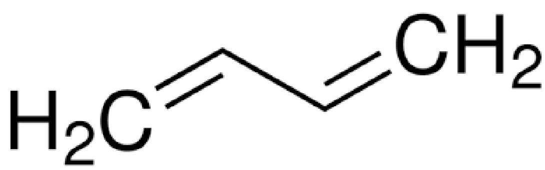
United States
Environmental Protection Agency

November 2024
Office of Chemical Safety and
Pollution Prevention

Draft General Population Exposure for 1,3-Butadiene

Technical Support Document for the Draft Risk Evaluation

CASRN: 106-99-0



November 2024

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

ABBREVIATIONS AND ACRONYMS

AAMG	Ambient Air Monitoring Group
ADAF	Age Dependent Adjustment Factor
ADC	Average daily concentrations
AERMOD	American Meteorological Society/Environmental Protection Agency Regulatory Model
AMTIC	Ambient Monitoring Technology Information Center
CMAQ	Community Multiscale Air Quality Modeling System
COU	Conditions of Use
EPA	Environmental Protection Agency
HEC	Human Equivalent Concentration
HEM	Human Exposure Model
IIOAC	Integrated Indoor Outdoor Air Calculator

IRIS	Integrated Risk Information System
LADC	Lifetime Average Daily Concentrations
MOE	Margin of Exposure
NAICS	North American Industry Classification System
NEI	National Emissions Inventory
OCSPP	Office of Chemical Safety and Pollution Prevention
OES	Occupational Exposure Scenario
OPPT	Office of Pollution Prevention and Toxics
POD	Point of Departure
SAB	Science Advisory Board
TRI	Toxic Release Inventory
TSCA	Toxic Substances Control Act

ACKNOWLEDGEMENTS

The Assessment Team gratefully acknowledges the participation, review, and input from U.S. Environmental Protection Agency (EPA or the Agency) Office of Pollution Prevention and Toxics (OPPT) and Office of Chemical Safety and Pollution Prevention (OCSPP) senior managers and science advisors. The Agency is also grateful for assistance from the following EPA contractors for the preparation of this draft technical support document: ICF (Contract No. 68HERC23D0007).

Docket

Supporting information can be found in the public docket, Docket ID: EPA-HQ-OPPT-2024-0425.

Disclaimer

Reference herein to any specific commercial products, process or service by trade name, trademark, manufacturer, or otherwise does not constitute or imply its endorsement, recommendation, or favoring by the United States Government.

Authors: Kiet Ly

Contributors: Sheila Healy and Kevin Vuilleumier

Technical Support: Mark Gibson, Hillary Hollinger, and Grace Kaupas

This draft technical support document was reviewed and cleared for release by OPPT and OCSPP leadership.

SUMMARY

This draft technical document is in support of the Toxic Substances Control Act (TSCA) *Draft Risk Evaluation for 1,3-Butadiene* (U.S. EPA, 2024h). See the draft risk evaluation for a complete list of all the technical support documents for 1,3-butadiene.

Key Points: General Population Exposure Assessment

The following bullets summarize the key points of this draft general population exposure assessment:

- 1,3-Butadiene is ubiquitous in the ambient air; therefore, EPA quantitatively assessed human exposure to 1,3-butadiene via the ambient air pathway.
- EPA presents both measured and modeled concentrations of 1,3-butadiene from multiple lines of evidence, data, and analyses in this draft ambient air exposure assessment to evaluate and contextualize 1,3-butadiene exposures under multiple Toxic Substances Control Act (TSCA) conditions of use (COU).
- EPA used Integrated Indoor/Outdoor Air Calculator (IIOAC) and Human Exposure Model (HEM) to model industrial releases reported to TRI for the years 2016 through 2021 (Sections 2.2.2 and 2.2.3)
- Exposures from industrial releases of 1,3-butadiene that can be attributed to TSCA COUs based on the IIOAC 95th percentile modeled concentrations ranged from 0.0 to 109.5 $\mu g/m^3$ 100 to 1,000 m from facility releases.
- Exposures from industrial releases of 1,3-butadiene that can be attributed to TSCA COUs based on the HEM 95th percentile modeled concentrations ranged from 0.0 to 383.4 $\mu g/m^3$ 10 to 50,000 meters from facility releases.
- EPA considered the last 6 years (2016–2021) of monitored 1,3-butadiene concentrations extracted from EPA's Ambient Monitoring Technology Information Center (AMTIC) dataset for this draft exposure assessment (Section 2.3.1).
- The Agency acknowledges this ambient monitoring data is generally representative of a total aggregate concentration from all 1,3-butadiene sources (both TSCA and other sources), but taken together with other data sources allows EPA to contextualize modeled concentrations relative to the monitored concentrations from AMTIC.
- Monitored 1,3-butadiene concentrations extracted from AMTIC between 2016 and 2021 ranged from 0.0 to 122.8 $\mu g/m^3$ across all monitored 24-hour sampling values.
- Comparing modeled concentrations in relation to the other data sources considered, EPA found that modeled concentrations were within the same order of magnitude as the AMTIC monitoring data.
- Additional analysis includes the 2020 AirToxScreen data (a screening analysis representing 1,3-butadiene contributions from 38 different sources categories that include fuel use and combustion related emissions [Section 2.3.2]).
- EPA is confident in the characterization of exposures to 1,3-butadiene via the ambient air pathway-inhalation route in this draft assessment resulting from industrial facility releases. The greatest uncertainty is associated with the contribution of 1,3-butadiene to the total ambient monitoring data due to other sources related to fuel use, combustion, and mobile emissions.

1 INTRODUCTION

1,3-Butadiene is a colorless gas that is produced during petroleum processing and is primarily used for synthetic rubber production, with small amounts found in plastics and fuel. IT is released into the environment by industrial operations involved with manufacturing, processing, formulation, disposal, and other practices (U.S. EPA, 2024c). 1,3-Butadiene is also released into the ambient air through motor vehicle emissions, combustion, and other activities related to fuel use and products.

This draft assessment describes the use of reasonably available information to evaluate exposure of the general population to 1,3-butadiene. EPA evaluated the reasonably available information for releases of 1,3-butadiene from facilities that use, manufacture, or process it under industrial and/or commercial conditions of use (COUs) subject to Toxic Substances Control Act (TSCA) regulations, as detailed in the *Draft Environmental Releases and Occupational Exposure Assessment for 1,3-Butadiene* (U.S. EPA, 2024c). In the *Draft Environmental Media Concentrations for 1,3-Butadiene* (U.S. EPA, 2024a), EPA evaluated the presence of 1,3-butadiene in different media pathways (air, water, and land) through reported concentrations in peer-reviewed literature, gray literature and monitoring databases. Based on 1,3-butadiene's chemical properties and fate parameters detailed in the *Draft Physical Chemistry and Fate Assessment for 1,3-Butadiene* (U.S. EPA, 2024g) and further supported by data described in the *Draft Environmental Media Concentrations for 1,3-Butadiene* (U.S. EPA, 2024a), exposures to 1,3-butadiene for the general population are only expected through the air pathway. Therefore, EPA conducted a quantitative assessment by modeling ambient air concentrations based on facility releases to assess general population exposure to 1,3-butadiene from ambient air.

As detailed in the *Draft Environmental Releases and Occupational Exposure Assessment for 1,3-Butadiene* (U.S. EPA, 2024c), releases are reported to occur to the ambient air. Although subject to direct and indirect photolysis in the ambient air, 1,3-butadiene is ubiquitous— especially in the urban setting due to industrial releases and combustion related activities—and has consistently been found to be present in air based on testing and ambient monitoring implemented under multiple EPA programs. The Agency analyzed data from the Toxic Release Inventory (TRI) to evaluate facility air releases of 1,3-butadiene for the 2016 to 2021 reporting years..

This document evaluates how releases of 1,3-butadiene impact the general population through ambient air exposure. As described in Section 2, using the TRI release data as input, EPA modeled predicted concentrations of 1,3-butadiene in ambient air starting with the EPA's IIOAC (Section 2.2.2) and further refining with HEM (Section 2.2.3). When possible, the modeled concentrations were compared to environmental monitoring data (Section 2.3.1).

The modeling for this draft ambient air assessment focused specifically on exposures to individuals potentially living near industrial facilities (within 100 to 1,000 meters [0.062 to 0.62 miles]) reporting releases of 1,3-butadiene that are associated with TSCA COUs. TRI reported release data from 2016 through 2021 across 8 occupational exposure scenarios (OESs) associated with 11 TSCA COUs were used as model input. Because results from IIOAC (Appendix A.1) showed preliminary cancer risk screening at or above the 1 in a million benchmark (*i.e.*, 1×10^{-6}) at the 1,000 m distance, refined modeling was conducted using HEM to quantify exposures for additional distances (up to 50,000 m) based on site-specific days of operation and localized regional meteorological data (Section 2.2.3). In addition, HEM used the 2020 census data to estimate risks due to ambient air exposures at census blocks that are within 50 km to 1,3-butadiene facility release points.

To provide context for modeled ambient air concentrations based on TRI releases, HEM modeled concentrations were compared to the measured concentrations of 1,3-butadiene in ambient air available in the Ambient Monitoring Technology Information Center Ambient Monitoring Archive database (AMTIC). The ranges for both modeled and measured concentrations were within the same order of magnitude (Section 2.3.1). However, EPA recognizes that this is not a direct comparison since modeled concentrations are based on facility releases while monitoring data extracted from AMTIC represent 24-hour measured concentrations collected at air monitoring stations that vary in distance from TRI facilities. In addition, AMTIC measured concentrations reflect all possible contributing sources—including sources associated with TSCA COUs and other sources not within the scope of this assessment (*e.g.*, vehicular mobile sources, residential wood combustion, wildfires).

To provide context for the contribution to ambient air concentrations from other sources, EPA evaluated existing modeled data from the 2020 AirToxScreen Assessments (Section 2.3.2). AirToxScreen is based on releases reported to the National Emissions Inventory (NEI). A summary of NEI release data is presented in the *Draft Environmental Release and Occupational Exposure Assessment for 1,3-Butadiene* (U.S. EPA, 2024c), but NEI release data were not used as input for modeling of exposures to the general population in this draft assessment. EPA intends to incorporate exposures and risks analyses based on the 2017 and 2020 NEI reported releases for the finalized draft risk evaluation.

1.1 Scope of the Risk Evaluation

The TSCA risk evaluation of 1,3-butadiene comprises several human health, environmental, fate, and exposure assessment modules, and a risk evaluation document. A diagram showing the relationships between assessments is provided in Figure 1-1. This general population exposure assessment is one of five technical support documents that are outlined in green.

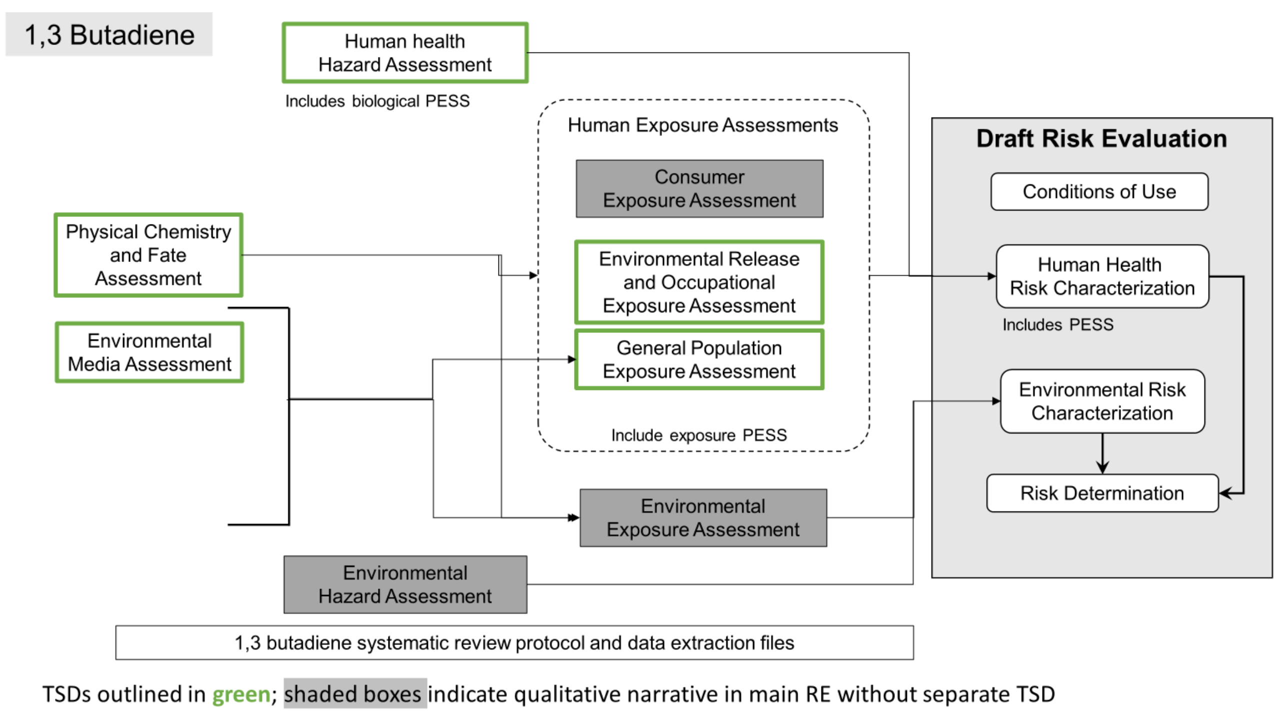


Figure 1-1. Risk Assessment Document Map Summary

1.2 Summary of the Chemistry, Fate, and Transport Assessment

1,3-Butadiene is primarily transformed in ambient air by indirect photolysis through reaction with ozone, nitrates, and hydroxy radicals to form other chemicals. Studies indicate 1,3-butadiene has a halflife range of 0.76 to 9 hours, with the longer half-lives corresponding to periods without sunlight. Industrial releases and vehicular emissions are major sources. 1,3-Butadiene can also be formed in ambient air as a product of combustion of organic matter such as petroleum products, wood, and coal. 1,3-Butadiene is volatile and will evaporate from water and soil and does not sorb to sediment. For these reasons, air is expected to be the major pathway of concern for 1,3-butadiene in the environment while water, sediment, and soil are expected to be minor compartments. Figure 1-2 below depicts the transportation and partitioning of 1,3-butadiene in the environment. For more details, see the *Draft Physical Chemistry and Fate Assessment for 1,3-Butadiene* (U.S. EPA, 2024g).

