**United States**
**Environmental Protection Agency**

**Office of Chemical Safety and**
**Pollution Prevention**

# User's Guide:
# Integrated Indoor-Outdoor Air Calculator

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# 1 Introduction

## 1.1 Overview and Purpose

The EPA Office of Pollution Prevention and Toxics (OPPT) assesses a wide variety of chemical substances that are released to air from facility (stack, incinerator, and fugitive), area soil, and area water sources. In addition to existing chemicals, OPPT must also assess air emissions for new chemical submissions. Site-specific information is often not known when assessing new chemical submissions. For example, location, size, number of stacks, and/or incinerator characteristics may all be unknowns when modeling air concentrations and exposures stemming from facility releases. Therefore, a versatile approach was developed to estimate outdoor and indoor air concentrations, as well as particle deposition, resulting from air releases by distance from the source.

Thus, OPPT designed the Integrated Indoor-Outdoor Air Calculator (IIOAC), a user-friendly Excel-based tool that estimates indoor and outdoor air concentrations, as well as particle deposition, by distance, from chemical releases to air. IIOAC allows for different meteorological stations and local land cover, release durations, particle/vapor scenarios, urban/rural settings, and types of sources. Releases may occur through facility (stack, incinerator, and fugitive), area soil, and area water sources. Daily-averaged and annual-averaged air concentrations are used to estimate chemical exposure doses. IIOAC was developed to process multiple scenarios from multiple sources at once; the tool allows for intermittent releases and variation in meteorological conditions to account for potential variability in exposure conditions. OPPT reviewed available air modeling applications and determined that a tool meeting these needs is not currently available (see Section 2).

IIOAC is able to quickly process new and existing chemicals from multiple sources and multiple releases for release and exposure potential. The tool uses pre-run results from a suite of AERMOD dispersion scenarios run in a variety of meteorological and land-use settings. AERMOD is a modeling system comprised of several modeling routines that work together to estimate time-average air concentrations and deposition rates around emissions sources. AERMOD is fully promulgated as a replacement to the Industrial Source Complex (ISC3) Dispersion Models, in accordance with the Revisions to the Guideline on Air Quality Models (US EPA, 2017d).

This user's guide describes OPPT's development of IIOAC. The guide is intended to allow a user to:

1. Learn how to use IIOAC, and
2. Thoroughly understand the modeling approaches and input parameters to aid with output interpretation.

Sections 2 and 3 provide an overview of existing model applications and a description of IIOAC. Section 4 uses screen shots and instructions to teach the user how to simulate various combinations of exposure scenarios. Sections 5 through 11 document modeling inputs and approaches, including how the AERMOD model was configured, how ambient air concentrations are estimated for different release types, how indoor concentrations are estimated from ambient concentrations, and how doses are calculated. Section 12 provides an example application of IIOAC. Finally, Section 13 discusses remaining uncertainties in and potential updates to the model.

## 1.2 Acknowledgements and Disclaimer

This work was conducted under work assignment 4-53 of EPA's contract EP-W-12-010 with ICF.

*The views expressed in this report do not represent the policies of the U.S. Environmental Protection Agency. Mention of trade names of commercial products should not be interpreted as an endorsement by the U.S. Environmental Protection Agency*

# 2 Available Air Modeling Tools

The primary component of IIOAC is the use of AERMOD to simulate the transport of a pollutant to receptors. As part of the overall design effort, available EPA air modeling tools were reviewed. A brief summary of each is provided in this section along with a discussion of other applications of these models for exposure assessment.

## 2.1 ISC3, AERSCREEN, and SCREEN3

ISC3 is a steady-state Gaussian plume model that evaluates pollutant concentrations from a range of different industrial sources while accounting for: settling and dry deposition of particles; downwash; volume, area, point, and line sources; plume rise; point source separation; and limited terrain adjustment. ISC3 operates in short-term (ISCST3) and long-term (ISCLT3) modes, and both operate under the same assumptions but require different meteorological data. ISCST3 tends to be overly conservative in stable conditions, but performs somewhat better under neutral conditions (US EPA, 1995b).

SCREEN3 and AERSCREEN are simplistic models that quickly estimate worst-case air concentrations using a limited set of inputs. SCREEN3 is a screening version of ISC3 and is incorporated into E-FAST 2.0. AERSCREEN is a screening version of AERMOD. They create random combinations of meteorological parameters that are not site-specific and that are used in order to identify the combinations of parameters that lead to worst-case air concentrations in the modeling. SCREEN3 and AERSCREEN do not calculate deposition, and their outputs do not include a variety of averaging times that the user might be interested in (US EPA 1995a; US EPA 2016a).

