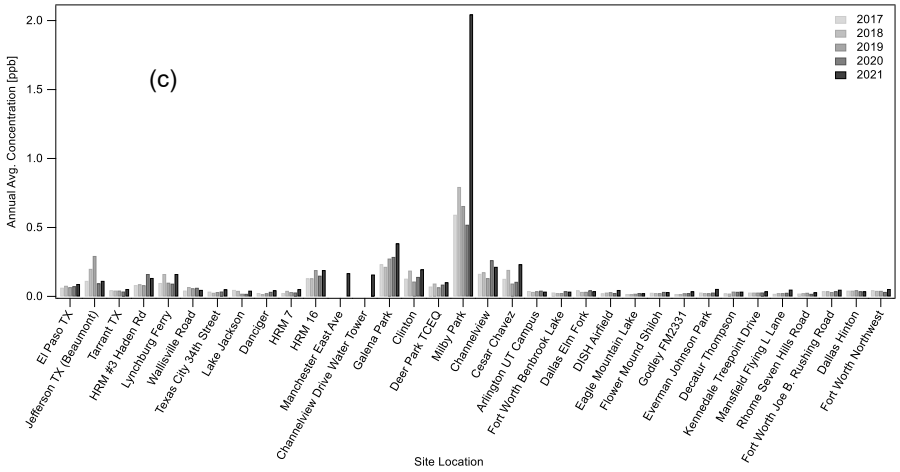


Figure 6: 1,3-butadiene annual average concentrations at (a) several EPA nationwide sites, (b) Louisiana sites, (c) Texas sites

Taking a closer look at Figure 6 (c), it appears that sites in Harris County, TX (TCEQ Region 12, sites from HRM#3 to Cesar Chavez) have slightly higher 1,3-butadiene concentrations compared to sites in Dallas, TX (TCEQ Region 4). A more detailed discussion on potential reasons for this is provided in Section **Error! Reference source not found.** of this report.

Table 9 presents the same 1,3-butadiene annual average concentrations as Figure 6 in a tabulated format. The rows highlighted in light green (HRM-3, HRM-16, and Milby Park) correspond to select sites with higher-than-average concentrations of 1,3-butadiene (compared to nationwide averages).

Table 9: Annual average 1,3-butadiene concentrations (ppb) at various nationwide air monitoring sites (2017-2021)

(TCEQ) Region	Site Name	Site Description	Annual Average 1,3-Butadiene Concentration [ppb]				
			2017	2018	2019	2020	2021
12	Site_22_3	HRM #3 Haden Rd	0.081	0.087	0.080	0.16	0.13
12	Site_23_2	Lynchburg Ferry	0.097	0.16	0.099	0.092	0.16
12	Site_24_1	Wallisville Road	0.042	0.067	0.058	0.062	0.047
12	Site_25_1	Texas City 34th Street	0.034	0.026	0.031	0.035	0.051
12	Site_26_1	Lake Jackson	0.047	0.040	0.019	0.018	0.041
12	Site_28_1	Danciger	0.024	0.016	0.022	0.033	0.044
12	Site_47_2	HRM 7	0.024	0.040	0.031	0.028	0.052
12	Site_48_1	HRM 16	0.13	0.13	0.18	0.15	0.23
12	Site_55_3	Manchester East Ave	–	–	–	–	0.17
12	Site_56_2	Channelview Drive Water Tower	–	–	–	–	0.16
12	Site_72_5	Galena Park	0.23	0.21	0.27	0.29	0.38
12	Site_A_2	Clinton	0.13	0.19	0.11	0.14	0.20
12	Site_H_1	Deer Park_TCEQ	0.071	0.093	0.065	0.085	0.10
12	Site_K_2	Milby Park	0.59	0.79	0.66	0.52	2.04
12	Site_R_2	Channelview	0.16	0.17	0.13	0.26	0.21
12	Site_V_1	Cesar Chavez	0.13	0.19	0.093	0.10	0.23
4	C1018_Site_2A_1	Arlington UT Campus	0.038	0.032	0.036	0.041	0.034
4	C1503_Site_2B_1	Fort Worth Benbrook Lake	0.028	0.023	0.024	0.037	0.034
4	C1505_Site_2C_1	Dallas Elm Fork	0.043	0.032	0.033	0.043	0.037
4	C1013_Site_2D_2	DISH Airfield	0.021	0.027	0.030	0.024	0.046
4	C75_Site_2E_2	Eagle Mountain Lake	0.016	0.016	0.019	0.023	0.022