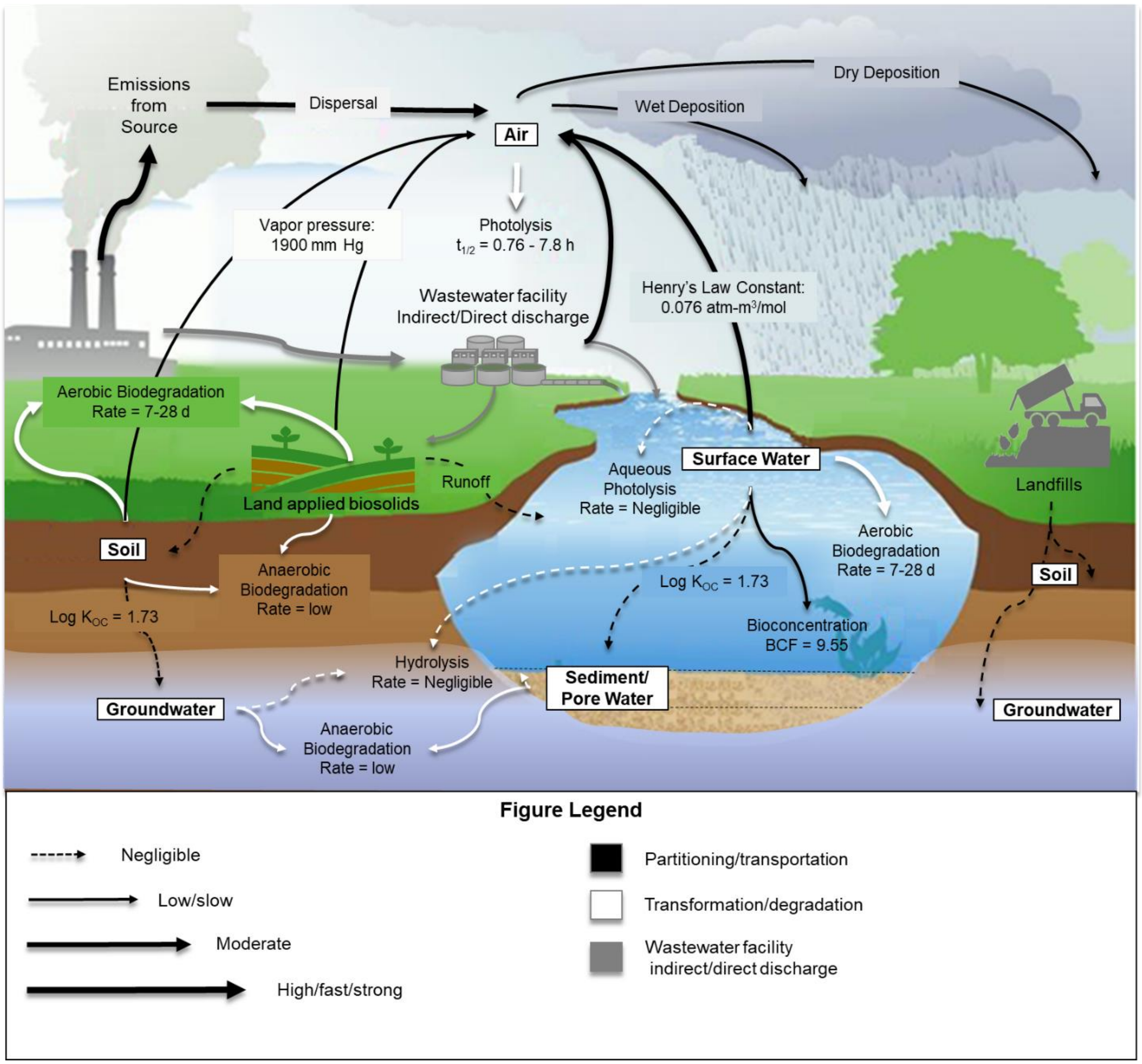


Figure 1-2. Transport, Partitioning and Degradation of 1,3-Butadiene in the Environment

The diagram depicts the distribution (grey arrows), transport and partitioning (black arrows) as well as the transformation and degradation (white arrows) of 1,3-butadiene in the environment. The width of the arrow is a qualitative indication of the likelihood that the indicated partitioning will occur or the rate at which the indicated degradation will occur (*i.e.*, wider arrows indicate more likely partitioning or more rapid degradation).

2 APPROACH AND METHODOLOGY

As described in Section 1, 1,3-butadiene exposures to the general population are expected to occur only through the air pathway. Modeling approaches were used to estimate general population exposures to

1,3-butadiene due to reported releases from industrial facilities. Measurement data obtained from ambient air monitoring networks were used to provide context for aggregate concentrations from both TSCA sources and other sources.

Given the complexities of the exposure assessment of 1,3-butadiene in ambient air as previously described, multiple yet complimentary lines of evidence were considered to understand and contextualize the ambient air concentrations of 1,3-butadiene resulting from TSCA COUs. These evidence streams are summarized below and detailed in the following subsections:

1. ***Modeled 1,3-Butadiene Concentrations from TSCA COUs:*** This draft assessment uses EPA's IIOAC to model 1,3-butadiene ambient air concentrations near releasing facilities, based on reported 1,3-butadiene release data from the TRI for TSCA COUs (Section 2.2.2). EPA's HEM v4.2 was also used to obtain geographically refined estimates of 1,3-butadiene ambient air concentrations based on site-specific TRI releases, site-specific meteorological data, and 2020 U.S. census blocks and population data (Section 2.2.3).
2. ***Measured 1,3-Butadiene Concentrations:*** Measurement data from ambient air monitoring networks available through EPA's AMTIC database (U.S. EPA, 2022) was used together with measurement data extracted from peer-reviewed studies to provide context for aggregate concentrations of 1,3-butadiene in ambient air and for the modeled concentrations of 1,3-butadiene from TSCA sources (Section 2.3.1).
3. ***Relative Source Contributions In Ambient Air:*** This draft assessment includes discussion of the 2020 Air Toxics Screening Assessment Tool (AirToxScreen) to provide context for the relative contributions of 1,3-butadiene in ambient air from multiple source categories (Section 2.3.2).

2.1 General Population Exposure Scenarios

EPA expects the ambient air pathway to be the predominant human exposure pathway to 1,3-butadiene in the outdoor environment as shown in Figure 2-1. In summary, 1,3-butadiene is released from industrial facilities as uncontrolled fugitive releases such as process equipment leaks, process vents, building windows, building doors, and roof vents. It is also released from industrial facilities as stack releases, which may be either uncontrolled (*e.g.*, direct releases out a stack) or controlled with a pollution control device (*e.g.*, baghouse, scrubber, thermal oxidizer). Once released to ambient air, 1,3-butadiene can move off-site into the surrounding areas where human populations may be exposed through inhalation. This draft ambient air exposure assessment focuses on exposures to a subset of the general population living near industrial facilities that are releasing 1,3-butadiene to the ambient air.

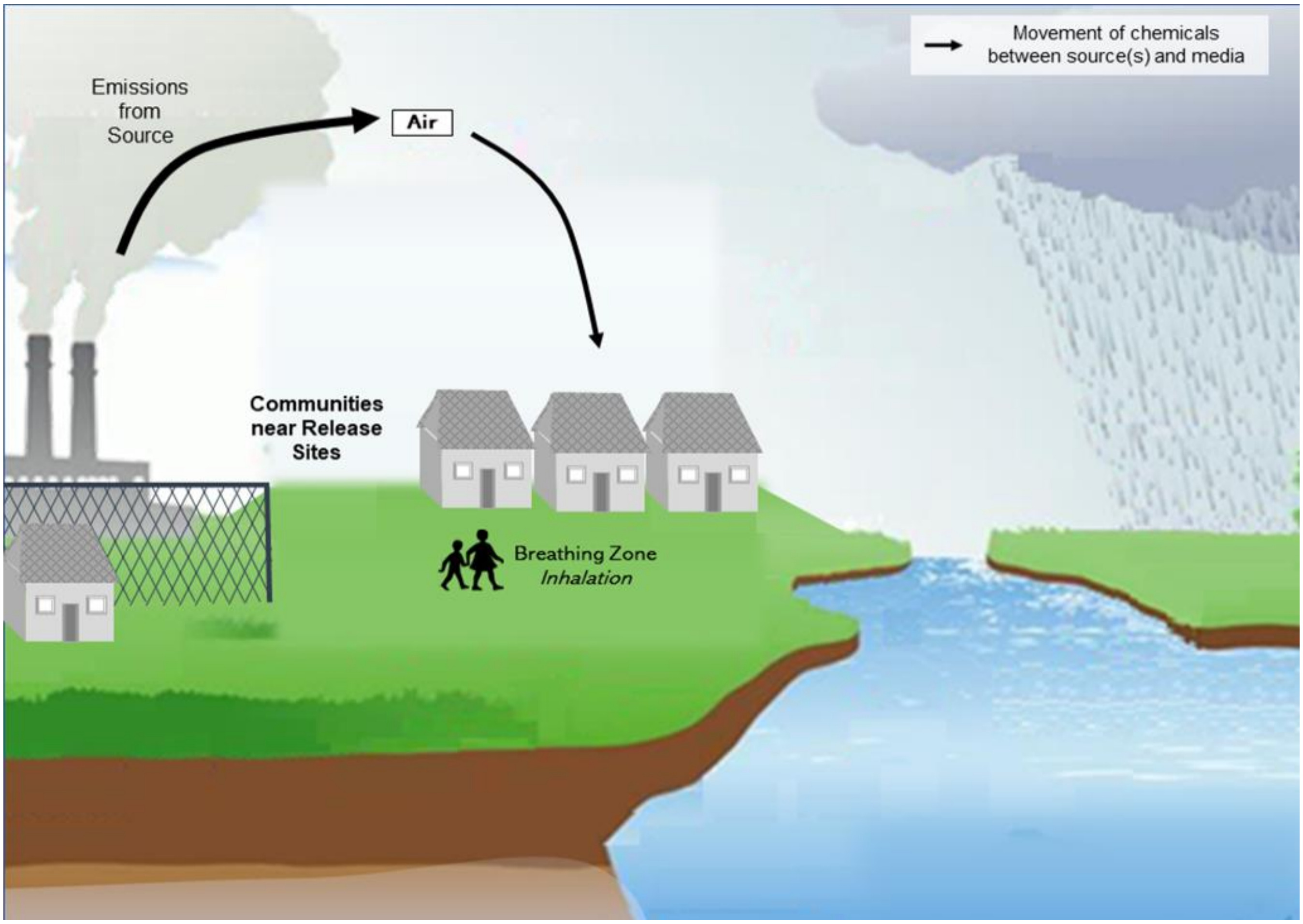


Figure 2-1. Industrial Releases to the Environment and Pathways by Which Exposures of the General Population to 1,3-Butadiene May Occur

2.2 Inhalation Exposure Modeling Assessment

2.2.1 Environmental Releases to Air

Air release estimates of 1,3-butadiene from the 2016 to 2021 TRI were used as inputs to modeling tools described in subsequent sections. Facilities must meet TRI reporting criteria for the number of full-time employees, specific NAICS codes and a chemical threshold of manufacturing and processing (>25,000 lb) or otherwise using 1,3-butadiene (>10,000 lb). A bulk run of all facilities reporting air releases of 1,3-butadiene to TRI was conducted to obtain aggregated location-specific air concentrations at a national scale. The TRI database included 229 reporting facilities across the 6 years of reporting data queried, for a total of 1,169 individual reported releases. Total annual fugitive releases ranged from 140,613 to 167,970 kg, while total annual stack releases ranged from 325,629 to 471,927 kg. These TRI facilities are each assigned to an occupational exposure scenario. OESs are established based on similarities or differences in release and exposure sources, worker activities, and use patterns occurring at a facility. OESs are then mapped to COUs shown in Table 1-1 of the *Draft Environmental Release and Occupational Exposure Assessment for 1,3-Butadiene* (U.S. EPA, 2024b), which, along with its associated supplemental files, provide detailed descriptions of the methods used to extract release data and summarize the individual facility releases. In addition to the TRI reported releases, EPA also modeled ambient concentrations for an additional OES related to adhesives and sealants based on EPA estimated releases detailed in the *Draft Environmental Releases and Occupational Exposures Assessment* (U.S. EPA, 2024c). For the purposes of this assessment, the modeled air concentrations are based on facility-specific releases and, therefore, general population exposures are associated with facility-specific assigned OESs and COUs.

2.2.2 Integrated Indoor/Outdoor Air Calculator Model (IIOAC)

IIOAC is a spreadsheet-based tool that estimates indoor and outdoor ambient air concentrations at different distances from sources that release chemical substances to the air. The tool uses pre-run results from a suite of dispersion scenarios within EPA's American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD). While the pre-run scenarios include a variety of meteorological and land-use settings, the IIOAC model is still limited by the parameterizations utilized for those pre-run scenarios (meteorologic data, stack heights, distances, exposed population, etc.). Additional information on IIOAC can be found in the user guide (EPA, 2019).

EPA used the IIOAC Model to estimate daily-averaged and annual-averaged 1,3-butadiene ambient air concentrations at predefined distances (100, 100–1,000, and 1,000 m) from facilities releasing 1,3-butadiene to the ambient air. IIOAC model results are used to evaluate potential exposures for the general population living near industrial releases of 1,3-butadiene. IIOAC serves as an initial screening tool to determine whether refined modeling is required to further assess general population exposures. Complete results of IIOAC modeling are provided in the supplemental file *Draft Integrated Indoor Outdoor Air Calculator (IIOAC) TRI 2016-2021 Exposure and Risk Analysis for 1,3-Butadiene* (U.S. EPA, 2024f).

2.2.2.1 Exposure Scenarios

IIOAC can model a variety of user defined input parameters and exposure scenarios, including varying release scenarios/patterns, release types, release durations, urban/rural settings (topography), and meteorological conditions. Releases from individual facilities reported in TRI 2016 to 2021 were reported as stack and/or fugitive releases; with facilities reporting both types of releases. Stack and fugitive releases were modeled separately and then aggregated together for facilities that reported both in the same TRI reporting year. EPA modeled stack and fugitive releases using the default release parameters integrated within the IIOAC Model, along with a user-defined length and width for fugitive releases as listed in Table 2-1. For facilities with both stack and fugitive releases, the modeled concentrations were summed together as a total concentration for that facility.

Table 2-1. IIOAC Default Input Parameters for Stack and Fugitive Air Releases

Stack Release Parameters	Value	Fugitive Release Parameters	Value
Stack height (m)	10	Length (m)	10
Stack diameter (m)	2	Width (m)	10
Exit velocity (m/sec)	5	Angle (°)	0
Exit temperature (K)	300	Release height (m)	3.05

For this general population exposure assessment, modeled air concentrations from IIOAC are based on the following:

1. The annual release values reported by individual facilities (assigned to OESs and mapped to respective TSCA COUs for the TRI 2016–2021 datasets), assuming the total annual reported releases are continuous and equally distributed across all days of operation.
2. An operating scenario representing industrial facilities releasing 1,3-butadiene to the ambient air

operating 24 hours/day, 7 days/week, 365 days/year. This is a conservative assumption for this screening-level estimate, in which, facilities are constantly releasing 1,3-butadiene every day at every hour throughout the year.