## 2.2 AERMOD

OPPT's recommended modeling system for steady-state air quality dispersion is AERMOD, a Gaussian plume dispersion model based on planetary boundary layer principles. The AERMOD modeling system is comprised of several modeling routines that work together to estimate time-average air concentrations and deposition rates around emission sources. AERMOD can incorporate a variety of emission source characteristics, chemical deposition properties, complex terrain, and site-specific hourly meteorology to estimate air concentrations and deposition amounts at user-specified receptors and at a variety of averaging times. AERMOD is fully promulgated as a replacement to ISC3, in accordance with the Revisions to the Guideline on Air Quality Models (US EPA, 2017c).

## 2.3 Air Modeling Applications

The air models described above have been used in various applications to estimate chemical releases to various media. A brief description of three applications is provided below, with a comparison of the applications in Table 1. Two additional tools, the Volatilization algorithm in the Pesticide in Water Calculator (PWC) and European Union System for the Evaluation of Substances (EUSES), were also included as they estimate air concentration due to chemical release; however, these two tools do not use the air models described above.

- **Risk-Screening Environmental Indicators (RSEI)** (US EPA, 2017a): EPA's RSEI tool is a screening tool that incorporates risk-related perspective to quickly assess the potential health and environmental impacts from industrial chemical releases. RSEI uses AERMOD to estimate air concentrations from stack and fugitive releases to air, given source parameters and meteorological input data. These air concentrations are used to calculate doses, which can be translated into a risk-related score when population data and toxicity weights are accounted for. RSEI scores are used for comparison purposes to rank and prioritize chemicals and industry sectors. Values calculated from RSEI are only meaningful when compared to other values produced from RSEI.
- **Exposure and Fate Assessment Screening Tool (E-FAST)** (Versar, Inc., 2007): EPA's E-FAST is a screening-level tool that estimates industrial and household chemical releases to air, water, and land, and uses these values to calculate inhalation and ingestion exposure. E-FAST uses SCREEN3 to model air concentrations from stack and fugitive sources, given release information and meteorological parameters. The estimated air concentrations are then used to calculate inhalation acute and chronic exposure doses for individuals who breathe the air containing the chemical.
- **Volatilization Screening Tool (VST)** (US EPA, 2014a): EPA's Volatilization Screening Tool estimates air concentrations downwind of fields treated with semi-volatile pesticides using pre-run AERSCREEN results. The inputs of the tool are application rates of chemical onto soil and meteorological and land surface input parameters to estimate downwind air concentrations. The Volatilization Screening Tool provides a fast estimate of values previously calculated by the resource-intensive Probabilistic Exposure and Risk model for FUMigants (PERFUM).

- **Volatilization algorithm in the Pesticide in Water Calculator (PWC)** (US EPA, 2015b): Within the EPA's PWC, the volatilization algorithm calculates the chemical release of land-applied pesticide to air and water. None of the air models described above are used; rather, the algorithm uses chemical parameters such as Henry's Law constant to calculate daily mass flux into air over a specified time period and is used for bare soil and pre-emergent applications of fumigant and conventional pesticides. The algorithm should not be used for foliar applications or for semi-volatile chemicals with Henry's law constant below $10^{-7}$ $\text{atm}\cdot\text{m}^3/\text{mol}$. Inhalation exposure due to vapor-phase concentrations cannot be evaluated as the daily average flux is not precise enough to capture spikes over short time scales.
- **European Union System for the Evaluation of Substances (EUSES)** (European Chemicals Agency, 2016): Developed by the European Commission, the EUSES tool is used to conduct environmental exposure assessments to industrial chemicals and biocides. EUSES follows Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) requirements, a European Union regulation. Air concentration is estimated using the Gaussian plume model Operational Priority Substance (OPS), along with chemical parameters such as vapor pressure and Henry's Law constant. EUSES uses multiple interactive forms to facilitate data entry to parameterize the chemical being released, the process releasing it, environmental parameters helping govern chemical fate and transport, and exposure parameters leading to estimates of chemical exposure and risk.