4	C1007_Site_2F_2	Flower Mound Shiloh	0.026	0.023	0.023	0.032	0.031
4	C1501_Site_2G_1	Godley FM2331	0.016	0.017	0.021	0.023	0.036
4	C1009_Site_2J_2	Everman Johnson Park	0.027	0.023	0.022	0.027	0.054
4	C88_Site_2T_2	Decatur Thompson	0.021	0.020	0.034	0.033	0.034
4	C1062_Site_62_1	Kennedale Treepoint Drive	0.027	0.027	0.027	0.028	0.036
4	C1063_Site_63_1	Mansfield Flying L Lane	0.018	0.023	0.023	0.026	0.049
4	C1064_Site_64_1	Rhome Seven Hills Road	0.020	0.022	0.026	0.018	0.029
4	C1065_Site_65_1	Fort Worth Joe B. Rushing Road	0.037	0.037	0.031	0.037	0.048
4	C60_Site_E_3	Dallas Hinton	0.041	0.041	0.044	0.036	0.036
4	C13_Site_F_10	Fort Worth Northwest	0.043	0.040	0.040	0.032	0.053
National	4_13_4003	Maricopa AZ	0.088	0.12	0.07	0.08	0.10
National	6_73_1	San Diego CA	0.042	0.039	0.031	0.042	0.030
National	11_1_43	District of Columbia DC	0.022	0.0040	0.11	0.12	0.024
National	13_89_2/**3**	DeKalb GA	--	0.13	0.17	0.15	0.10
National	18_89_22/34/**35**/2008	Lake IN	0.041	0.045	0.006	0.075	0.14
National		Capitol LA	0.061	0.065	0.037	0.032	0.035
National		Dutchtown LA	0.031	0.018	0.024	0.028	0.026
National	23_5_29	Cumberland ME	0.26	0.075	0.050	0.036	
National	24_5_3001	Baltimore MD	0.12	0.12	0.069	0.026	0.033
National	27_3_1003	Anoka MN	0.023	0.023	--	--	--
National	32_3_540	Clark NV	--	0.16	--	--	--
National	33_11_5001	Hillsborough NH	0.031	0.0060	0.0035	0.00042	0.0027
National	33_15_18	Rockingham NH	0.021	0.015	0.0059	0.0041	0.039
National	34_23_11	Middlesex NJ	0.020	0.019	0.012	0.014	0.11
National	36_5_110	Bronx NY	0.030	0.029	0.028	0.035	0.019
National	37_119_41	Mecklenburg NC	0.42	0.35	0.021	0.28	0.18

National	39_61_47	Hamilton OH	0.055	0.028	--	--	--
National	44_7_22	Providence RI	0.028	0.019	0.018	0.018	0.020
National	48_113_69	Dallas TX	0.042	0.042	0.046	0.038	0.038
National	48_141_44	El Paso TX	0.063	0.077	0.066	0.073	0.089
National	48_245_1035	Jefferson TX (Beaumont)	0.11	0.20	0.29	0.094	0.11
National	48_439_1002	Tarrant TX	0.044	0.042	0.042	0.035	0.053
National	49_11_4	Salt Lake UT	0.014	0.015	0.012	0.010	0.010

Building on the discussion in Section 1.4.2 of this report, the annual average measured concentration of 1,3-butadiene for the year 2019 at the HRM-16 (near-fenceline) site was 0.18 ppb or 0.40 µg/m^3 which was considerably less than the TSCA pre-screening (annual average) model output of 4.84 ppb or 10.75 µg/m^3, less than TSCA full-screen model maximum output of 0.47 ppb or 1.04 µg/m^3, and of similar magnitude to the Facility-Specific AERMOD maximum concentration of 0.20 ppb or 0.44 µg/m^3. Note that the model outputs are the 95th percentile result for the TSCA pre-screening model (IIOAC) and the maximum concentration result for the TSCA full-screen model and Facility-Specific AERMOD. Additionally, the TSCA pre-screening model output discussed here is the concentration directly at the fenceline whereas the TSCA full-screen output and the ambient concentrations are measured at a nearby air monitoring site (HRM-16, 0.82 miles from modeled facility). These results highlight the conservative nature of the TSCA pre-screening approach which is not predictive of real ambient concentrations, where the suggested model predicts concentrations that are higher than those measured by air monitoring stations near the facility. The data from monitoring sites reflects aggregate exposures from multiple industrial sites and other sources, and is impacted by environmental and seasonal effects which are not necessarily captured in screening models. As such, it is expected that a realistic model would provide an output concentration of 1,3-butadiene that is considerably lower than the ambient annual average concentration which incorporates several (industrial and non-industrial) sources. In that regard, the Facility-Specific AERMOD, which is considered the best available science, provides more realistic predicted ambient concentrations, albeit still conservative, for this case-study facility. The Facility-Specific modeled concentration is considered conservative as model outputs are only based on modeling the sources in a single case-study facility, whereas measured concentrations are based on all industrial, and non-industrial (mobile and area) sources in the monitoring location.