3. Application of the meteorology patterns from the Lake Charles, Louisiana, meteorological station to every facility (regardless of the facility's geographic location), and assumption of a "rural" land designation for every facility. These assumptions result in conservative air concentration results appropriate for a screening-level model. This designation of meteorology and land designation is recommended in the IIOAC user guide (EPA, 2019) for use when conservative estimates are desired.

2.2.2.2 IIOAC Model Output

The IIOAC model provides output values for daily-average and annual-averaged high-end (95th percentile) and mean ambient air concentrations in circular rings 100, 100 to 1,000 and 1,000 m from releasing facilities. These distances are also referred to as "fenceline," "community," and "outer-boundary" rings, respectively, in IIOAC.

For the two finite distances (100 and 1,000 m), IIOAC considers a polar grid of 16 modeled exposure receptors evenly spaced around each distance ring. For the area between 100 and 1,000 m from the releasing facility, IIOAC uses a cartesian grid of 228 receptors and 234 receptors, for stack and fugitive releases, respectively, placed at 100 m intervals across the entire area. Since IIOAC considers 6 years of environmental release data (TRI 2016–2021) and the exposure scenario assumes 365 days of operation each year (366 for a leap year), this results in a total of 2,192 separate daily-averaged concentrations. That is, hourly concentrations averaged over 1 day, and annual-averaged concentrations (*i.e.*, the hourly concentrations averaged over 1 year, for each modeled exposure receptor). Since IIOAC was modeled based on facilities releasing 1,3-butadiene to the ambient air with a steady, continuous release over time, operating 24 hours/day, 7 days/week, 365 days/year, the modeled daily-averaged and annual-averaged concentrations are equal.

The 95th percentile concentration at each distance ring (100, 100–1,000, and 1000 m) is the 95th percentile modeled concentration across the entire distribution of modeled concentrations at each distance per facility per TRI reporting year. Generally, the 95th percentile represents a downwind concentration at a modeled exposure point where a resident lives downwind of the industrial release, considering a non, site-specific estimate for dispersion and dilution. Additional information on IIOAC model outputs can be found in the user guide (EPA, 2019).

95th percentile results for ambient modeled concentrations across all facilities, reporting years and modeled distances (100, 100–1000 and 1000 m) ranged from 0 to 109.5 μg/m^3 with the highest modeled concentrations at 100 m). Mean modeled concentration results are shown in Table_Apx A-3. For full IIOAC modeling results, see the supplemental file: *Draft Integrated Indoor Outdoor Air Calculator (IIOAC) TRI 2016-2021 Exposure and Risk Analysis for 1,3-Butadiene* (U.S. EPA, 2024f).

2.2.2.3 Screening-Level Risk Estimates

For the purposes of this draft risk evaluation, EPA assumes that an individual's personal exposure is equivalent to the ambient, outdoor concentration at the individual's home address (further assuming that the individual lives at the same address for their full lifetime). Therefore, the annual-averaged ambient concentration results from IIOAC are assumed to be equal to chronic exposure concentrations, for the purposes of calculating chronic non-cancer and cancer screening-level risk estimates. This screening level assessment was done to determine whether refined modeling for estimated exposures may be warranted.

Exposure concentrations, chronic non-cancer, and cancer screening-level risk estimates based on IIOAC modeled results are presented and summarized in Appendix A. Hazard values used to calculate screening-level risk estimates are described in the *Draft Human Health Risk Assessment for 1,3-Butadiene* (U.S. EPA, 2024e). Margin of exposures (MOEs) were calculated at each distance (100, 100–1,000, and 1000 m) using the 95th percentile IIOAC modeled ambient air concentrations as conservative exposure estimates for each individual facility and for every reporting year. No resulting MOEs were below the chronic non-cancer benchmark; therefore, there is no expectation of non-cancer risks to the general population from TRI facility releases. However, screening-level cancer risks calculated using the 95th percentile and mean concentrations were at or above the 1 in a million benchmark up to 1,000 m from facility releases. Because the screening-level risk estimates derived using IIOAC results were above this benchmark, EPA utilized HEM to conduct a more geographically-refined analysis of ambient air concentrations using localized meteorological data and site-specific parameters (when available). EPA includes additional information from the HEM outputs related to population at the census block level used for the *Draft Risk Evaluation for 1,3-Butadiene* (U.S. EPA, 2024h) .

2.2.3 Human Exposure Model (HEM)

EPA used HEM 4.2 to model geographically refined 1,3-butadiene concentrations surrounding releasing facilities. HEM 4.2 has two components: (1) an atmospheric dispersion model, AERMOD, with included regional meteorological data; and (2) U.S. Census Bureau population data at the census block level. The current HEM version utilizes 2020 census data. AERMOD estimates the magnitude and distribution of chemical concentrations in ambient air in the vicinity of each releasing facility within user-defined radial distances out to 50 km (about 30 miles). HEM can also provide risk estimates based on modeled chemical concentrations in ambient air at the centroid of over 8 million census blocks across the United States. The model estimates cancer risks and noncancer hazards at census blocks using ambient concentration estimates from the built-in AERMOD modeling combined with user provided hazard data. HEM automatically utilizes regional meteorological data for each release point, as well as local topographic information, to inform the release dispersion model. In summary, modeling with HEM allowed for the following refinements over the IIOAC approach:

1. The AERMOD dispersion model within HEM allows for modeling of 1,3-butadiene ambient air concentrations at radial distances greater than 1,000 m from facility releases.
2. The AERMOD model utilizes regional meteorological data matched to the release facility's location, as well as local topographic information for each release point to inform the dispersion model.
3. Within HEM, site-specific values for facility operating days and hours were used, when available

Refer to the HEM v4.2 User Guide for more details about these and other capabilities.

2.2.3.1 Exposure Scenario

EPA evaluated site-specific releases from 225 TRI facilities directly reporting to TRI with Form R using HEM v4.2. Similar to the IIOAC modeling, stack and fugitive releases were modeled separately, each using the same set of default parameters integrated into the IIOAC model for comparability (Table 2-2).

Table 2-2. HEM Input Parameters for Stack and Fugitive Air Releases

Stack Release Parameters	Value	Fugitive Release Parameters	Value
Stack height (m)	10	Length (m)	10
Stack diameter (m)	2	Width (m)	10
Exit velocity (m/sec)	5	Angle (degrees)	0
Exit temperature (°K)	300	Release height (m)	3.05

The exposure scenario modeled with HEM utilized site-specific releases and parameters for operating hours and days, when available, as reported to TRI for 2016 to 2021. For hours of operation, EPA assumed facilities operated 24 hours/day. For days of operation, EPA used site-specific reported data which varied from 250 to 350 days a year.

To obtain refined ambient air concentrations of 1,3-butadiene surrounding release facilities to inform analysis of cancer risk, HEM was run with 11 rings of receptors placed at varying radial distances from the facility center: 10, 30, 60, and 100 m, and 1, 2.5, 5, 10, 15, 25, and 50 km. In addition, HEM was manually configured to output ambient air concentrations at two area distances at 30 to 60 m and 100 to 1,000 m. Each ring comprises 16 evenly spaced receptors. Annual, facility-specific TRI releases were used as input to HEM, which then provides as output annual-average ambient concentrations at each receptor along each modeled distance ring. The HEM results allow for evaluation of ambient air concentrations at refined distances from facility releases, and comparison of the relative contributions from fugitive and stack releases.

To obtain refined estimates of cancer risk, the option to apply HEM at the census block level was implemented. Annual, facility-specific TRI releases were used as input to HEM, along with inhalation unit risk (IUR) values for 1,3-butadiene from the *Draft Human Health Risk Assessment for 1,3-Butadiene* (U.S. EPA, 2024e). HEM explicitly models concentrations at census blocks near facilities (typically 3 km) and interpolates concentrations at census blocks further away out to 50 km. Details on how the HEM model interpolates from ambient concentrations at ring receptors to obtain concentrations at census block centroids can be found in the HEM v4.2 User Guide. Outputs of this model application include cancer risks at each census block surrounding a facility, together with U.S. census population counts corresponding to the census block.

See Appendix B.1 for details on HEM inputs.

2.2.3.2 HEM Modeling Results by Discrete Distances

Releases from individual facilities reported in TRI 2016 to 2021 were reported as stack and/or fugitive releases; with some facilities reporting both types of releases. Stack and fugitive releases were modeled separately and then aggregated together for facilities that reported both in the same TRI reporting year. This resulted in over 2,200 release scenarios modeled through HEM (225 TRI facilities with stack and/or fugitive source emissions across 5 reporting years). The 95th percentile concentrations at each distance ring modeled by HEM were grouped together based on the facility's assigned OESs and associated COUs and summarized across the distances 10 to 50,000 m from facility release points.

95th percentile modeled ambient air concentrations from HEM across all facility releases and all distances (10 to 50,000 m) reporting from 2016 to 2021 ranged from 0.0 to 383.4 μg/m³, with the greatest concentrations modeled within the first 60 m from industrial facilities. To simplify presentation of results, EPA focused on modeled air concentrations at distances 100, 100 to 1,000, and 1,000 m.

These distances are also consistent with the community populations living near facilities as described in the fenceline methodology (Draft Screening Level Approach for Assessing Ambient Air and Water Exposures to Fenceline Communities Version 1.0). 95th percentile modeled results from HEM ranged from 0.0 to 91.2 $\mu g/m^3$ across all facilities for the 100, 100 to 1,000 and 1,000 m distances. This range is similar to the IIOAC 95th percentile results, which ranged from 0.0 to 109.5 $\mu g/m^3$ for the same distance rings. Table 2-3 includes the HEM 95th percentile modeled concentrations for the 100, 100 to 1,000, and 1000 m distances for each OES. Tables for the 95th and 50th percentile modeled concentrations across all distances are provided in Appendix B.2. Similar to the IIOAC results, the OESs and COUs associated with plastic and rubber compounding, manufacturing, and processing as a reactant resulted in the highest modeled concentrations. For the full results of HEM modeled concentrations, including the 50th and 10th percentile, see supplemental file *Draft Human Exposure Model (HEM) TRI 2016-2021 Exposure and Risk Analysis for 1,3-Butadiene* (U.S. EPA, 2024d).

Table 2-3. HEM 95th Percentile Modeled Concentrations (μg/m^3)

Life Cycle Stage	Category	Subcategory	OES	TRI Facilities	Stat	Ambient Concentration across Facilities within OES by Distance from All Sources (m) (Based on 95th Percentile Modeled Concentrations μg/m^3)		
						100	100–1,000	1,000
Manufacture	Import	Import	Manufacturing	40	Maximum	7.8E01	1.3E01	4.6E00
					Mean	1.20E01	1.91E00	5.97E−01
					Median	3.29E00	5.74E−01	1.61E−01
					Minimum	0.00E00	0.00E00	0.00E00
Processing	Processing as a reactant	Other: Monomer used in polymerization process in: Plastic material and resin manufacturing; Manufacturing synthetic rubber and plastics	Plastics and Rubber Compounding	33	Maximum	9.1E01	7.3E00	2.1E00
					Mean	1.10E01	1.23E00	3.18 E−01
					Median	3.40E00	4.85E−01	1.28E−01
					Minimum	8.33E−04	3.61E−04	1.42E−04
Processing	Processing – incorporation into article	Other: Polymer in: Rubber and plastic product manufacturing	Plastics and Rubber Converting	1	Maximum	5.3E−07	1.5E−07	4.3E−08
					Mean	5.26E−07	1.45E−07	4.30E−08
					Median	5.26E−07	1.45E−07	4.30E−08
					Minimum	5.26E−07	1.45E−07	4.30E−08
Processing	Processing – incorporation into formulation, mixture, or reaction product	Processing aids, not otherwise listed in: Petrochemical manufacturing	Processing Incorporation into formulation, mixture, or reaction product	53	Maximum	1.7E01	6.6E00	3.1E00
					Mean	1.04E00	2.09E−01	7.95E−02
					Median	1.32E−01	1.87E−02	5.59E−03
					Minimum	0.00E00	0.00E00	0.00E00

Life Cycle Stage	Category	Subcategory	OES	TRI Facilities	Stat	Ambient Concentration across Facilities within OES by Distance from All Sources (m) (Based on 95th Percentile Modeled Concentrations µg/m^3)		
						100	100–1,000	1,000
Processing	Processing as a reactant	Intermediate in: Adhesive manufacturing; All other basic organic chemical manufacturing; Fuel binder for solid rocket fuels; Organic fiber manufacturing; Petrochemical manufacturing; Petroleum refineries; Plastic material and resin manufacturing; Propellant manufacturing; Synthetic rubber manufacturing; Wholesale and retail trade	Processing as a reactant	57	Maximum	3.0E01	3.0E00	7.7E−01
					Mean	2.75E00	3.12E−01	8.65E−02
					Median	4.08E−01	6.38E−02	1.70E−02
					Minimum	0.00E00	0.00E00	0.00E00
Disposal	Disposal	Disposal	Recycling	11	Maximum	7.1E−01	8.5E−02	2.2E−02
					Mean	2.60E−01	3.24E−02	9.19E−03
					Median	1.90E−01	2.33E−02	6.12E−03
					Minimum	1.23E−03	3.00E−04	1.48E−04
Manufacturing	Import	Import	Repackaging	23	Maximum	2.0E01	2.4E00	5.1E−01
					Mean	2.08E00	2.11E−01	6.10E−02
Processing	Repackaging	Intermediate in: Wholesale and retail trade			Median	9.16E−02	1.43E−02	3.19E−03
					Minimum	1.38E−04	3.41E−05	1.40E−05
Disposal	Disposal	Disposal	Waste handling, disposal, treatment, and recycling	7	Maximum	1.8E−01	2.1E−02	6.9E−03
					Mean	3.97E−02	5.07E−03	1.57E−03
					Median	1.34E−03	3.47E−04	1.18E−04
					Minimum	2.85E−04	3.05E−05	8.34E−06
			Total	**225**				

2.2.3.1 HEM Modeling Results by Census Blocks

As described in Section 2.2.3, HEM provides results at the census block level for refined evaluation of cancer risk. HEM calculates an aggregated cancer risk value, the maximum individual risk (MIR), for each census block within 50 km of facility releases. This risk value is calculated by multiplying the aggregate census block ambient air concentration by the IUR. A general population IUR, which incorporates an age dependent adjustment factor (ADAF) of IUR of 4.4×10^{-6} risk per µg/m³ from the *Draft Human Health Risk Assessment for 1,3-Butadiene* (U.S. EPA, 2024e), was applied for 1,3-butadiene in this modeling approach. For specific HEM output values of cancer risk at the census block level, and overall risk characterization for general population exposures, see *the Draft Risk Evaluation for 1,3-Butadiene* (U.S. EPA, 2024h).