Table 1. Overview of existing air modeling applications.

| | | | **Air Modeling Application or Tool** | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | **IIOAC** | **RSEI** | **E-FAST** | **VST** | **PWC** | **EUSES** |
| **Features** | | | | | | | | |
| | Air Model | | AERMOD | AERMOD | SCREEN3 | AERSCREEN | n/a | OPS[a] |
| | Screening tool | | ✓ | ✓ | ✓ | ✓ | | |
| Inputs | Source types (Releasing to air) | Point | ✓ | ✓ | ✓ | | | ✓ |
| | | Fugitive | ✓ | ✓ | ✓ | | | ✓ |
| | | Area soil | ✓ | | | ✓ | ✓ | |
| | | Area water | ✓ | ✓ | | | | ✓ |
| | Source origins | Consumer products | | | ✓ | | | ✓ |
| | | Industrial activities | ✓ | ✓ | ✓ | | | ✓ |
| | Urban conditions considered | | ✓ | ✓ | ✓ | | | |
| | Particle phase considered | | ✓ | | | N/A | N/A | ✓ |
| | Intermittent releases possible | | ✓ | | | | | ✓ |
| | Atmospheric transformation considered | | | ✓ | | | | ✓ |
| | Terrain considered | | | ✓ | ✓ | ✓<br>Only simple, uniform terrain | ✓ | |
| | Choice of meteorology conditions | | ✓ | ✓ | ✓ | | ✓ | |
| | Choice of land cover conditions | | ✓<br>By selecting different meteorology sites | ✓ | ✓ | | | |
| | Building downwash considered | | | | ✓ | | ✓<br>Exposure to runoff and leaching | |

|  |  |  | Air Modeling Application or Tool |  |  |  |  |  |
|---|---|---|---|---|---|---|---|---|
|  |  |  | **IIOAC** | **RSEI** | **E-FAST** | **VST** | **PWC** | **EUSES** |
|  | Multiple releases processed at once |  | ✓ |  | ✓ |  |  |  |
| Outputs | Conservative estimates |  |  | ✓ | ✓ | ✓ |  | ✓ |
|  | Deposition modeled |  | ✓ |  |  |  |  | ✓ |
|  | Outputs at different distances from source |  | ✓ | ✓ | ✓ | ✓ |  |  |
|  | Exposure doses calculated |  | ✓ |  | ✓ |  |  |  |
|  | Indoor air concentrations calculated |  | ✓ |  |  |  |  |  |
|  | Averaging periods used | 1-hr |  |  | ✓ | ✓ |  |  |
|  |  | Daily | ✓ |  |  |  | ✓ |  |
|  |  | Annual | ✓ | ✓ | ✓ |  |  | ✓ |

[a]: OPS = Operational Priority Substances

# 3 General Description of IIOAC

While there are a variety of tools to estimate air concentrations resulting from chemical releases, the comparison outlined in Table 1 shows the need for a tool that is able to quickly and simultaneously process multiple emission scenarios for multiple sources, while allowing for intermittent releases and variation in meteorological conditions. To meet this need, OPPT designed the IIOAC tool.

## 3.1 General Description

IIOAC is a tool that assesses the release to air and exposure potential for new and existing chemicals. A key feature of the tool is the grouping of inputs to define emission scenarios. An emission scenario is a collection of releases featuring one or multiple source types, each with different temporal patterns and emission rates. For each emission scenario, the tool provides output summarizing air concentrations, particle deposition, and exposure doses at different receptor distances for each source type. A general overview of the Excel-based tool is illustrated in Figure 1.