A similar analysis for the year 2021 shows that the measured annual average concentration of 1,3-butadiene at the HRM-16 (near-fenceline) site was 0.23 ppb or 0.51 µg/m^3 which was less than the TSCA pre-screening model output of 4.36 ppb or 9.69 µg/m^3 and the TSCA full-screen model maximum of 0.33 ppb or 0.74 µg/m^3, and of similar magnitude to the Facility-Specific AERMOD which had model maximum concentrations of 0.21 ppb or 0.46 µg/m^3. Here we note again that the Facility-Specific model is still considered conservative as model outputs are only based on the sources within this case-study facility, whereas measured concentrations are based on all industrial and non-industrial sources in the monitoring location.

An EPA Memorandum titled “Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze”[44] discusses how to compare model outputs to observed (measurement) data. In that work, cases with factors of 2 under- and over-prediction are considered to meet “performance criteria”, i.e. the model results are acceptable when compared to measurement data. The memorandum suggests that less abundant species should have less stringent proposed “performance goals” (close to best achievable results) and “performance criteria” (acceptable results). Although no qualitative benchmark is provided for less abundant species (such as 1,3-butadiene), the memorandum recommends allowing for larger bias and error when the ambient concentration of any species falls below 2 µg m^{-3}, as the model’s ability to make accurate predictions decreases at lower concentrations. Additionally, the EPA recommends against the use of such benchmarks in a pass/fail mode but only as

[44] https://www3.epa.gov/ttn/naaqs/aqmguide/collection/cp2_old/20070418_page_guidance_using_models.pdf

a means of assessing general confidence in data, alongside other qualitative or quantitative procedures to assess overall model performance (e.g. the discussion of Positive Matrix Factorization in the forthcoming section of this report).

Figure 7 presents historical trends of 1,3-butadiene based on work from Hendler et al. (2010)[45] (shown in grey) compared to data analysis conducted as part of this report (shown in red). The graphics show that for almost all Houston sites (with minor exceptions), concentrations of 1,3-butadiene have substantially reduced since 1995-2009.