2.3 Other Assessments

2.3.1 Measured Ambient Air Concentrations

The Agency identified and summarized monitoring data for 1,3-butadiene extracted from EPA's AMTIC database (U.S. EPA, 2022)—a collection of data from air monitoring networks across the United States. EPA also identified and summarized measured data from peer-reviewed literature, gray literature, and databases that were included in EPA's systematic review process detailed in the *Draft Systematic Review Protocol for 1,3-Butadiene* (U.S. EPA, 2024i). For the purposes of this general population exposure assessment, EPA focused on comparing modeled concentrations to the AMTIC database because measurements in AMTIC are more representative of measured ambient air concentrations of 1,3-butadiene across the United States compared to studies evaluated during systematic review. The studies evaluated during systematic review were limited and vary by sample size, geographic location and temporally (*i.e.*, time of year samples were collected, sampling durations and sample collection methods).

AMTIC includes ambient air quality monitoring data collected for high priority air pollutants and is overseen by the EPA Ambient Air Monitoring Group (AAMG). Submitted air quality monitoring data must meet the collection and quality assurance criteria set by AMTIC to be included in the database. Ambient air concentration data was pulled in August of 2024 capturing monitoring data from 2016 to 2021, to be consistent with TRI reporting years being evaluated. The concentrations ranged from 0.0 to 122.8 µg/m^3 across all monitored 24-hour sampling values. For more details on AMTIC monitoring data and measured ambient air concentrations from systematic review, see the *Draft Environmental Media Concentrations for 1,3-Butadiene* (U.S. EPA, 2024a).

2.3.2 Air Toxics Screening Assessment Tool (AirToxScreen)

EPA evaluated existing modeled data from the 2020 AirToxScreen Assessment to provide context for the relative contributions to 1,3-butadiene ambient air concentrations from 38 source categories that include agriculture, residential wood burning and vehicular and other mobile sources. The 2020 AirToxScreen uses the Community Multiscale Air Quality (CMAQ) chemical transport model and the AERMOD dispersion model to estimate annual average outdoor ambient air concentrations across the United States using release data from the 2020 NEI database. Because NEI release data can be differentiated by source category, AirToxScreen outputs allow for a comparison of the relative contributions of different source categories (including both TSCA and other sources) to aggregate 1,3-butadiene ambient concentrations.

The AirToxScreen 2020 assessment modeled concentrations of 1,3-butadiene using the 2020 NEI data and 2020 census block information. Figure 2-2 shows modeled concentrations of 1,3-butadiene across the United States from all 38 source categories. Table 2-4 provides a summary of 1,3-butadiene ambient concentrations from the AirToxScreen 2020 assessment by EPA Region. Concentrations across all 10 regions ranged from 3.75×10^{-7} to 4.05 µg/m^3 with the lowest minimum concentration modeled in Region 10 and highest maximum concentration modeled in Region 7. Highest median and mean concentrations modeled were in Region 10.

EPA recognizes that activities related to fuel use and combustion are major sources of 1,3-butadiene and uses AirToxScreen to help characterize those emission sources. Figure 2-3 is a plot of the 1,3-butadiene concentrations for source categories related to fuel use and combustion and Figure 2-4 is a plot of the 1,3-butadiene concentrations for source categories not related to fuel use and combustion. For source categories related to fuel use and combustion, residential wood burning, wildfires, oil and gas, commercial cooking, airports, and light duty vehicles were contributing source categories while waste disposal, commercial lawn and commercial equipment were contributing source categories not related to fuel use and combustion. TRI facilities fall under the stationary point source category and may have fuel use and combustion related activities. TRI facilities may also fall under other source categories such as oil and gas, solvents and coatings, waste disposal, and industrial.

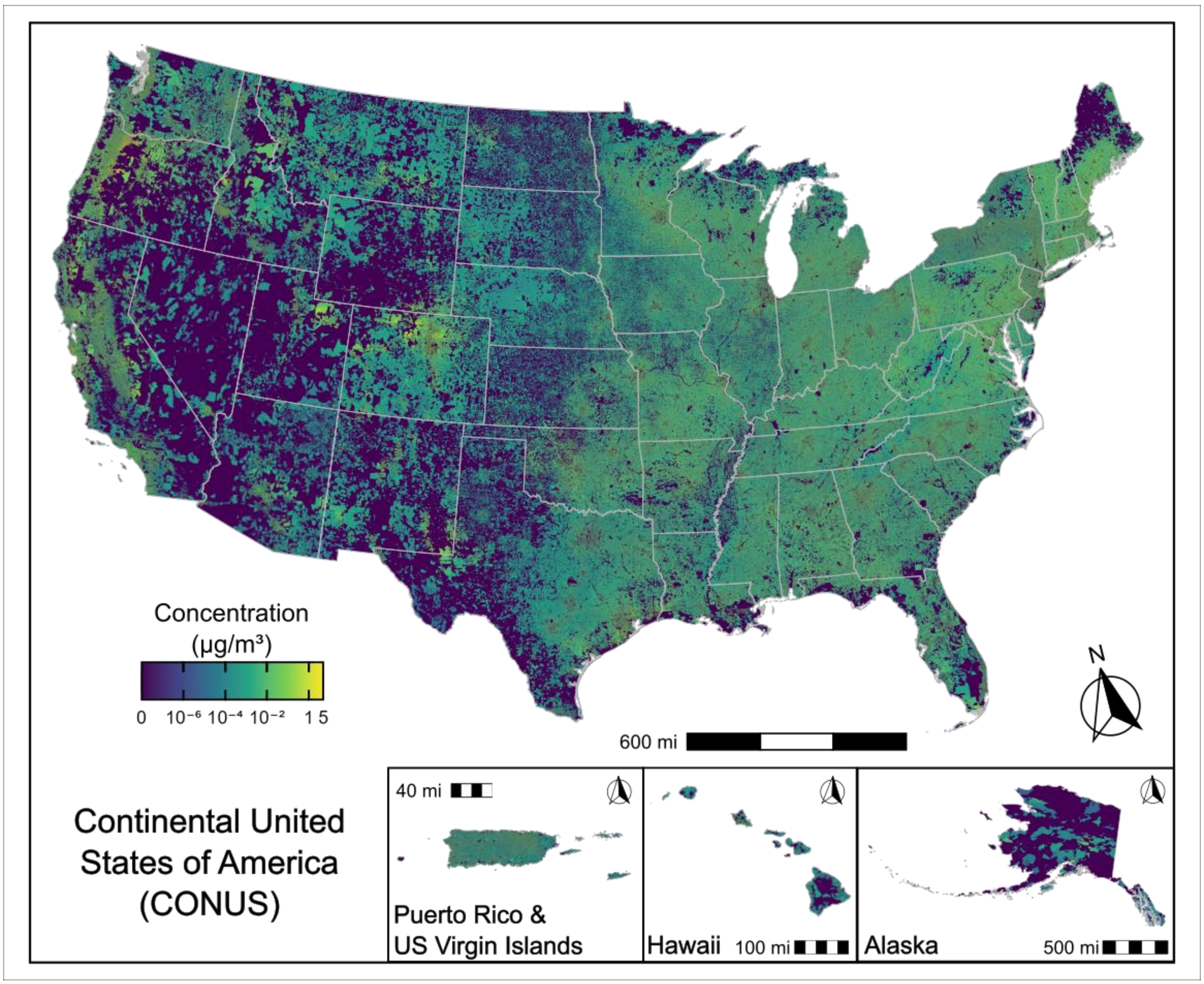


Figure 2-2. Map of Contiguous United States with AirToxScreen 2020 Results Based on NEI 2020 Releases Aggregated and Summarized by Census Block

Table 2-4. Summary of 1,3-Butadiene Ambient Concentrations from AirToxScreen 2020

Region	States	Ambient Concentrations ($\mu g/m^3$)				
		Minimum	Median	Maximum	Mean	Standard Deviation
Region 1	CT, ME, MA, NH, RI, and VT	5.63E−04	2.09E−02	*8.50E-02*	2.11E−02	9.53E−03
Region 2	NJ, NY, Puerto Rico, and U.S. Virgin Islands	3.48E−05	1.84E−02	1.16E−01	2.09E−02	1.42E−02
Region 3	DE, DC, MD, PA, VA, and WV	**7.26E-04**	1.52E−02	1.62E−01	1.72E−02	1.03E−02
Region 4	AL, FL, GA, KY, MS, NC, SC, and TN	4.17E−05	7.50E−03	8.10E−01	9.06E−03	5.73E−03
Region 5	IL, IN, MI, MN, OH, and WI	1.46E−04	9.59E−03	1.35E00	1.19E−02	8.47E−03
Region 6	AR, LA, NM, OK, and TX	1.05E−05	6.41E−03	1.32E00	9.82E−03	1.32E−02
Region 7	IA, KS, MO, and NE	1.17E−04	*4.85E-03*	**4.05E00**	*8.03E-03*	9.66E−03
Region 8	CO, MT, ND, SD, UT, and WY	5.55E−05	5.48E−03	6.28E−01	1.63E−02	2.22E−02
Region 9	AZ, CA, HI, NV	2.93E−05	1.69E−02	5.51E−01	2.08E−02	2.11E−02
Region 10	AK, ID, OR, and WA	*3.75E-07*	**2.78E-02**	1.43E00	**4.35E-02**	5.94E−02

Bold = highest value in the column; *Italics* = lowest value in the column

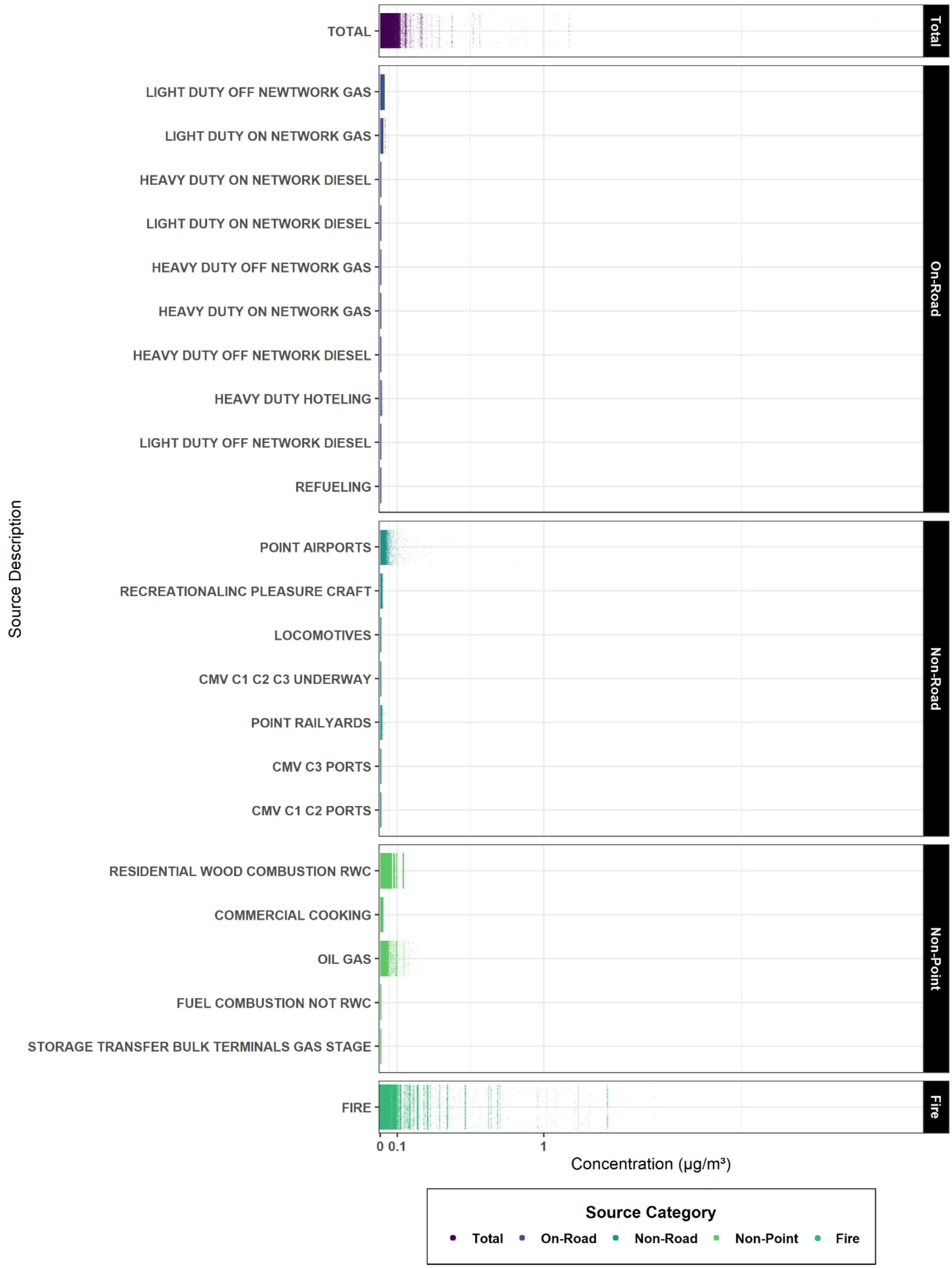


Figure 2-3. 1,3-Butadiene Ambient Air Concentrations and Combustion Sources from AirToxScreen 2020