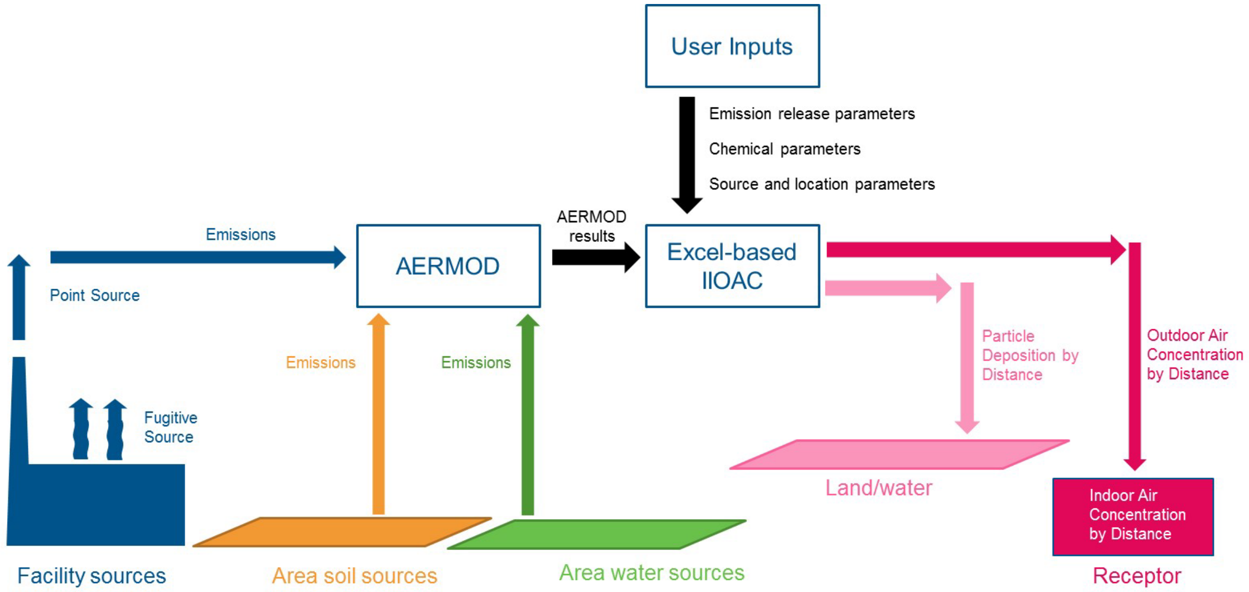


Figure 1. Schematic of the different components of IIOAC.

IIOAC considers releases from the following emission source types:

- Facility sources (point and fugitive) – point sources are defined as stack and incineration releases,
- Area soil sources, and
- Area water sources (batch and continuous-flow systems).

For each source type, a suite of generic AERMOD (version 16216r) runs have been designed and pre-run; the resulting air concentrations and particle depositions were post-processed in R and packaged into lookup tables as part of IIOAC (see Section 4.1 for downloading and operating IIOAC. Note, the zip file needs to be located in the same folder as IIOAC). Running the Excel-based IIOAC involves specifying emission scenario inputs so that the applicable AERMOD run is selected and the associated concentrations and depositions are adjusted to account for the particular emission rate and if applicable, area size. Three types of user inputs are required to characterize each emission scenario:

- Emission parameters: source type, emission rate, and number of releases per year,
- Chemical and system parameters: area source size or chemical-specific parameters, and
- Location parameters: facility parameters, climate region, urban/rural, and particle sizes.

Each of these types are explained in greater detail in Section 3.2.

IIOAC allows these inputs to be either imported via an input file or manually entered. IIOAC is currently designed to allow for up to a maximum of 100 release profiles (i.e., the combination of number of releases per year and the emission rate) per source type. Based on the user inputs, the tool will automatically calculate and display, for each emission scenario and at pre-defined receptor distances, the resulting outdoor and indoor air concentrations (by applying an indoor-outdoor ratio, see Section 10); particle deposition to surfaces; and acute and chronic dose at pre-defined life stages. An export feature is available that allows the user inputs and associated outputs to be saved into a separate Excel workbook.

## 3.2 User Inputs

### 3.2.1 Emission Parameters

For each site of interest, users have the option to import an Excel data file or manually input information on the emission source type, number of emission scenarios, number of releases per scenario, and for each release, the mass released per day and the number of release days.

Table 2 provides an example of user-defined emission scenarios and release profiles. In the example in Table 2, three types of emission scenarios occur and are given the following names: manufacturing, processing, and use. Multiple source types with multiple releases can occur for each emission scenario. For example, in the Use scenario, there are four different releases from both fugitive and area land sources. IIOAC can process all source types and emission scenarios at once and provide a summary of results as described in Section 3.3. Note the default release duration is 24 hours for all source types. However, the user has the option of selecting release durations of 1, 4, and 8 hours for point (stack, incinerators) and fugitive sources.

Table 2. Example of multiple emission scenarios entered by user for each site.

| Emission Scenario # | Emission Scenario | Source Type | Release # | Mass Released per Day (kg/day) | # of Release Days per Year |
|---|---|---|---|---|---|
| 1 | Manufacturing | Incineration | 1 | 100 | 5 |
| 1 | Manufacturing | Fugitive | 1 | 10 | 100 |
| 2 | Processing | Incineration | 1 | 50 | 12 |
| 2 | Processing | Incineration | 2 | 1 | 100 |
| 2 | Processing | Fugitive | 1 | 100 | 5 |
| 2 | Processing | Fugitive | 2 | 10 | 50 |
| 2 | Processing | Area Water | 1 | 1 | 250 |
| 2 | Processing | Area Water | 2 | 1 | 100 |
| 2 | Processing | Area Water | 3 | 0.1 | 250 |
| 2 | Processing | Area Water | 4 | 0.01 | 365 |
| 3 | Use | Fugitive | 1 | 1 | 5 |
| 3 | Use | Fugitive | 2 | 0.5 | 12 |
| 3 | Use | Fugitive | 3 | 0.25 | 100 |
| 3 | Use | Fugitive | 4 | 0.001 | 365 |
| 3 | Use | Area Soil | 1 | 100 | 1 |
| 3 | Use | Area Soil | 2 | 10 | 5 |
| 3 | Use | Area Soil | 3 | 1 | 12 |
| 3 | Use | Area Soil | 4 | 0.1 | 30 |