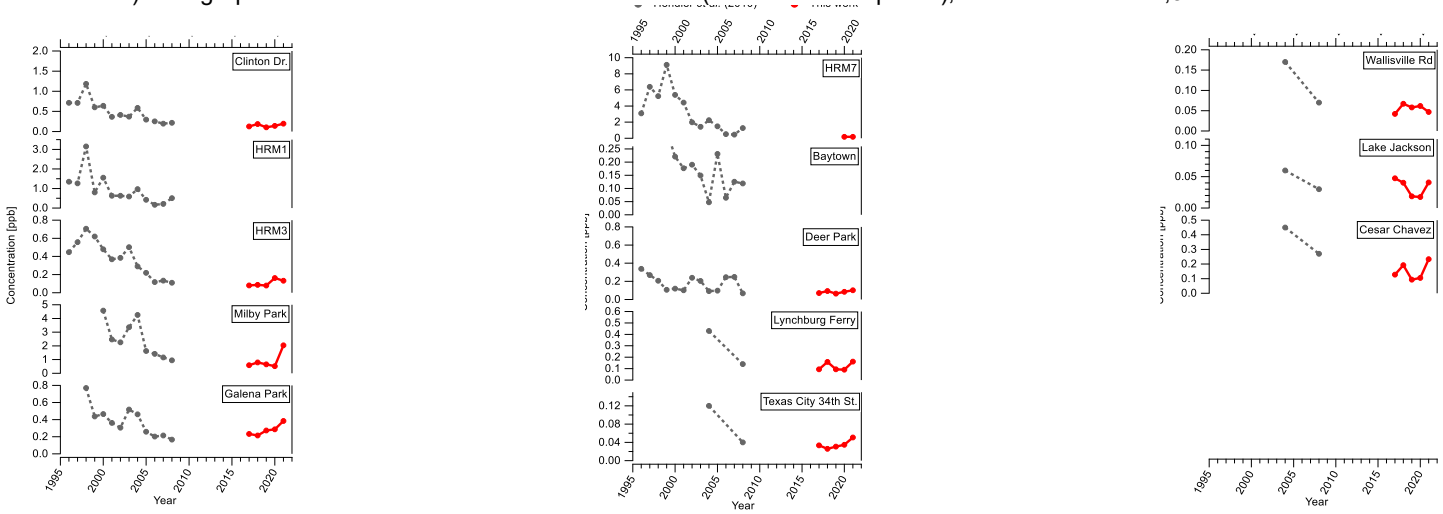


Figure 7: Historical trends of 1,3-butadiene concentrations at various Region 12 sites (1995 - 2023 YTD)

[45] Hendler AH, Goodmanson Bunch AT, Crow WL. Long-term trends in ambient air 1,3-butadiene levels in Houston, Texas. Environ Sci Technol. 2010 Oct 1;44(19):7383-90.

A similar trend is seen in Figure 8 where 1,3-butadiene emissions reported to EPA's TRI have fallen since 2009 (black trace, left axis). A comparison of ambient annual average concentrations from 2017-2021 (red traces, right axis) show similar trends to the TRI-reported values, especially for years 2017-2020. The zip code 77017 was chosen for this analysis as that is where the TCEQ's Milby Park and Cesar Chavez air monitoring sites are located. The uptick in Milby Park concentrations for the year 2021 may be related to severe weather events in 2021 namely the winter storm Uri that affected several cities in Texas including Houston (where Milby Park and Cesar Chavez are located). Not shown in Figure 7 is the Milby Park annual average concentration in 2022 (0.713 ppb) which was similar to the annual average concentration in 2020 (0.519), which further supports the idea that the 2021 annual average was an anomalously high value due to extreme weather conditions.

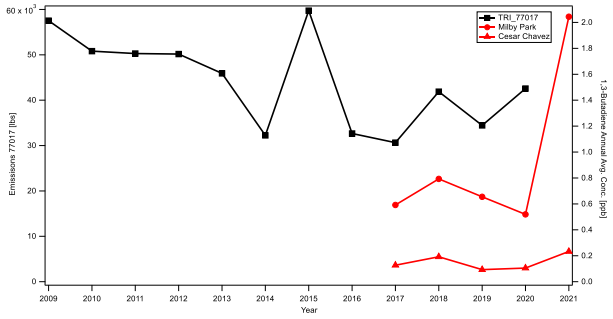


Figure 8: Comparison of 2009-2020 Toxic Release Inventory data within zip code 77017 (left) to 2017-2021 ambient monitoring data (right)

5. Conclusions

In this work, we assessed the EPA's TSCA Screening Level Approach (EPA Document# EPA-744-D-22-001) by examining the Pre-Screening and Full-Screening methodologies proposed. We chose a case study facility that has reported 1,3-butadiene emissions, and which was previously evaluated by the EPA as part of the Office of Air's Residual Risk Assessment for the MON in support of the 2020 Risk and Technology Review (Docket EPA-HQ-OAR-2018-0746).

We compared the Pre-Screening and Full-Screening models to an air dispersion model that is set up following the example provided in the 2020 MON RTR using emissions data from 2019 and 2021. The modeled maximum concentrations for both years showed similar trends where TSCA Pre-screening (IIOAC) outputs consistently had the highest values (10.75 $\mu g/m^3$ and 9.69 $\mu g/m^3$ for years 2019 and 2021 respectively), followed by the TSCA Full-Screening AERMOD (1.04 $\mu g/m^3$ and 0.74 $\mu g/m^3$), with the MON-RTR or "permit-style" AERMOD run producing the lowest output concentrations (0.44 $\mu g/m^3$ and 0.46 $\mu g/m^3$).