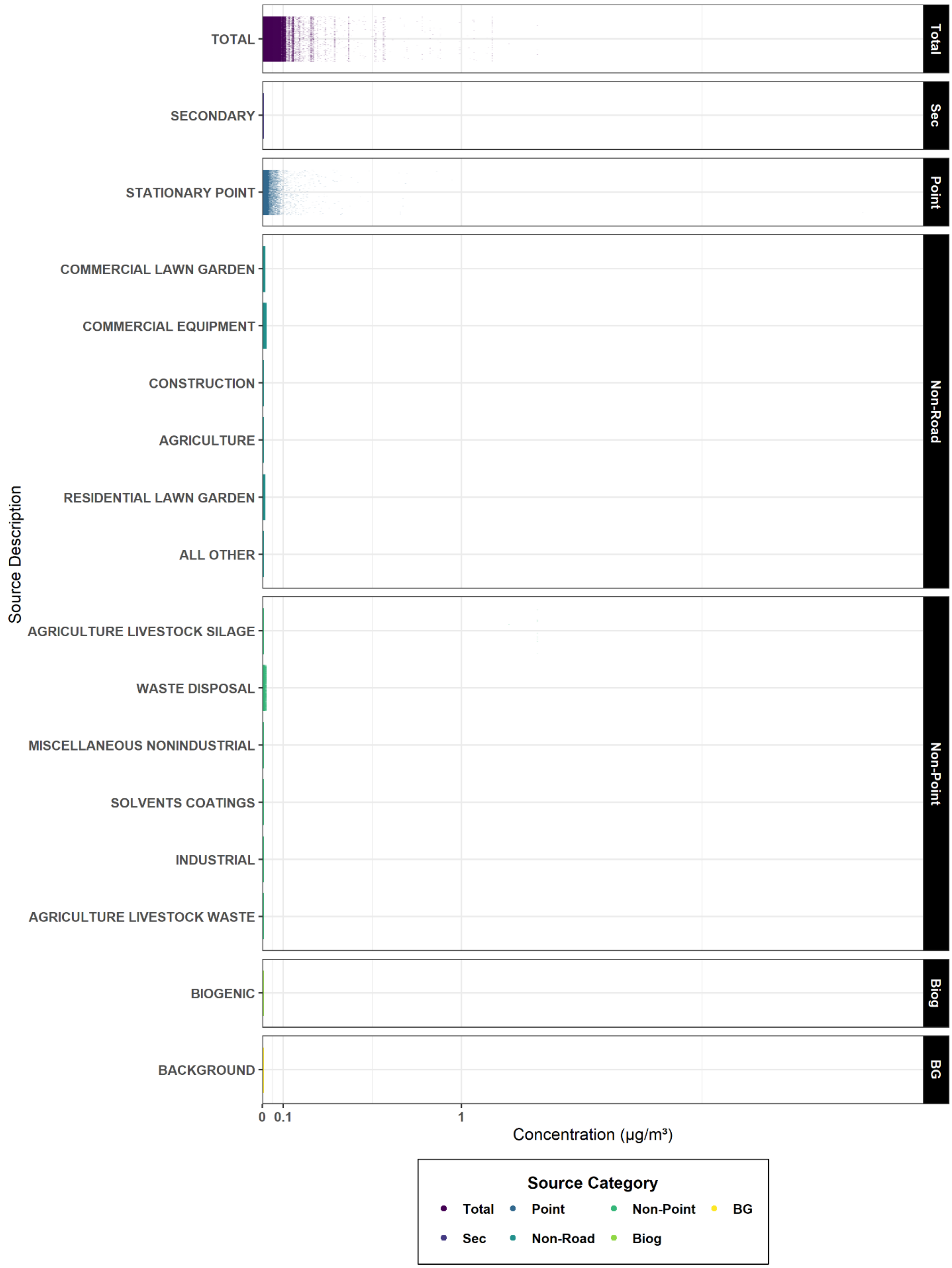


Figure 2-4. 1,3-Butadiene Ambient Air Concentrations and Non-combustion Sources from AirToxScreen 2020

3 STRENGTHS AND LIMITATIONS, ASSUMPTIONS, UNCERTAINTY, AND CONFIDENCE STATEMENT

3.1 Integrated Indoor/Outdoor Air Calculator Model (IIOAC)

The approach and methodology presented in this ambient air exposure assessment replicates previously peer reviewed approaches and methods, and incorporates several additional components recommended by peer reviewers to provide a more comprehensive exposure assessment. As such, EPA has high confidence in the IIOAC modeling and use of the results to characterize exposures and derive risk estimates for individuals living nearby releasing facilities.

Strengths of this ambient air exposure assessment include use of actual environmental release data from across multiple years which are reported by industry, as required by statute, and undergoes repeatable quality assurance quality control reviews (U.S. EPA, 2024c). These release data are used as direct inputs to two separate EPA's peer-reviewed models to estimate concentrations at several distances from releasing facilities where individuals may reside for many years.

Although IIOAC was used as a screening tool, a general limitation of IIOAC is that the modeling is based on pre-run scenarios within AERMOD. As such, default input parameters for IIOAC are confined to those input parameters utilized for those pre-run AERMOD scenarios and cannot be changed, including default stack parameters, 2011 to 2015 meteorological data, and the lack of site-specific information like building dimensions, stack heights, elevation, and land use.

3.2 Human Exposure Model (HEM)

The HEM 4.2 dispersion calculations are handled by EPA's AERMOD, which has undergone peer review and evaluation as part of the regulatory models process. A description of its promulgation as a regulatory model is included in Appendix W in 40 CFR Part 51. Due to its regular application in assessments to inform regulatory decisions, EPA has high confidence in the modeling results. A limitation of the model is the exclusion of photodegradation processes, which may be relevant to ambient air concentrations of 1,3-butadiene. Without modeled decreases in concentration due to photodegradation, the results presented in this document are more conservative (*i.e.*, protective).

3.3 AirToxScreen

AirToxScreen has been previously reviewed by EPA's Science Advisory Board (SAB). As such, EPA has confidence in the modeled data. Similarly, these data are based on the NEI, which has been rated as a high-quality data source according to the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances, Version 1.0: A Generic TSCA Systematic Review Protocol with Chemical-Specific Methodologies* (also called "Draft Systematic Review Protocol") (U.S. EPA, 2021b).

The strengths of these data are that they show the various potential sources of 1,3-butadiene in the coterminous United States. The limitations of these data are that they cannot be directly compared to TSCA COUs as they are not representative of facility-scale releases and subsequent ambient air concentrations. A key assumption of AirToxScreen is that it cannot provide a precise exposure and risk for a specific person. Instead, these results are best applied to understand differences in potential sources of 1,3-butadiene. An additional limitation is that AirToxScreen is largely dependent on state-reported emissions inventories to which hazardous air pollutants (HAPs; *e.g.*, 1,3-butadiene) are voluntarily reported.

3.4 Ambient Monitoring Technology Information Center (AMTIC) Dataset

AMTIC data has been previously reviewed and verified by the AMTICs Ambient Air Monitoring Group, which has taken various quality assurance steps to ensure data quality and has been certified in accordance to 40 CFR Part 58.15. EPA has high confidence in the AMTIC ambient air data set (U.S. EPA, 2022), which received a high-quality rating from EPA's systematic review process (U.S. EPA, 2021a).

The primary limitations of the AMTIC data are as presented in this ambient air exposure assessment, the data has not been annualized and therefore represents a diverse collection of sampling durations (none of which are annual averages) that are not directly comparable to IIOAC, HEM, or AirToxScreen data. Additionally, because monitored data represents a total aggregate concentration from all sources of 1,3-butadiene contributing to ambient air concentrations, the AMTIC data cannot be associated with TSCA COUs for purposes of characterizing exposures from TSCA COUS.

3.5 Weight of Scientific Evidence

EPA has robust confidence in the overall characterization of exposures for this ambient air exposure assessment as it relies upon direct reported releases from databases that received a high-quality rating from EPA's systematic review process and peer-reviewed models to derive exposure concentrations at distances from releasing facilities where individuals reside for many years. Use of additional peer-reviewed models (AirToxScreen and HEM) along with monitoring data (AMTIC) to further contextualize ambient air concentrations of 1,3-butadiene provide added strength and confidence to the approaches and methods used in this draft ambient air exposure assessment. This confidence statement is consistent with the Draft Systematic Review Protocol (U.S. EPA, 2021b).

The use of release data across multiple years of data provide a more comprehensive ambient air exposure assessment and ensure higher release years are not missed. Furthermore, use of actual reported releases minimizes uncertainties around estimated releases using theoretical distributions and provides added confidence that modeled concentrations and exposures are real and not hypothetical apart from EPA estimated releases for the Adhesives and sealants OES.

4 CONCLUSIONS

EPA modeled ambient air concentrations using both the IIOAC and HEM models to assess general population exposures to 1,3-butadiene based on TRI release data. EPA used monitoring data from the AMTIC (U.S. EPA, 2022) to groundtruth results from the models and to reflect aggregate 1,3-butadiene ambient air concentrations from all sources. To contextualize and characterize other sources of 1,3-butadiene, EPA also evaluated existing modeled data from the 2020 AirToxScreen to show how different source categories contribute to total ambient air concentrations of 1,3-butadiene nationwide.

Modeled results from IIOAC for exposure concentrations to populations living near industrial facilities (within 100–1,000 m [0.062–0.62 miles]) releasing 1,3-butadiene to the ambient air ranged from 0.0 to 109.5 µg/m^3. Refined model results from HEM ranged from 0.0 to 91.2 µg/m^3 for populations living 100 to 1,000 m (0.062 to 0.62 miles). For all distances modeled with HEM 10 to 50,000 m (0.006–31.06 miles), the concentration range was 0.0 to 383.4 µg/m^3, with the highest concentrations modeled within the first 30 to 60 m away from the release point. Monitored 1,3-butadiene concentrations extracted from AMTIC (2016–2021) ranged from 0.0 to 122.8 µg/m^3 across all monitored 24-hour sampling values. The AirToxScreen 2020 Assessment based on NEI 2020 data, modeled a range of 3.75×10^{-7} to 4.05 µg/m^3 across all 10 EPA regions. AirToxScreen modeled 1,3-butadiene concentrations are attributable to 38 source categories that include point sources, nonpoint sources, and on-road/non-road sources.

Taken together, these results show that modeled 1,3-butadiene ambient air concentrations using IIOAC and HEM were in the same order of magnitude as measured 1,3-butadiene concentrations from AMTIC monitoring data. To characterize exposures associated with TSCA COUs, for purposes of informing regulatory decisions under TSCA, it is necessary to recognize modeled concentrations may contribute to some part of the total concentrations, captured by monitored data but are independent and exclusive of other sources like mobile on-road and off-road sources. More specifically, exposures presented in this draft ambient air assessment of 1,3-butadiene resulting from TSCA COUs are representative of exposures from TSCA COUs alone. Total exposure to 1,3-butadiene at a given location in the ambient air all exposures from all sources (*e.g.*, TSCA COUs, on-road and off-road sources, etc.) are additive. This means a total exposure at a given location is derived from adding the contribution of 1,3-butadiene from TSCA COUs to the contribution of 1,3-butadiene from every other source of 1,3-butadiene. Although it is possible to present “total exposure” to 1,3-butadiene in ambient air resulting from every source (TSCA COUs and other sources), it is not appropriate for this assessment of 1,3-butadiene because TSCA only provides authority to regulate exposures resulting from TSCA COUs and does not provide authority to regulate beyond TSCA COUs.

Based on the modeled concentrations using IIOAC and HEM, the following TSCA COUs-OESs resulted in the highest 1,3-butadiene concentrations (Table 4-1).

Table 4-1. Occupational Exposure Scenarios (OESs) and Conditions of Use (COUs) with Highest Modeled Concentrations

Life Cycle Stage	Category	Subcategory	OES
Manufacture	Import	Import	Manufacturing
Processing	Processing as a reactant	Other: Monomer used in polymerization process in: Plastic material and resin manufacturing; Manufacturing synthetic rubber and plastics	Plastics and rubber compounding
		Intermediate in: Adhesive manufacturing; All other basic organic chemical manufacturing; Fuel binder for solid rocket fuels; Organic fiber manufacturing; Petrochemical manufacturing; Petroleum refineries; Plastic material and resin manufacturing; Propellant manufacturing; Synthetic rubber manufacturing; Wholesale and retail trade	Processing as a reactant
	Processing – incorporation into formulation, mixture, or reaction product	Processing aids, not otherwise listed in: Petrochemical manufacturing	Processing – incorporation into formulation, mixture, or reaction product

EPA has robust confidence in the overall characterization of exposures for this general population exposure assessment. Exposure results relied upon peer-reviewed models and direct reported releases, which can be tied to TSCA COUs to derive exposure concentrations at distances from releasing facilities where those within the general population typically reside for many years. The similarity between monitoring data and the modeled concentrations provides added confidence to EPA's use of modeled results to characterize human exposures to 1,3-butadiene via the ambient air pathway.

5 REFERENCES

EPA, US. (2019). User's Guide: Integrated Indoor-Outdoor Air Calculator (IIOAC). Washington, DC: U.S. EPA.

U.S. EPA (U.S. Environmental Protection Agency). (2021a). Best practices for review and validation of ambient air monitoring data. (EPA-454/B-21-007).

U.S. EPA (U.S. Environmental Protection Agency). (2021b). Draft systematic review protocol supporting TSCA risk evaluations for chemical substances, Version 1.0: A generic TSCA systematic review protocol with chemical-specific methodologies. (EPA Document #EPA-D-20-031). Washington, DC: Office of Chemical Safety and Pollution Prevention. https://www.regulations.gov/document/EPA-HQ-OPPT-2021-0414-0005

U.S. EPA (U.S. Environmental Protection Agency). (2022). Ambient Monitoring Technology Information Center (AMTIC) - Ambient Monitoring Archive for HAPs [Database]. Washington, DC. Retrieved from https://www.epa.gov/amtic/amtic-ambient-monitoring-archive-haps

U.S. EPA (U.S. Environmental Protection Agency). (2024a). Draft Environmental Media Concentrations for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.

U.S. EPA. (2024b). Draft Environmental Release Assessment for Formaldehyde. Washington, DC: U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics.

U.S. EPA (U.S. Environmental Protection Agency). (2024c). Draft Environmental Release for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.

U.S. EPA (U.S. Environmental Protection Agency). (2024d). Draft Human Exposure Model (HEM) TRI 2016-2021 Exposure and Risk Analysis for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.

U.S. EPA (U.S. Environmental Protection Agency). (2024e). Draft Human Health Hazard Assessment for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.

U.S. EPA (U.S. Environmental Protection Agency). (2024f). Draft Integrated Indoor Outdoor Air Calculator (IIOAC) TRI 2016-2021 Exposure and Risk Analysis for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.

U.S. EPA (U.S. Environmental Protection Agency). (2024g). Draft Physical Chemistry and Fate Assessment for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.

U.S. EPA (U.S. Environmental Protection Agency). (2024h). Draft Risk Evaluation for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.

U.S. EPA (U.S. Environmental Protection Agency). (2024i). Draft Systematic Review Protocol for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.

APPENDICES

Appendix A INTEGRATED INDOOR/OUTDOOR AIR CALCULATOR MODELING

A.1 IIOAC Screening Assessment Results

A total of 225 TRI reporting facilities reported releases of 1,3-butadiene to the ambient air. The following three OESs had the highest modeled 95th percentile concentrations relative to the other calculated exposure concentrations evaluated:

- Plastics and Rubber Compounding (109.5 μg/m^3);
- Manufacturing (80.0 μg/m^3) and;
- Processing as a Reactant (41.1 μg/m^3).

In addition to the TRI reported releases, EPA also modeled estimated releases for an additional OES involving adhesives and sealants.

IIOAC-modeled exposure concentrations results were used to calculate non-cancer and cancer risks in the following section as a screening tool to determine whether refined modeling was required.

A.1.1 Risk Calculations

A.1.1.1 Inhalation Margin of Exposure

EPA used a margin of exposure (MOE) approach using high-end exposure estimates to determine if the pathway analyzed is a pathway of concern. The MOE is the ratio of the non-cancer hazard value (or point of departure [POD]) divided by a human exposure dose. The chronic MOEs for non-cancer inhalation risks were calculated using Equation_Apx A-1 below.