### 3.2.2 Chemical and System Parameters

Depending on the source type selected, the user will also be asked to enter chemical-specific and/or system-specific parameters. All emission scenarios with a given source type use the same system parameters. Table 3 outlines the required user inputs:

Table 3. Chemical and system-specific parameters required for IIOAC.

| User Input | Symbol | Source Type | | | | |
|---|---|---|---|---|---|---|
| | | Point | Fugitive | Soil | Water – Batch[a] | Water – Continuous flow[b] |
| System-specific parameters | | | | | | |
| (Surface) Area ($m^2$) | $A$ | | ✓ | ✓ | ✓ | ✓ |
| Depth of water (m) | $D$ | | | | ✓ | ✓ |
| Flowrate ($m^3$/day) | $Q$ | | | | | ✓ |
| Chemical-specific parameters | | | | | | |
| Vapor pressure (Torr) | $VP$ | | | ✓ | ✓ | ✓ |
| Solubility (mg/L) | $Sol$ | | | ✓ | | |
| Organic carbon sorption | $K_{oc}$ | | | ✓ | | |

|  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|
| coefficient (mL/g) |  |  |  |  |  |  |
| Volatilization half-life (1/day) | $t_{1/2}$ |  |  |  | ✓ | ✓ |
| Molecular weight (g/mol) |  |  |  | ✓ | ✓ | ✓ |

[a]: batch water sources are considered to be area water sources with no flow in or out of the system, e.g., lake, surface impoundment for wastewater, open tanks

[b]: continuous flow water sources have a constant flowrate in and out of the system, e.g., river, aeration tank in wastewater treatment process

### 3.2.3 Location Parameters

For each source type selected, Table 4 lists the location and deposition parameters that must be provided by the user. Further information on each of the inputs is described in Sections 5.3-5.5.

Table 4. Location parameters required for IIOAC.

| **User Input** | **Source Type** |  |  |  |  |
|---|---|---|---|---|---|
|  | **Point** | **Fugitive** | **Soil** | **Water – Batch[a]** | **Water – Continuous flow[b]** |
| Urban or rural setting | ✓ | ✓ | ✓ | ✓ | ✓ |
| Particle size or vapor | ✓ | ✓ |  |  |  |
| Climate region | ✓ | ✓ | ✓ | ✓ | ✓ |

[a]: batch water sources are considered to be area water sources with no flow in or out of the system, e.g., lake, surface impoundment for wastewater, open tanks

[b]: continuous flow water sources have a constant flowrate in and out of the system, e.g., river, aeration tank in wastewater treatment process

## 3.3 IIOAC Outputs

The meteorology data used in IIOAC varies hourly throughout the year and results in a wide range of air concentrations for a given set of emission inputs. As a result, for each emission scenario defined by the user, IIOAC will provide output metrics for two groups of receptors: inner ring or fenceline ring receptors, and near-facility community receptors. A description of these receptor groups, along with the number of receptors for each AERMOD run, are provided in Section 5.6.

For each group of receptors, the meteorology data is used to calculate the following parameters:

- Daily-averaged air concentration (i.e., hourly concentrations averaged over one day),
- Annual-averaged air concentration values (i.e., hourly concentrations averaged over one year), and
- Annual-averaged total annual particle deposition (wet and dry) (i.e., hourly deposition averaged over one year).

IIOAC then calculates and reports the central-tendency and high-end values, defined as the average (mean) and 95th percentile, respectively, of all values of the above three parameters.

While total annual particle deposition (total, wet, dry) is not used further in IIOAC, these results can be used as inputs to models that estimate soil and surface water concentrations.

In addition to air concentrations and particle deposition, the mean and high-end acute and chronic exposure doses are also calculated using the mean and high-end daily- and annual-averaged air concentrations (see Section 11). Exposure doses are provided for the following age groups:

- Young toddler (1- <2 years),
- Adult (16- <78 years), and
- Lifetime (0- <78 years) – calculated for chronic exposure doses only.

Table 5 provides an example IIOAC output for one run. Output metrics are calculated for each emission scenario. The stack and incinerator sources are aggregated into one source called point source. For fugitive and area sources, IIOAC outputs are calculated based on the user-specified area size. However, these outputs can be scaled to a different area size if needed, using regression coefficients in Appendix A.