The modeling study highlights the conservative results from the TSCA Screening Level Approach methodologies, where the concentrations from the Pre-screening stage are an order of magnitude greater than the Full-screening stage, and the Full-screening stage concentrations are almost twice as high as concentrations from the MON RTR-based AERMOD run. Examining the modeled concentrations at various receptors extending from near-fenceline to ~5 miles away showed that **concentrations dropped considerably as distance from the facility increased**. The facility-specific AERMOD following the EPA's 2020 MON RTR methodology, which is considered the best available science, produced the most predictive (albeit still conservative) concentrations of all three models, because it utilized the most specific multi-variable inputs.

To put the air dispersion modeling studies into context, ambient air concentrations of 1,3-butadiene measured at various nationwide sites with automated gas chromatography (auto-GC) measurements from years 2017 to 2021 were analyzed and all concentrations (with the exception of one Texas site in 2021) were found to be below 1 ppb.

This work used the 1,3-butadiene-emitting case study facility to highlight the overly conservative nature of the methodologies proposed in the TSCA Screening Level Approach. Using facility data and guidelines available in the MON RTR final rule published by the EPA's Office of Air and a more refined air dispersion model run produced modeled concentrations that are more realistic, and more closely match with ambient measurements. Thus, in keeping with EPA's commitment to leverage existing data and resources, we encourage referral to the methodology followed in the EPA's MON RTR docket to provide refinement to the methodologies suggested in the TSCA Screening Level Approach.