Equation_Apx A-1. Margin of Exposure Calculation

$$MOE = \frac{Non\text{–}\ cancer\ Hazard\ Value\ (POD)}{Human\ Exposure}$$

Where:

MOE	=	Margin of exposure for acute, short-term, or chronic risk comparison (unitless)
Non-cancer Hazard Value (POD)	=	Human equivalent concentration (HEC, μg/m^3)
Human Exposure	=	Exposure estimate (μg/m^3)

MOE risk estimates may be interpreted in relation to benchmark MOEs. Benchmark MOEs are typically the total uncertainty factor for each non-cancer POD. The MOE estimate is interpreted as a human health risk of concern if the MOE estimate is less than the benchmark MOE (*i.e.*, the total uncertainty factor). On the other hand, for this screening level analysis, if the MOE estimate is equal to or exceeds the benchmark MOE, the exposure pathway is not analyzed further. Typically, the larger the MOE, the more unlikely it is that a non-cancer adverse effect occurs relative to the benchmark. When determining whether a chemical substance presents unreasonable risk to human health or the environment, calculated risk estimates are not "bright-line" indicators of unreasonable risk, and EPA has the discretion to consider other risk-related factors in addition to risks identified in the risk characterization.

Briefly, after considering hazard identification and evidence integration, dose-response evaluation, and weight of the scientific evidence of POD candidates, EPA chose one non-cancer endpoint for general population chronic exposure with a human equivalent concentration (HEC) value of 2.5 ppm (5500 $\mu g/m^3$) and a benchmark of 30. For more details on the non-cancer hazard values used to screen for risk, see the Draft Human Health Hazard Assessment for 1,3-Butadiene (U.S. EPA, 2024e). No calculated MOE was below the benchmark of 30 for all IIOAC modeled concentrations from 100 to 1000 m across all TRI facilities.

A.1.1.2 Inhalation Cancer Risk

Lifetime cancer risk is calculated with Equation_Apx A-2 using the LADC based on the 95th modeled annual air concentration and the general population Inhalation Unit Risk (IUR) of 4.4 x 10-6 per $\mu g/m^3$ from the *Draft Human Health Hazard Assessment for 1,3-Butadiene* (U.S. EPA, 2024e):

Equation_Apx A-2. Lifetime Cancer Risk Calculation

$$Lifetime\ Cancer\ Risk = \mathrm{LADC} \times \mathrm{IUR}$$

$$Lifetime\ Cancer\ Risk = LADC(\frac{\mu g}{m^3}) \times \frac{4.4E^{-6}}{\mu g/m^3}$$

Where:

LADC = Lifetime Average Daily Concentration
IUR = Inhalation Unit Risk (risk per unit of exposure ($\mu g/m^3$)

If the calculated lifetime cancer risk is above the cancer risk benchmark of 1 in a million, or $1{\times}10^{-6}$, then risk is potentially identified and warrants further evaluation. Table_Apx A-1 summarizes the 95th percentile IIOAC modeled concentrations at each distance and number of facilities in each OES while Table_Apx A-2 summarizes the calculated risks at each distance and number of facilities in each OES that surpassed the benchmark cancer risk of 1 in a million based on based on 95th percentile IIOAC modeled concentrations. Lifetime cancer risk ranged from 0 to $3.1{\times}10^{-4}$ across the 100, 100 to 1,000 m and 1,000 m distances. Out of the 225 TRI facilities, 132 facilities resulted in cancer risk above the 1 in a million benchmark based on 95th percentile IIOAC modeled concentrations; lifetime cancer risks based on mean IIOAC modeled concentrations (Table_Apx A-3) resulted in 128 out of 225 facilities (Table_Apx A-4). For adhesives and sealants, only the 95th percentile modeled concentrations based on 95th percentile estimated fugitive releases resulted in a cancer risk above the 1 in a million benchmark at the 100 m distance (Table_Apx A-5).

790 **Table_Apx A-1. IIOAC 95th Percentile Modeled Concentrations (µg/m³)**

IIOAC 95th Percentile Modeled Concentrations (µg/m³)			Distance		
OES	**TRI Facility Count**	**Stat**	**Fenceline (100m)**	**Community (100–1,000 m)**	**Outer-Boundary (1,000 m)**
Manufacturing	40	Max	8.0E01	1.1E01	5.3E00
		Mean	8.7E00	1.2E00	5.0E−01
		Median	2.1E00	3.0E−01	1.4E−01
		Min	0.0E00	0.0E00	0.0E00
Plastics and rubber compounding	33	Max	1.1E02	1.3E01	5.2E00
		Mean	9.4E00	1.2E00	4.8E−01
		Median	3.2E00	4.1E−01	1.7E−01
		Min	3.0E−04	9.4E−05	5.0E−05
Plastics and rubber converting	1	Max	3.5E−07	1.1E−07	5.8E−08
		Mean	3.5E−07	1.1E−07	5.8E−08
		Median	3.5E−07	1.1E−07	5.8E−08
		Min	3.5E−07	1.1E−07	5.8E−08
Processing – incorporation into formulation, mixture, or reaction product	53	Max	9.8E00	3.1E00	1.6E00
		Mean	6.0E−01	9.0E−02	4.0E−02
		Median	5.4E−02	9.6E−03	4.6E−03
		Min	0.0E00	0.0E00	0.0E00
Processing as a reactant	57	Max	4.1E01	4.9E00	2.0E00
		Mean	2.1E00	2.6E−01	1.1E−01
		Median	3.4E−01	4.5E−02	1.9E−02
		Min	0.0E00	0.0E00	0.0E00
Recycling	11	Max	1.2E00	1.4E−01	5.5E−02
		Mean	2.0E−01	2.6E−02	1.1E−02
		Median	1.1E−01	1.5E−02	6.8E−03
		Min	2.2E−04	7.1E−05	3.8E−05
Repackaging	23	Max	2.0E01	2.5E00	1.0E00
		Mean	1.4E00	1.7E−01	6.9E−02
		Median	5.8E−02	6.8E−03	2.7E−03
		Min	0.0E00	0.0E00	0.0E00

IIOAC 95th Percentile Modeled Concentrations (µg/m³)			Distance		
OES	**TRI Facility Count**	**Stat**	**Fenceline (100m)**	**Community (100–1,000 m)**	**Outer-Boundary (1,000 m)**
Waste handling, disposal, treatment, and recycling	7	Max	2.5E−01	2.9E−02	1.2E−02
		Mean	1.9E−02	3.2E−03	1.5E−03
		Median	8.8E−04	1.4E−04	6.5E−05
		Min	2.3E−05	3.0E−06	1.3E−06
Total	**225**				

Table_Apx A-2. IIOAC 95th Percentile Cancer Risks

Cancer Risk Based on IIOAC 95th Percentile Modeled Concentrations				Distance		
OES	**TRI Facility Count**	**Number of Facilities above 1E−06**	**Stat**	**Fenceline (100m)**	**Community (100–1,000m)**	**Outer-Boundary (1,000m)**
Manufacturing	40	30	Max	3.6E−04	5.1E−05	2.3E−05
			Mean	3.9E−05	5.2E−06	2.2E−06
			Median	9.5E−06	1.4E−06	6.2E−07
			Min	0.0E00	0.0E00	0.0E00
Plastics and rubber compounding	33	30	Max	4.9E−04	5.8E−05	2.3E−05
			Mean	4.2E−05	5.2E−06	2.2E−06
			Median	1.4E−05	1.8E−06	7.5E−07
			Min	1.3E−09	4.2E−10	2.2E−10
Plastics and rubber converting	1	0	Max	1.6E−12	4.9E−13	2.6E−13
			Mean	1.6E−12	4.9E−13	2.6E−13
			Median	1.6E−12	4.9E−13	2.6E−13
			Min	1.6E−12	4.9E−13	2.6E−13
Processing – Incorporation into formulation, mixture, or reaction product	53	24	Max	4.4E−05	1.4E−05	7.3E−06
			Mean	2.7E−06	4.0E−07	1.8E−07
			Median	2.4E−07	4.3E−08	2.0E−08
			Min	0.0E00	0.0E00	0.0E00
Processing as a Reactant	57	36	Max	1.8E−04	2.2E−05	8.8E−06
			Mean	9.1E−06	1.2E−06	4.8E−07
			Median	1.5E−06	2.0E−07	8.5E−08
			Min	0.0E00	0.0E00	0.0E00

Cancer Risk Based on IIOAC 95th Percentile Modeled Concentrations				Distance		
OES	**TRI Facility Count**	**Number of Facilities above 1E−06**	**Stat**	**Fenceline (100m)**	**Community (100–1,000m)**	**Outer-Boundary (1,000m)**
Recycling	11	3	Max	5.2E−06	6.1E−07	2.4E−07
			Mean	9.0E−07	1.2E−07	4.9E−08
			Median	4.8E−07	6.5E−08	3.0E−08
			Min	1.0E−09	3.2E−10	1.7E−10
Repackaging	23	8	Max	9.0E−05	1.1E−05	4.5E−06
			Mean	6.2E−06	7.5E−07	3.1E−07
			Median	2.6E−07	3.0E−08	1.2E−08
			Min	0.0E00	0.0E00	0.0E00
Waste handling, disposal, treatment, and recycling	7	1	Max	1.1E−06	1.3E−07	5.2E−08
			Mean	8.4E−08	1.4E−08	6.5E−09
			Median	3.9E−09	6.3E−10	2.9E−10
			Min	1.0E−10	1.4E−11	5.8E−12
Total	**225**	**132**				

Table_Apx A-3. IIOAC Mean Modeled Concentrations (µg/m^3)

IIOAC Mean Modeled Concentrations (µg/m^3)			Distance		
OES	**TRI Facility Count**	**Stat**	**Fenceline (100 m)**	**Community (100–1,000 m)**	**Outer-Boundary (1,000 m)**
Manufacturing	40	Max	7.3E01	1.0E01	4.5E00
		Mean	8.0E00	1.0E00	4.3E−01
		Median	1.9E00	2.7E−01	1.2E−01
		Min	0.0E00	0.0E00	0.0E00
Plastics and Rubber Compounding	33	Max	1.0E02	1.1E01	4.4E00
		Mean	8.6E00	1.0E00	4.1E−01
		Median	2.9E00	3.6E−01	1.4E−01
		Min	2.6E−04	8.2E−05	4.3E−05

IIOAC Mean Modeled Concentrations (µg/m³)			Distance		
OES	**TRI Facility Count**	**Stat**	**Fenceline (100 m)**	**Community (100–1,000 m)**	**Outer-Boundary (1,000 m)**
Plastics and rubber converting	1	Max	3.0E−07	9.7E−08	5.1E−08
		Mean	3.0E−07	9.7E−08	5.1E−08
		Median	3.0E−07	9.7E−08	5.1E−08
		Min	3.0E−07	9.7E−08	5.1E−08
Processing – incorporation into formulation, mixture, or reaction product	53	Max	8.6E00	2.7E00	1.4E00
		Mean	5.5E−01	8.0E−02	3.4E−02
		Median	4.9E−02	8.4E−03	3.9E−03
		Min	0.0E00	0.0E00	0.0E00
Processing as a reactant	57	Max	3.8E01	4.3E00	1.7E00
		Mean	1.9E00	2.3E−01	9.2E−02
		Median	3.1E−01	4.0E−02	1.6E−02
		Min	0.0E00	0.0E00	0.0E00
Recycling	11	Max	1.1E00	1.2E−01	4.6E−02
		Mean	1.8E−01	2.3E−02	9.3E−03
		Median	9.8E−02	1.3E−02	5.7E−03
		Min	2.0E−04	6.2E−05	3.3E−05
Repackaging	23	Max	1.8E01	2.2E00	8.5E−01
		Mean	1.3E00	1.5E−01	5.8E−02
		Median	5.3E−02	6.0E−03	2.3E−03
		Min	0.0E00	0.0E00	0.0E00
Waste handling, disposal, treatment, and recycling	7	Max	2.3E−01	2.6E−02	9.7E−03
		Mean	1.7E−02	2.8E−03	1.3E−03
		Median	8.0E−04	1.2E−04	5.6E−05
		Min	2.1E−05	2.7E−06	1.1E−06
Total	**225**				

Table_Apx A-4. IIOAC Mean Cancer Risks

Cancer Risk Based on IIOAC Mean Modeled Concentrations				Distance		
OES	**TRI Facility Count**	**Number of Facilities above 1E-06**	**Stat**	**Fenceline (100m)**	**Community (100–1,000 m)**	**Outer-Boundary (1,000 m)**
Manufacturing	40	30	Max	2.0E−04	2.8E−05	1.3E−05
			Mean	2.2E−05	2.9E−06	1.2E−06
			Median	5.4E−06	7.5E−07	3.3E−07
			Min	0.0E00	0.0E00	0.0E00
Plastics and rubber compounding	33	30	Max	2.8E−04	3.2E−05	1.2E−05
			Mean	2.4E−05	2.9E−06	1.1E−06
			Median	8.2E−06	1.0E−06	4.0E−07
			Min	7.2E−10	2.3E−10	1.2E−10
Plastics and rubber converting	1	0	Max	8.5E−13	2.7E−13	1.4E−13
			Mean	8.5E−13	2.7E−13	1.4E−13
			Median	8.5E−13	2.7E−13	1.4E−13
			Min	8.5E−13	2.7E−13	1.4E−13
Processing – incorporation into formulation, mixture, or reaction product	53	22	Max	2.4E−05	7.6E−06	4.0E−06
			Mean	1.5E−06	2.2E−07	9.6E−08
			Median	1.4E−07	2.4E−08	1.1E−08
			Min	0.0E00	0.0E00	0.0E00
Processing as a reactant	57	36	Max	1.1E−04	1.2E−05	4.7E−06
			Mean	5.3E−06	6.5E−07	2.6E−07
			Median	8.8E−07	1.1E−07	4.5E−08
			Min	0.0E00	0.0E00	0.0E00
Recycling	11	3	Max	3.0E−06	3.4E−07	1.3E−07
			Mean	5.2E−07	6.5E−08	2.6E−08
			Median	2.7E−07	3.6E−08	1.6E−08
			Min	5.5E−10	1.7E−10	9.1E−11

Cancer Risk Based on IIOAC Mean Modeled Concentrations				Distance		
OES	**TRI Facility Count**	**Number of Facilities above 1E-06**	**Stat**	**Fenceline (100m)**	**Community (100–1,000 m)**	**Outer-Boundary (1,000 m)**
Repackaging	23	7	Max	5.2E−05	6.1E−06	2.4E−06
			Mean	3.6E−06	4.2E−07	1.6E−07
			Median	1.5E−07	1.7E−08	6.4E−09
			Min	0.0E00	0.0E00	0.0E00
Waste handling, disposal, treatment, and recycling	7	0	Max	6.3E−07	7.2E−08	2.7E−08
			Mean	4.8E−08	7.8E−09	3.5E−09
			Median	2.2E−09	3.5E−10	1.6E−10
			Min	5.9E−11	7.6E−12	3.1E−12
Total	**225**	**128**				

Table_Apx A-5. Adhesive and Sealants IIOAC Exposure and Risk Results

OES	Source Type	Release Stat	Average Daily Concentration (ADC) (µg/m^3)						Cancer Risk = ADC*IUR IUR = 4.4E−06 risk per µg/m^3					
			High End 95th Percentile			Central Tendency Mean			High-End 95th Percentile			Central Tendency Mean		
			Fenceline Avg (100 m)	Outer-Boundary Avg (1,000 m)	Community Avg (100–1,000 m)	Fenceline Avg (100 m)	Outer-Boundary Avg (1,000 m)	Community Avg (100–1,000 m)	Fenceline Avg (100 m)	Outer-Boundary Avg (1,000 m)	Community Avg (100–1,000 m)	Fenceline Avg (100 m)	Outer-Boundary Avg (1,000 m)	Community Avg (100–1,000 m)
Adhesives and sealants	Fugitive	95th	1.64E00	7.62E−02	1.90E−01	1.47E00	6.33E−02	1.67E−01	7.20E−06	3.35E−07	8.34E−07	6.49E−06	2.79E−07	7.34E−07
		50th	1.27E−01	5.77E−03	1.45E−02	1.10E−01	4.72E−03	1.24E−02	5.61E−07	2.54E−08	6.40E−08	4.83E−07	2.08E−08	5.47E−08
	Stack	95th	4.73E−02	7.93E−03	1.48E−02	3.90E−02	6.48E−03	1.24E−02	2.08E−07	3.49E−08	6.52E−08	1.71E−07	2.85E−08	5.47E−08
		50th	4.13E−03	7.11E−04	1.29E−03	2.92E−03	4.87E−04	9.30E−04	1.82E−08	3.13E−09	5.68E−09	1.28E−08	2.14E−09	4.09E−09

Appendix B Human Exposure Modeling

B.1 HEM Model Inputs

B.1.1 Introduction

EPA requested use of release data from the EPA's TRI, with the EPA Human Exposure Model (HEM Version 4.2), to estimate air concentrations resulting from air releases of 1,3-butadiene, modeled at census block receptors and co-located receptors surrounding the release sources. This appendix describes the setup of these model runs.