Table 5. Example IIOAC output. Outputs for stack and incinerators are aggregated into point source. High-end values are defined as the 95th percentile.

| Source Type | Emission Scenario | Statistic | Location | Outdoor Air Concentration (µg/$m^3$) | | Indoor Air Concentration (µg/$m^3$) | | Deposition (g/$m^2$) | | | Acute Dose (mg/kg/day) | | Chronic Dose (mg/kg/day) | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | Daily | Annual | Daily | Annual | Tot | Wet | Dry | Young Toddler | Adult | Young Toddler | Adult | Lifetime |
| Point | Manufacturing | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| | Processing | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| | Use | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| Fugitive | Manufacturing | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| | Processing | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| | Use | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| Area Water | Manufacturing | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| | Processing | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| | Use | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| Area Soil | Manufacturing | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| | Processing | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |
| | Use | High-End & Mean | Fenceline | | | | | | | | | | | | |
| | | | Community | | | | | | | | | | | | |

# 4 Using IIOAC

## 4.1 Downloading and Operating IIOAC

To use IIOAC, two files **must be downloaded and saved to the same folder**. These are an Excel file containing the main program file (IIOAC_Locked_v1.0.xlsm), and a “zip” file (i.e., a file format commonly used for compression and transmission of large computer files) of pre-run AERMOD results (IIOAC_RunFiles.zip). **Files from the zip file should not be extracted and should remain within the zip file.** The user will not directly access the zip file; rather, the main program file will call on files within the zip file.

## 4.2 Hardware and Software Requirements for IIOAC

The hardware and software requirements to run IIOAC are listed below. Note that higher specifications will lead to increased performance and decreased runtime.

Hardware (Windows Vista Business Requirements):

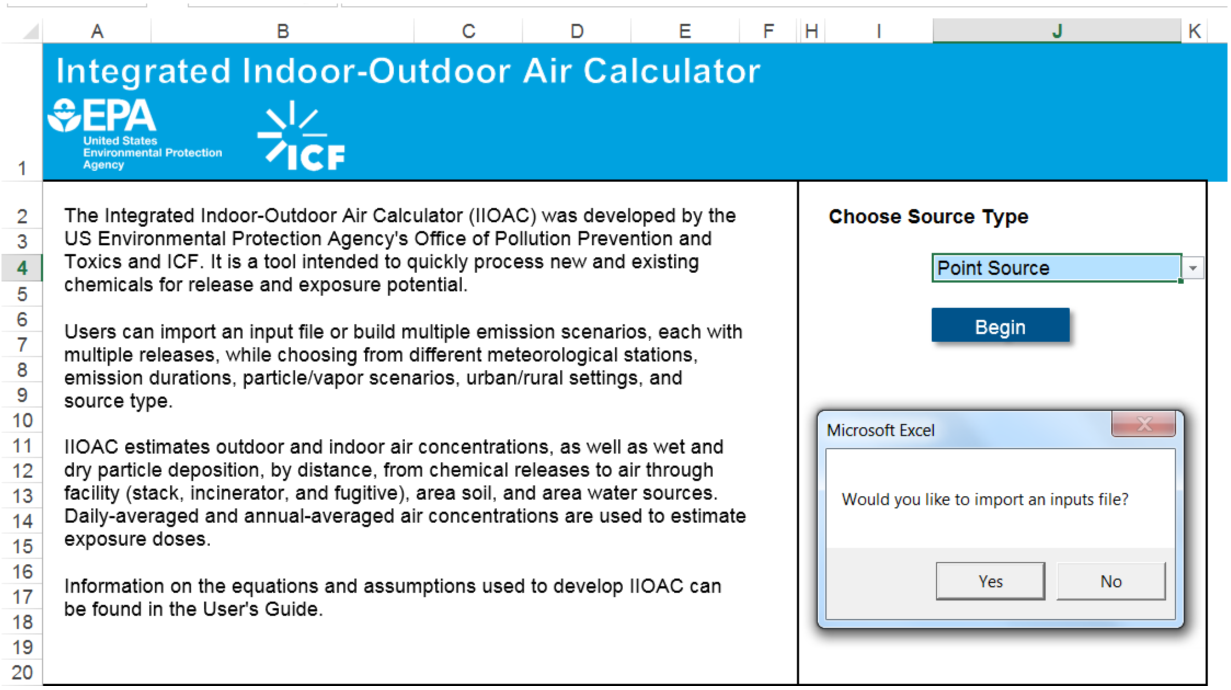
- 1-gigahertz (GHz) 32-bit (x86) processor or 1-GHz 64-bit (x64) processor,
- 1 GB of system memory, and
- 128 MB of graphic memory (minimum).