Appendix A

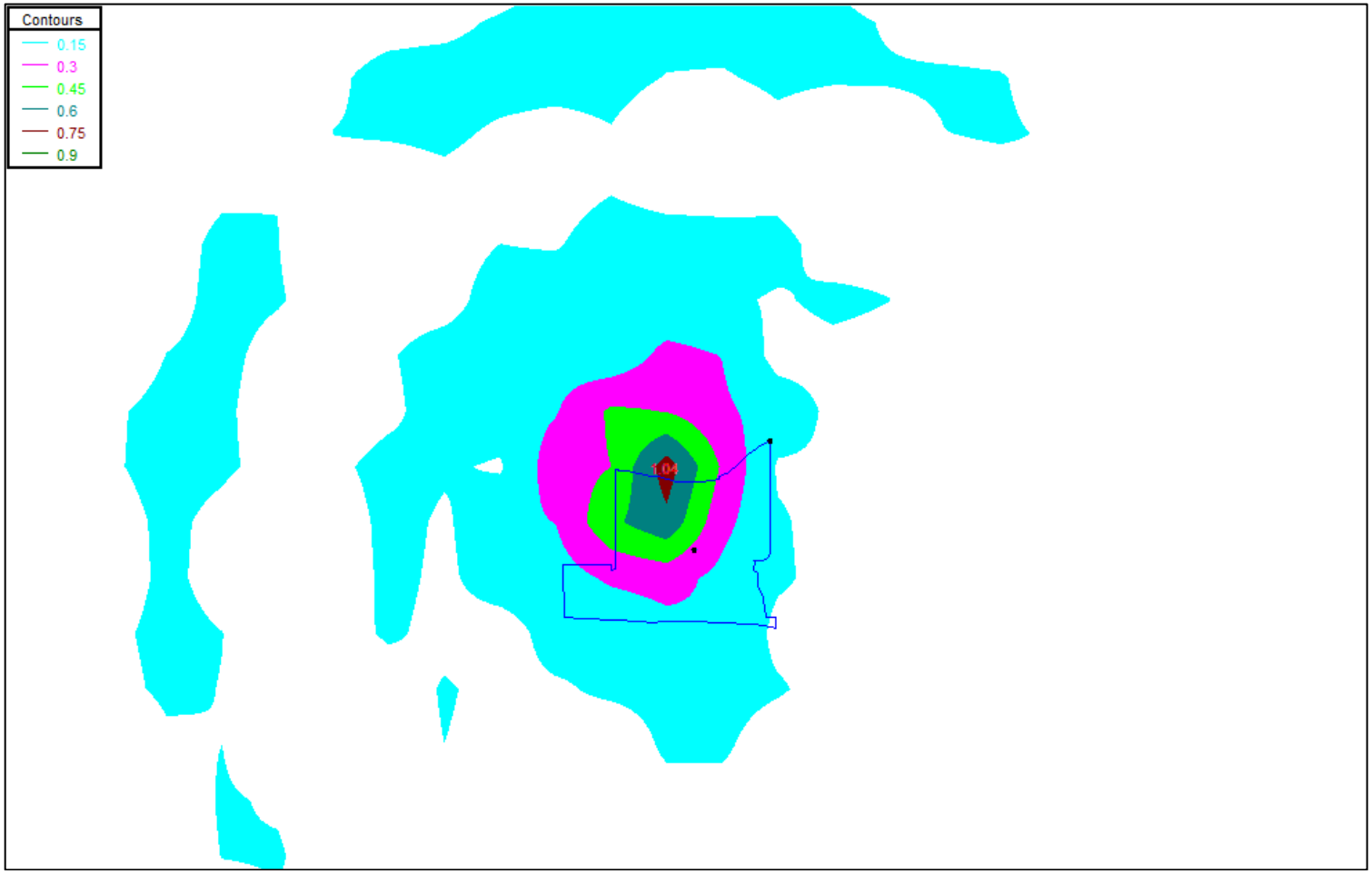


Figure A- 1 AERMOD Output Concentrations (µg m^{-3}) Contour Plot for TSCA Full Screen model for Year 2019