B.1.2 HEM

HEM 4.2 has two components: (1) an atmospheric dispersion model, AERMOD[1], with included meteorological data; and (2) U.S. Census Bureau population data at the block level. The current HEM version utilizes 2020 Census data—including all 50 states, the District of Columbia, Puerto Rico, and the U.S. Virgin Islands.[2] AERMOD estimates the magnitude and distribution of chemicals concentrations in ambient air in the vicinity of each releasing facility within a user-defined radial distances out to 50 km (about 30 miles). HEM also provides chemical concentrations in ambient air at the centroid of over 8 million census blocks across the United States. The model also is able to combine the estimated chemical concentrations with dose-response data to estimate cancer risks and noncancer hazards, and the population data to inform cancer incidence, and other risk measures. HEM automatically utilizes meteorological data for each release point, as well as local topographic information, to inform the release dispersion model. Refer to the HEM 4.2 User Guide for more details about these and other capabilities.

B.1.3 Model Settings

EPA produced a workbook of estimated air release information for (*1,3-Butadiene 2016-2021 TRI Release Assessment 2_15_2024*, received 15 February 2024), retrieved from 2016 to 2021 editions of the TRI. This information included facility names, locations, identifier codes, OES assignments, annual air releases (stratified by fugitive and point sources), the interday air-release patterns, and which TRI form the information was submitted under.

Table_Apx B-1 indicates the values and settings used in the HEM "facility list" input file, and
Table_Apx B-2,
Table_Apx B-3, and Table_Apx B-4 provide additional information on those values and settings. As shown in Table_Apx B-1, the model automatically matched a meteorology station to each facility by proximity. The meteorological dataset contains over 800 stations nationwide—most of which reflect 2019 meteorological conditions. The model automatically determined if the facility was in an urban location using 2020 census data. EPA explicitly modeled census block receptors within 3,000 m of each facility, with some exceptions noted in the tables, while the model interpolated results to other block receptors out to 50,000 m. All modeling scenarios utilized several rings of non-census receptors. The rings each had 16 had receptors placed every 22.5 ° (starting due north of the facility) for distances ranging from 10 to 50,000 m from the facility.

EPA modeled each year of TRI records separately. The Agency modeled TRI Form A and Form R records separately, such that there was one HEM run for all 2016 Form A facilities, one run for all 2016

[1] Page for AERMOD (American Meteorological Society/Environmental Protection Agency Regulatory Model.
[2] The HEM census file for the U.S. Virgin Islands has 0 people in each location. Block-level population data may not be currently available from the 2020 census.

Form R facilities, and so on for 2017 to 2021. This ensured that any multi-facility aggregate outputs that HEM produced per run were confined to release data from the same year. EPA kept Form A data separate from Form R data because Form A releases are specified as either all stack releases or all fugitive releases but not both, and within each Form A run the Agency ran each facility's stack or fugitive source as a separate "facility" to prevent aggregation of the facility's stack and fugitive concentrations. Form A modeling utilized an "S" or "F" suffix to each facility ID to designate that it was the stack source or fugitive source being modeled.

Table_Apx B-1. Settings for HEM's "Facility List" Input File

Parameter Group	Parameter	Value or Setting	Interpretation	Note
Dispersion Environment	met_station	[blank]	Model chose the meteorology station closest to each facility	
	rural_urban	[blank]	Model found the nearest census block to the facility center and determined whether that block was located in an urbanized area as designated by the 2020 Census	
	urban_pop	[blank]	Model used a default of 50,000 people for the urban population	
Modeling Domain Defined	max_dist	50,001	Model used a default of 50,000 m to define the modeling domain around each facility (entering 50,001 here forced a default of 50,000)	
	model_dist	50,001	Model used a default of 3,000 m to define the cutoff distance around each facility for explicitly modeling census block receptors, and then any block receptors beyond that had their modeling results interpolated from polar receptors (entering 50,001 here forced a default of 3,000)	For a small number of facilities, there were no populated block centroids within 3,000 m of the facility, and so this distance was set to 10,000 m, unless a larger value was needed to capture populated blocks (see Table_Apx B-2)
	radials	16	Model used polar receptors at the default of 16 radials	
	circles	11	Model used polar receptors at 11 concentric rings	
	overlap_dist	30	Model used a default 30 m to define the facility fenceline, inside which receptors were not considered as a point of maximum exposure/risk	
	ring1	10	Model used 10 m for the distance of the first ring of polar receptors	

Parameter Group	Parameter	Value or Setting	Interpretation	Note
	fac_center	L, [custom for each facility: latitude, longitude]	Model used the facility latitude and longitude from TRI	
	ring_dists	10, 30, 60, 100, 1,000, 2,500, 5,000, 10,000, 15,000, 25,000, 50,000	Model used concentric rings of polar receptors at these distances (in meters)	
Acute Options	acute	N	Model did not estimate short-term concentrations	
	hours	[blank]		
	multiplier	[blank]		
	high_value	[blank]		
Deposition and Depletion Parameters	dep	[blank]	Model did not estimate deposition	
	depl	[blank]		
	pdep	[blank]		
	pdepl	[blank]		
	vdep	[blank]		
	vdepl	[blank]		
Additional Options	elev	Y	Model included the elevation of receptors in the concentration estimates	
	user_rcpt	N	Model did not use additional user-specified receptors (beyond the polar grid and census blocks), which is the default choice	
	bldg_dw	N	Model did not estimate building downwash, which is the default choice	
	fastall	Y	Model used AERMOD's FASTALL option to conserve model run time by simplifying the dispersion algorithms, which is not the default choice	
	emiss_var	Y	Model used time-varying emissions, specified in a separate file	Separate file used AERMOD's MHRDOW7 format allowing emission rates to vary by month, hour

Parameter Group	Parameter	Value or Setting	Interpretation	Note
				of day, and the seven days of the week (see Table_Apx B-3 and Table_Apx B-4)
	annual	Y	Model used the default setting to calculate an annual average as a long-term concentration, which is the default choice	
	period_start	[blank]		
	period_end	[blank]		

Table_Apx B-2. Substitutions Made for the Facility List File's "model_dist" Parameter

TRI Facility ID	Modeled Distance
00851HSSLVLIMET	10,000
77503MCCHM1500N	10,000
77503MCCHM1500N_F [a]	10,000
77503MCCHM1500N_S [a]	10,000
77536DSPSL2525B	10,000
77536SFTYK2027B	10,000
77571QNTMC1515M	10,000
77643WSTMNHWY73	10,000
79086DMNDSSTARR	10,000
84029SFTYK11600	44,000
89003SCLGYHWY95	45,000

[a] This was a TRI Form A submission for this facility, where the stack emissions and fugitive emissions were modeled as separate "facilities" to prevent aggregation of the stack and fugitive results at the facility.

Table_Apx B-3. Assumptions for Intraday Emission-Release Duration

Hours per Day of Emissions	Assumed Hours of the Day Emitting
Unknown	All hours

Table_Apx B-4. Assumptions for Interday Emission-Release Pattern

Days per Year of Emissions	Release Pattern
250	Monday to Friday, except no Fridays in January to March

Days per Year of Emissions	Release Pattern
	Equals 247–249 days/year, depending on the year Emission factor when emissions on = 1.473
300	Monday to Saturday, except no Saturdays in January to March. Equals 200–201 days/year, depending on the year Emission factor when emissions on = 1.217
350	All days, except no Sundays in January to April. Equals 347–349 days/year, depending on the year Emission factor when emissions on = 1.05

Table_Apx B-5 indicates the physical source specifications used in the HEM "emission location" input file for point (stack) and area (fugitive) sources; these are the same default physical parameters as in EPA's IIOAC. In some cases, for a given year and TRI form, EPA provided multiple sets of stack releases or multiple sets of fugitive releases at a given facility; in these cases, the Agency aggregated the releases to one overall stack release and one overall fugitive release at the facility.

Table_Apx B-5. Physical Source Specifications

Source Type	Parameter	Value
Point (stack)	Stack height (m)	10
	Inside stack diameter (m)	2
	Exit gas velocity (m/sec)	5
	Exit gas temperature (Kelvin)	300
Area (fugitive)	Release height (m)	3.05
	Length (m)	10
	Width (m)	10
	Angle (°)	0

Note that the risk calculations were not completed at one facility, due to its U.S. Virgin Islands location and the population values being 0 in HEM's census files (see Table_Apx B-6). This facility was only in the 2020 Form R modeling.

Table_Apx B-6. Facilities Not Modeled for Risks

TRI Facility ID	Notes
00851HSSLVLIMET	The AERMOD run completed and concentration results were reported out. However, the risk calculations did not complete (HEM recorded it as a "skipped facility"), apparently due to there being no population values above 0 in vicinity. This is a U.S. Virgin Islands location. Although HEM's census library contains information on the Islands, all the population values are 0. HEM's risk evaluations at census locations may not operate correctly if all locations have 0 people.

When a HEM run completed, EPA also ran the model's risk summary reports that produce outputs which account for impacts on the same receptor from multiple neighboring facilities. The Agency also ran the demographics assessment which summarizes modeled impacts by various socioeconomic factors. EPA assumes that the skipped facility was not included in these aggregations; thus, these were temporarily remove the skipped facility from the 2020 Form R output folder to ensure successful completion of the demographics assessment.

HEM calculated risks using a cancer unit risk estimate (URE) of 4.4×10^{-6} $(\mu g/m^3)^{-1}$ for this set of modeling) and a chronic non-cancer reference concentration (RfC) of 0.002 mg/m^3 for reproductive hazards (from EPA's Integrated Risk Information System, IRIS.)

B.2 HEM Results

Table_Apx B-7. HEM TRI 2016–2021 95th Percentile Modeled Concentrations across All Distances by OESs and COUs

Life Cycle Stage	Category	Subcategory	OES	TRI Facilities	Stat	Ambient Concentration Across Facilities within OES by Distance from All Sources (m) (Based on 95th Percentile Modeled Concentrations µg/m^3)												
						10	**30**	**30-60**	**60**	**100**	**100–1,000**	**1,000**	**2,500**	**5,000**	**10,000**	**15,000**	**25,000**	**50,000**
Manufacture	Import	Import	Manufacturing	40	Max	1.2E02	2.0E02	1.6E02	1.1E02	7.8E01	1.3E01	4.6E00	1.4E00	5.4E−01	2.0E−01	1.1E−01	5.5E−02	1.9E−02
					Mean	2.19E01	3.94E01	3.03E01	2.13E01	1.20E01	1.91E00	5.97E−01	1.59E−01	5.86E−02	2.12E−02	1.17E−02	5.49E−03	1.99E−03
					Median	4.07E00	8.61E00	6.73E00	5.04E00	3.29E00	5.74E−01	1.61E−01	5.65E−02	2.16E−02	8.23E−03	4.61E−03	2.15E−03	7.54E−04
					Min	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00
Processing	Processing as a reactant	Other: monomer used in polymerization process in: plastic material and resin manufacturing; manufacturing synthetic rubber and plastics	Plastics and rubber compounding	33	Max	2.9E02	3.8E02	2.7E02	1.9E02	9.1E01	7.3E00	2.1E00	4.9E−01	1.7E−01	5.5E−02	2.9E−02	1.3E−02	4.3E−03
					Mean	3.26E01	4.45E01	3.34E01	2.28E01	1.10E01	1.23E00	3.18E−01	7.65E−02	2.63E−02	9.24E−03	4.99E−03	2.31E−03	8.24E−04
					Median	4.27E00	1.14E01	8.99E00	6.31E00	3.40E00	4.85E−01	1.28E−01	3.07E−02	1.04E−02	3.62E−03	1.92E−03	8.52E−04	3.05E−04
					Min	2.75E−09	4.19E−06	1.79E−04	3.30E−04	8.33E−04	3.61E−04	1.42E−04	3.85E−05	1.37E−05	5.09E−06	2.82E−06	1.31E−06	4.69E−07
Processing	Processing – incorporation into article	Other: Polymer in: Rubber and plastic product manufacturing	Plastics and rubber converting	1	Max	2.9E−12	3.0E−07	3.7E−07	4.1E−07	5.3E−07	1.5E−07	4.3E−08	1.9E−08	8.4E−09	3.6E−09	2.0E−09	1.0E−09	3.6E−10
					Mean	2.95E−12	3.02E−07	3.71E−07	4.13E−07	5.26E−07	1.45E−07	4.30E−08	1.87E−08	8.37E−09	3.55E−09	2.03E−09	9.98E−10	3.62E−10
					Median	2.95E−12	3.02E−07	3.71E−07	4.13E−07	5.26E−07	1.45E−07	4.30E−08	1.87E−08	8.37E−09	3.55E−09	2.03E−09	9.98E−10	3.62E−10
					Min	2.95E−12	3.02E−07	3.71E−07	4.13E−07	5.26E−07	1.45E−07	4.30E−08	1.87E−08	8.37E−09	3.55E−09	2.03E−09	9.98E−10	3.62E−10
Processing	Processing – incorporation into formulation, mixture, or reaction product	Processing aids, not otherwise listed in: Petrochemical manufacturing	Processing - incorporation into formulation, mixture, or reaction product	53	Max	1.5E01	3.9E01	3.3E01	2.4E01	1.7E01	6.6E00	3.1E00	8.6E−01	3.3E−01	1.2E−01	6.5E−02	3.0E−02	1.1E−02
					Mean	1.52E00	2.91E00	2.31E00	1.61E00	1.04E00	2.09E−01	7.95E−02	2.18E−02	8.22E−03	2.98E−03	1.64E−03	7.28E−04	2.67E−04
					Median	8.63E−02	2.09E−01	1.87E−01	1.59E−01	1.32E−01	1.87E−02	5.59E−03	1.72E−03	5.69E−04	2.15E−04	1.20E−04	4.78E−05	1.67E−05
					Min	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00