Software:

- Windows Operating System and
- MS Excel 2010 or greater.

## 4.3 Introduction Tab

In IIOAC, the **Introduction Tab** provides a general description of IIOAC and directs the user to choose a source type from the drop-down menu. The available options are: point source (stack or incineration), fugitive source, area soil source, area water source, and all sources (i.e., more than one type of source). After clicking **Begin**, the user has the option to import an input file or to manually enter scenario and release data (Figure 2).



Integrated Indoor-Outdoor Air Calculator

The Integrated Indoor-Outdoor Air Calculator (IIOAC) was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and ICF. It is a tool intended to quickly process new and existing chemicals for release and exposure potential.

Users can import an input file or build multiple emission scenarios, each with multiple releases, while choosing from different meteorological stations, emission durations, particle/vapor scenarios, urban/rural settings, and source type.

IIOAC estimates outdoor and indoor air concentrations, as well as wet and dry particle deposition, by distance, from chemical releases to air through facility (stack, incinerator, and fugitive), area soil, and area water sources. Daily-averaged and annual-averaged air concentrations are used to estimate exposure doses.

Information on the equations and assumptions used to develop IIOAC can be found in the User's Guide.

Choose Source Type: Point Source

Microsoft Excel

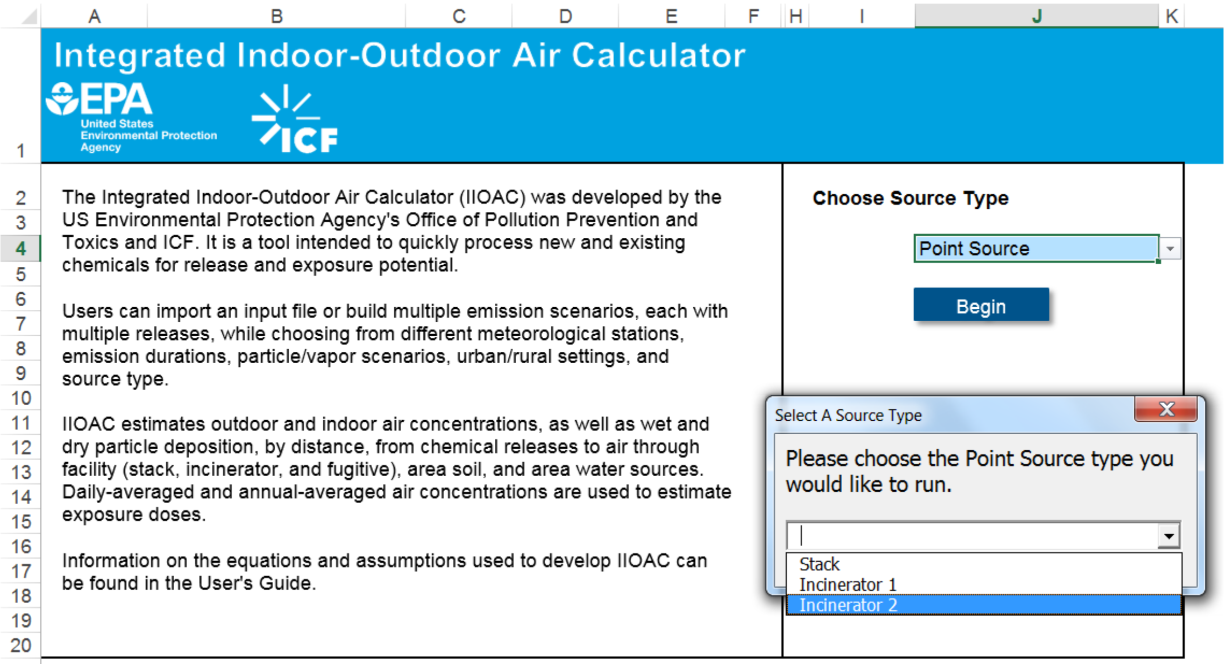
Would you like to import an inputs file?

Figure 2. Introduction Tab with the import file feature.

If the user chooses to import an input file, the input file must have column headers and the columns must be in the following order starting in column A:

- Scenario number: must be a whole number,
- Emission scenario: name or description of emission scenario,
- Source type: must be stack, fugitive, incineration, area soil, or area water (e.g., incinerator will not be recognized during the file import process),
- Release number: must be a whole number,
- Mass released per day, in kg/day: must be a number greater than zero, and
- Number of release days per year: must be a whole number between 1 and 365, inclusive.