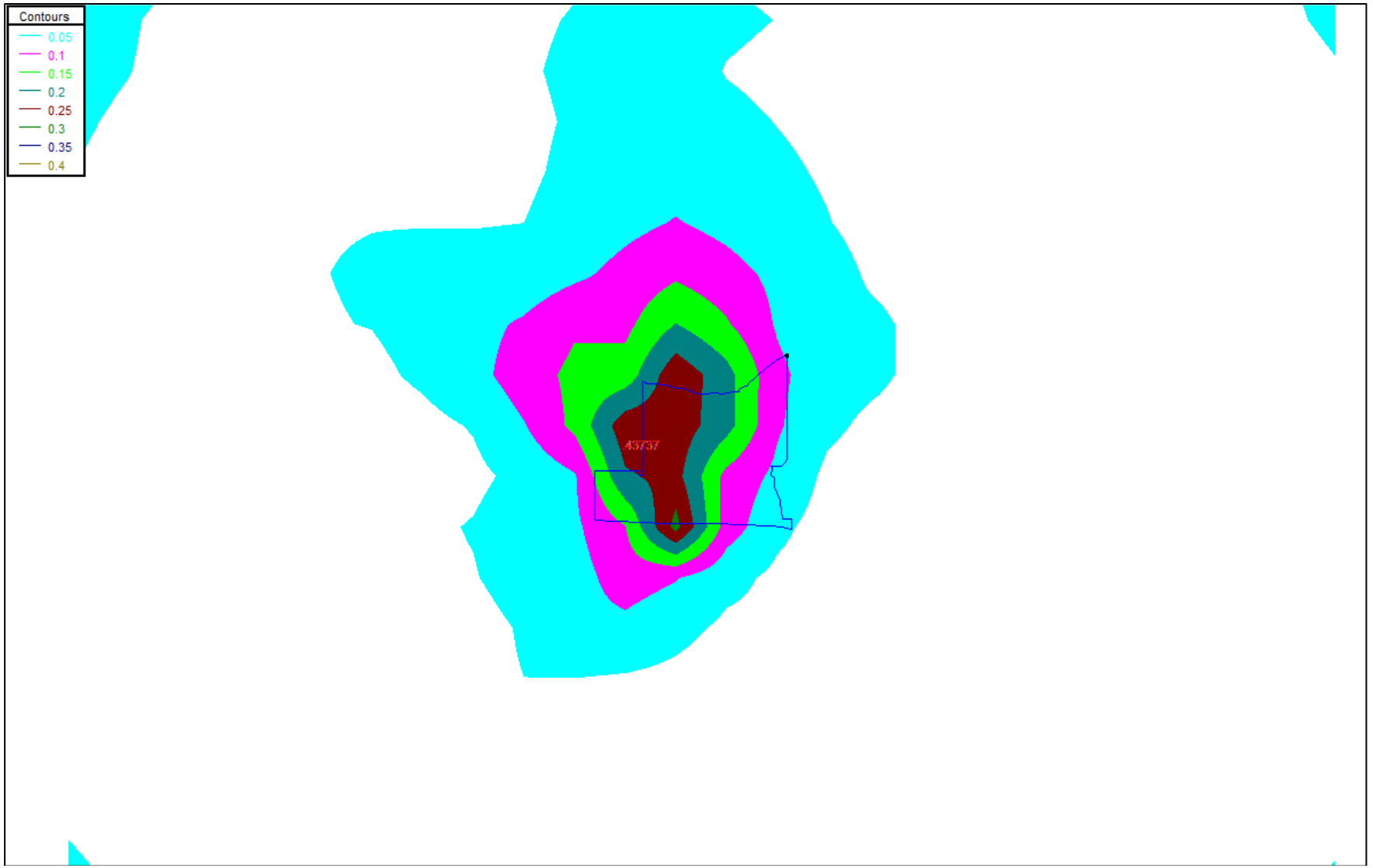


Figure A- 2 AERMOD Output Concentrations (µg m^{-3}) Contour Plot for Permit-style model for Year 2019

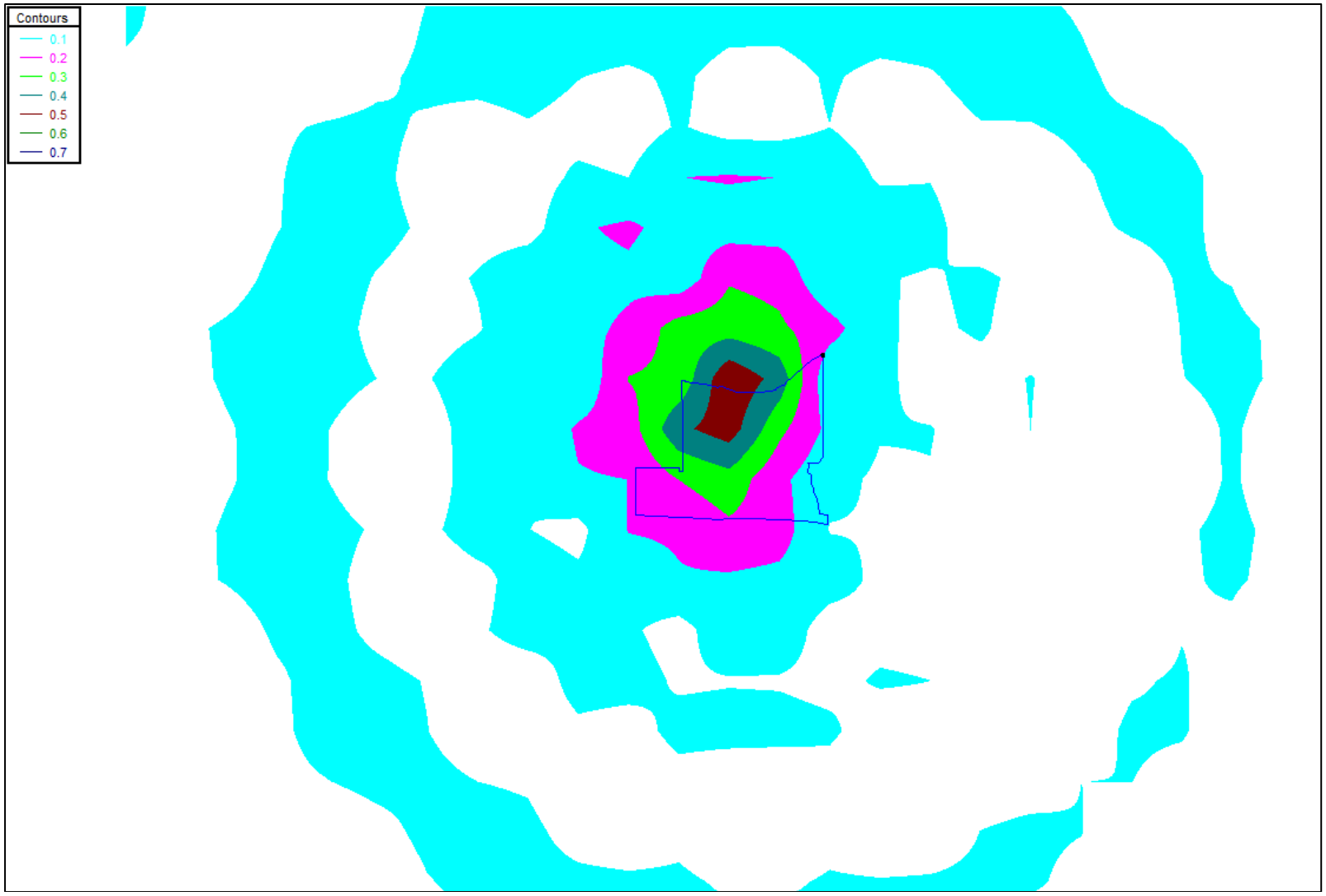


Figure A- 3 AERMOD Output Concentrations (µg m^{-3}) Contour Plot for TSCA Full Screen model for Year 2021