Life Cycle Stage	Category	Subcategory	OES	TRI Facilities	Stat	Ambient Concentration Across Facilities within OES by Distance from All Sources (m) (Based on 95th Percentile Modeled Concentrations µg/m³)												
						10	30	30-60	60	100	100–1,000	1,000	2,500	5,000	10,000	15,000	25,000	50,000
Processing	Processing as a reactant	Intermediate in: adhesive manufacturing; all other basic organic chemical manufacturing; fuel binder for solid rocket fuels; organic fiber manufacturing; petrochemical manufacturing; petroleum refineries; plastic material and resin manufacturing; propellant manufacturing; synthetic rubber manufacturing; wholesale and retail trade	Processing as a reactant	57	Max	8.3E01	1.2E02	1.1E02	7.1E01	3.0E01	3.0E00	7.7E−01	1.8E−01	6.2E−02	2.1E−02	1.1E−02	5.0E−03	1.8E−03
					Mean	6.16E00	1.01E01	8.10E00	5.56E00	2.75E00	3.12E−01	8.65E−02	2.20E−02	7.75E−03	2.75E−03	1.50E−03	6.96E−04	2.54E−04
					Median	7.93E−01	1.54E00	1.11E00	7.41E−01	4.08E−01	6.38E−02	1.70E−02	4.23E−03	1.25E−03	4.19E−04	2.18E−04	9.87E−05	3.56E−05
					Min	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00
Disposal	Disposal	Disposal	Recycling	11	Max	1.4E00	2.3E00	2.0E00	1.4E00	7.1E−01	8.5E−02	2.2E−02	5.3E−03	2.1E−03	7.1E−04	3.6E−04	1.5E−04	5.5E−05
					Mean	3.58E−01	7.62E−01	6.34E−01	4.84E−01	2.60E−01	3.24E−02	9.19E−03	2.21E−03	7.49E−04	2.53E−04	1.36E−04	5.77E−05	2.07E−05
					Median	1.26E−01	4.18E−01	3.50E−01	2.56E−01	1.90E−01	2.33E−02	6.12E−03	1.47E−03	4.66E−04	1.63E−04	1.28E−04	5.19E−05	1.84E−05
					Min	4.35E−09	1.09E−04	5.04E−04	7.07E−04	1.23E−03	3.00E−04	1.48E−04	5.19E−05	1.77E−05	5.94E−06	3.00E−06	1.28E−06	5.29E−07
Manufacturing	Import	Import	Repackaging	23	Max	6.2E01	9.3E01	6.6E01	4.2E01	2.0E01	2.4E00	5.1E−01	1.2E−01	4.1E−02	1.4E−02	7.6E−03	3.4E−03	1.2E−03
					Mean	4.78E00	8.78E00	6.23E00	4.19E00	2.08E00	2.11E−01	6.10E−02	1.46E−02	5.03E−03	1.74E−03	9.29E−04	4.21E−04	1.46E−04
Processing	Repackaging	Intermediate in: wholesale and retail trade			Median	1.90E−01	5.56E−01	3.87E−01	2.09E−01	9.16E−02	1.43E−02	3.19E−03	8.32E−04	3.05E−04	1.04E−04	5.71E−05	2.81E−05	1.02E−05
					Min	8.97E−10	8.10E−07	2.34E−04	2.19E−04	1.38E−04	3.41E−05	1.40E−05	5.60E−06	1.86E−06	6.24E−07	3.20E−07	1.57E−07	5.69E−08
Disposal	Disposal	Disposal	Waste handling, disposal, treatment, and recycling	7	Max	4.9E−01	7.3E−01	6.0E−01	3.8E−01	1.8E−01	2.1E−02	6.9E−03	2.0E−03	7.5E−04	2.6E−04	1.4E−04	6.6E−05	2.4E−05
					Mean	7.45E−02	1.17E−01	9.78E−02	6.59E−02	3.97E−02	5.07E−03	1.57E−03	4.10E−04	1.48E−04	5.08E−05	2.74E−05	1.25E−05	4.43E−06
					Median	6.78E−03	5.75E−03	4.51E−03	2.60E−03	1.34E−03	3.47E−04	1.18E−04	3.06E−05	1.07E−05	3.68E−06	1.94E−06	8.75E−07	3.06E−07
					Min	2.59E−08	2.06E−05	3.78E−04	4.76E−04	2.85E−04	3.05E−05	8.34E−06	2.88E−06	1.19E−06	5.15E−07	3.30E−07	1.68E−07	6.01E−08

Life Cycle Stage	Category	Subcategory	OES	TRI Facilities	Stat	Ambient Concentration Across Facilities within OES by Distance from All Sources (m) (Based on 95th Percentile Modeled Concentrations µg/m^3)												
						10	30	30-60	60	100	100–1,000	1,000	2,500	5,000	10,000	15,000	25,000	50,000
			Total	**225**														

Table_Apx B-8. HEM TRI 2016–2021 50th Percentile Modeled Concentrations across All Distances by OESs and COUs

Life Cycle Stage	Category	Subcategory	OES	TRI Facilities	Stat	Ambient Concentration Across Facilities within OES by Distance from All Sources (m) (Based on 50th Percentile Modeled Concentrations µg/m^3)												
						10	30	30-60	60	100	100–1,000	1,000	2,500	5,000	10,000	15,000	25,000	50,000
Manufacture	Import	Import	Manufacturing	40	Max	1.2E02	2.0E02	1.6E02	1.1E02	7.8E01	1.3E01	4.6E00	1.4E00	5.4E−01	2.0E−01	1.1E−01	5.5E−02	1.9E−02
					Mean	2.19E01	3.94E01	3.03E01	2.13E01	1.20E01	1.91E00	5.97E−01	1.59E−01	5.86E−02	2.12E−02	1.17E−02	5.49E−03	1.99E−03
					Median	4.07E00	8.61E00	6.73E00	5.04E00	3.29E00	5.74E−01	1.61E−01	5.65E−02	2.16E−02	8.23E−03	4.61E−03	2.15E−03	7.54E−04
					Min	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00
Processing	Processing as a reactant	Other: monomer used in polymerization process in: plastic material and resin manufacturing; manufacturing synthetic rubber and plastics	Plastics and rubber compounding	33	Max	2.9E02	3.8E02	2.7E02	1.9E02	9.1E01	7.3E00	2.1E00	4.9E−01	1.7E−01	5.5E−02	2.9E−02	1.3E−02	4.3E−03
					Mean	3.26E01	4.45E01	3.34E01	2.28E01	1.10E01	1.23E00	3.18E−01	7.65E−02	2.63E−02	9.24E−03	4.99E−03	2.31E−03	8.24E−04
					Median	4.27E00	1.14E01	8.99E00	6.31E00	3.40E00	4.85E−01	1.28E−01	3.07E−02	1.04E−02	3.62E−03	1.92E−03	8.52E−04	3.05E−04
					Min	2.75E−09	4.19E−06	1.79E−04	3.30E−04	8.33E−04	3.61E−04	1.42E−04	3.85E−05	1.37E−05	5.09E−06	2.82E−06	1.31E−06	4.69E−07
Processing	Processing – incorporation into article	Other: polymer in: rubber and plastic product manufacturing	Plastics and rubber converting	1	Max	2.9E−12	3.0E−07	3.7E−07	4.1E−07	5.3E−07	1.5E−07	4.3E−08	1.9E−08	8.4E−09	3.6E−09	2.0E−09	1.0E−09	3.6E−10
					Mean	2.95E−12	3.02E−07	3.71E−07	4.13E−07	5.26E−07	1.45E−07	4.30E−08	1.87E−08	8.37E−09	3.55E−09	2.03E−09	9.98E−10	3.62E−10
					Median	2.95E−12	3.02E−07	3.71E−07	4.13E−07	5.26E−07	1.45E−07	4.30E−08	1.87E−08	8.37E−09	3.55E−09	2.03E−09	9.98E−10	3.62E−10
					Min	2.95E−12	3.02E−07	3.71E−07	4.13E−07	5.26E−07	1.45E−07	4.30E−08	1.87E−08	8.37E−09	3.55E−09	2.03E−09	9.98E−10	3.62E−10

Life Cycle Stage	Category	Subcategory	OES	TRI Facilities	Stat	Ambient Concentration Across Facilities within OES by Distance from All Sources (m)												
						(Based on 50th Percentile Modeled Concentrations μg/m³)												
						10	**30**	**30-60**	**60**	**100**	**100–1,000**	**1,000**	**2,500**	**5,000**	**10,000**	**15,000**	**25,000**	**50,000**
Processing	Processing – incorpo-ration into formul-ation, mixture, or reaction product	Processing aids, not otherwise listed in: petrochemical manufacturing	Processing - incorporation into formulation, mixture, or reaction product	53	Max	1.5E01	3.9E01	3.3E01	2.4E01	1.7E01	6.6E00	3.1E00	8.6E−01	3.3E−01	1.2E−01	6.5E−02	3.0E−02	1.1E−02
					Mean	1.52E00	2.91E00	2.31E00	1.61E00	1.04E00	2.09E−01	7.95E−02	2.18E−02	8.22E−03	2.98E−03	1.64E−03	7.28E−04	2.67E−04
					Median	8.63E−02	2.09E−01	1.87E−01	1.59E−01	1.32E−01	1.87E−02	5.59E−03	1.72E−03	5.69E−04	2.15E−04	1.20E−04	4.78E−05	1.67E−05
					Min	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00
Processing	Processing as a reactant	Intermediate in: adhesive manufacturing; all other basic organic chemical manufacturing; fuel binder for solid rocket fuels; organic fiber manufacturing; petrochemical manufacturing; petroleum refineries; plastic material and resin manufacturing; propellant manufacturing; synthetic rubber manufacturing; wholesale and retail trade	Processing as a reactant	57	Max	8.3E01	1.2E02	1.1E02	7.1E01	3.0E01	3.0E00	7.7E−01	1.8E−01	6.2E−02	2.1E−02	1.1E−02	5.0E−03	1.8E−03
					Mean	6.16E00	1.01E01	8.10E00	5.56E00	2.75E00	3.12E−01	8.65E−02	2.20E−02	7.75E−03	2.75E−03	1.50E−03	6.96E−04	2.54E−04
					Median	7.93E−01	1.54E00	1.11E00	7.41E−01	4.08E−01	6.38E−02	1.70E−02	4.23E−03	1.25E−03	4.19E−04	2.18E−04	9.87E−05	3.56E−05
					Min	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00	0.00E00
Disposal	Disposal	Disposal	Recycling	11	Max	1.4E00	2.3E00	2.0E00	1.4E00	7.1E−01	8.5E−02	2.2E−02	5.3E−03	2.1E−03	7.1E−04	3.6E−04	1.5E−04	5.5E−05
					Mean	3.58E−01	7.62E−01	6.34E−01	4.84E−01	2.60E−01	3.24E−02	9.19E−03	2.21E−03	7.49E−04	2.53E−04	1.36E−04	5.77E−05	2.07E−05
					Median	1.26E−01	4.18E−01	3.50E−01	2.56E−01	1.90E−01	2.33E−02	6.12E−03	1.47E−03	4.66E−04	1.63E−04	1.28E−04	5.19E−05	1.84E−05
					Min	4.35E−09	1.09E−04	5.04E−04	7.07E−04	1.23E−03	3.00E−04	1.48E−04	5.19E−05	1.77E−05	5.94E−06	3.00E−06	1.28E−06	5.29E−07

Life Cycle Stage	Category	Subcategory	OES	TRI Facilities	Stat	Ambient Concentration Across Facilities within OES by Distance from All Sources (m) (Based on 50th Percentile Modeled Concentrations μg/m^3)												
						10	30	30-60	60	100	100–1,000	1,000	2,500	5,000	10,000	15,000	25,000	50,000
Manufacturing	Import	Import	Repackaging	23	Max	6.2E01	9.3E01	6.6E01	4.2E01	2.0E01	2.4E00	5.1E−01	1.2E−01	4.1E−02	1.4E−02	7.6E−03	3.4E−03	1.2E−03
					Mean	4.78E00	8.78E00	6.23E00	4.19E00	2.08E00	2.11E−01	6.10E−02	1.46E−02	5.03E−03	1.74E−03	9.29E−04	4.21E−04	1.46E−04
Processing	Repackaging	Intermediate in: Wholesale and retail trade			Median	1.90E−01	5.56E−01	3.87E−01	2.09E−01	9.16E−02	1.43E−02	3.19E−03	8.32E−04	3.05E−04	1.04E−04	5.71E−05	2.81E−05	1.02E−05
					Min	8.97E−10	8.10E−07	2.34E−04	2.19E−04	1.38E−04	3.41E−05	1.40E−05	5.60E−06	1.86E−06	6.24E−07	3.20E−07	1.57E−07	5.69E−08
Disposal	Disposal	Disposal	Waste handling, disposal, treatment, and recycling	7	Max	4.9E−01	7.3E−01	6.0E−01	3.8E−01	1.8E−01	2.1E−02	6.9E−03	2.0E−03	7.5E−04	2.6E−04	1.4E−04	6.6E−05	2.4E−05
					Mean	7.45E−02	1.17E−01	9.78E−02	6.59E−02	3.97E−02	5.07E−03	1.57E−03	4.10E−04	1.48E−04	5.08E−05	2.74E−05	1.25E−05	4.43E−06
					Median	6.78E−03	5.75E−03	4.51E−03	2.60E−03	1.34E−03	3.47E−04	1.18E−04	3.06E−05	1.07E−05	3.68E−06	1.94E−06	8.75E−07	3.06E−07
					Min	2.59E−08	2.06E−05	3.78E−04	4.76E−04	2.85E−04	3.05E−05	8.34E−06	2.88E−06	1.19E−06	5.15E−07	3.30E−07	1.68E−07	6.01E−08
			Total	225														