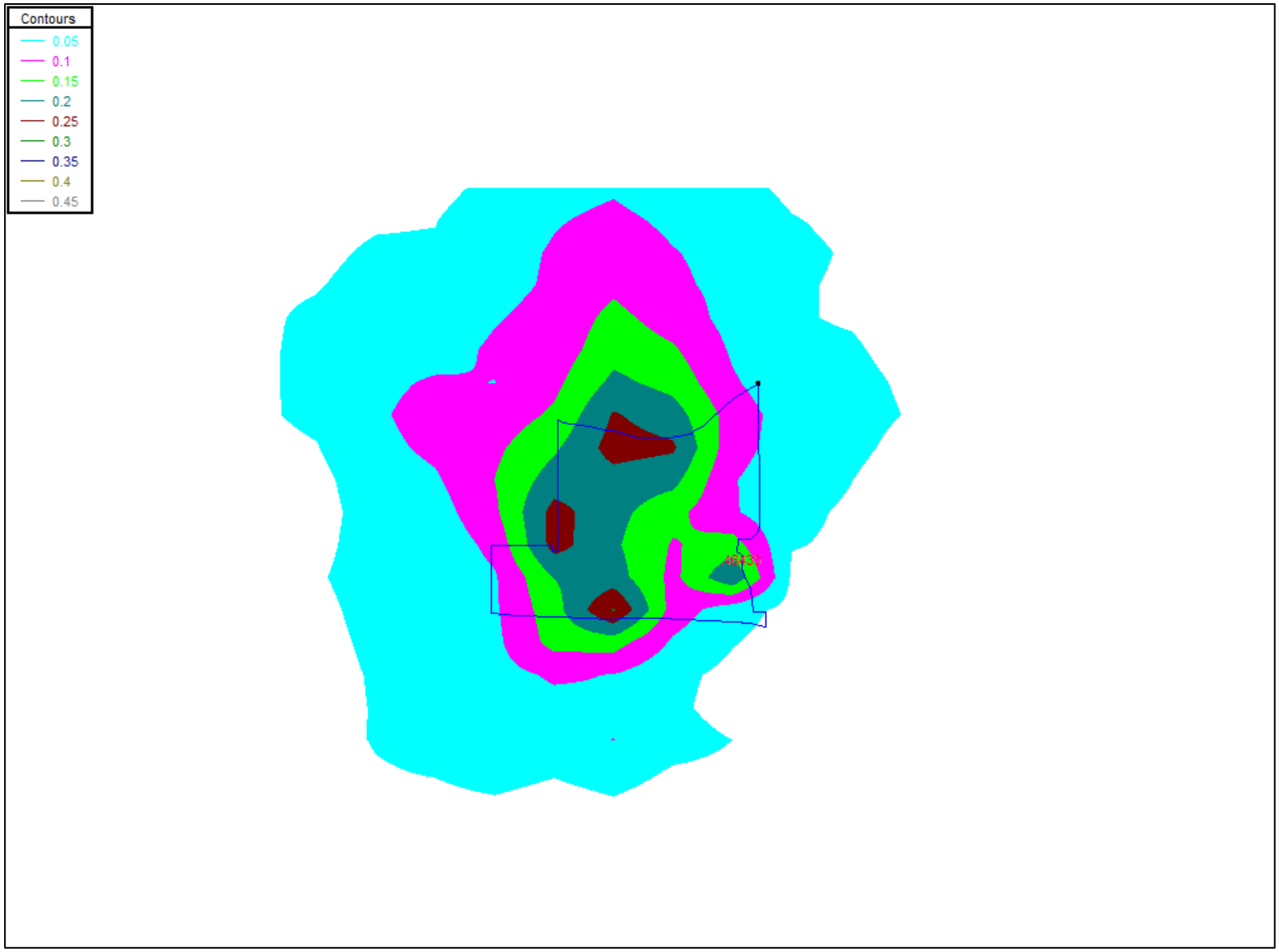


Figure A- 4 AERMOD Output Concentrations (µg m^{-3}) Contour Plot for Permit-style model for Year 2021