For the source type of point source, if the user selects the import inputs file option, an additional window appears (Figure 3), asking the user to specify if the point source is a stack, or one of two possible incinerator options (see Section 5.2.1 for parameters corresponding to these three point sources). Once selected, data from the inputs file is auto-populated into the **Source Inputs Tab** (see Section 4.5) and the user is automatically directed to the **Chemical Tab**. Note that when importing a file, the source type 'incineration' must be used in the inputs file instead of 'incinerator'.



Integrated Indoor-Outdoor Air Calculator

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Information on the equations and assumptions used to develop IIOAC can be found in the User's Guide.

Choose Source Type

Please choose the Point Source type you would like to run.

Figure 3. Options for point source.

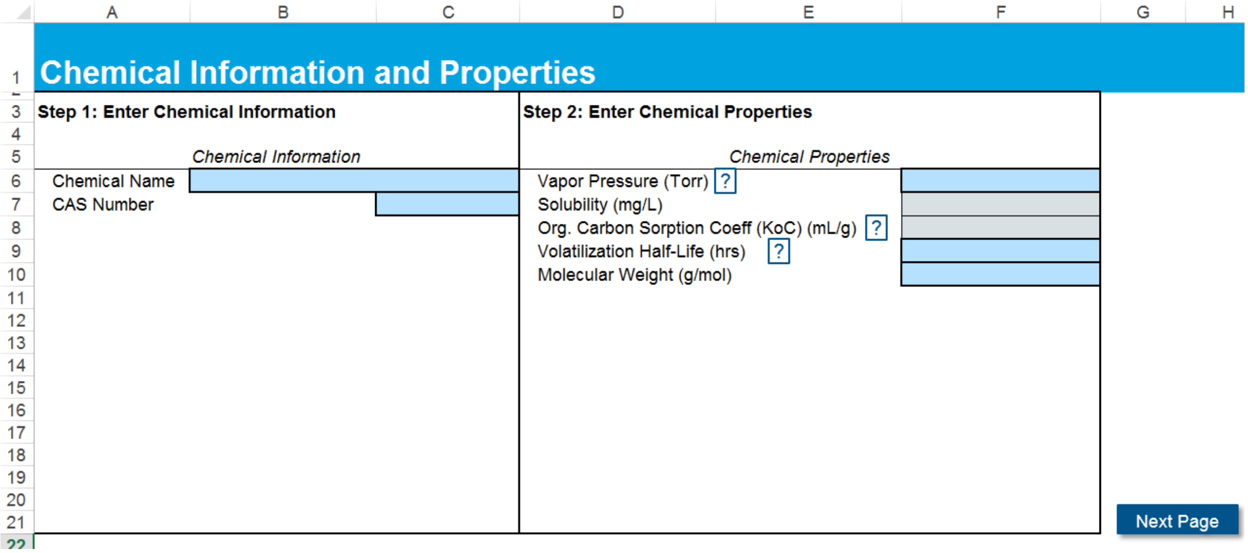
## 4.4 Chemical Tab

Depending on the source type selected, the user will be required to enter chemical-specific properties. In Figure 4, the boxes greyed out are not applicable to the source type and do not need to be filled in. For example, the source type selected in Figure 4 is for area water sources and therefore information on solubility and the organic carbon sorption coefficient are not needed. For the required information in blue boxes, IIOAC has built-in error messages if the user enters a value that is not valid (e.g., negative number for volatilization half-life). Question marks next to a chemical property provides additional information for the user. For example, the question mark next to vapor pressure provides the unit conversion from Torr to Pascal (Pa) or standard atmospheres (atm).

For volatilization half-life, the user can click on the question mark which leads to a pop-up window that provides a link to EPA's EPI Suite (US EPA, 2017b), a parameter estimation program. EPI Suite is a screening-level tool and should not be used if acceptable measured values are available. EPI Suite provides the following default values to estimate volatilization half-life:

- Water depth = 1 m (for both river and lake),
- Wind velocity = 5 m/s (river); 0.5 m/s (lake), and
- Current velocity = 1 m/s (river); 0.05 m/s (lake).

Volatilization half-life values are used in flux calculations for area water sources and should differ between batch and continuous-flow sources by entering a flowrate value of zero for batch sources.


Chemical Information and Properties

Step 1: Enter Chemical Information

*Chemical Information*

Chemical Name

CAS Number

Step 2: Enter Chemical Properties

*Chemical Properties*

Vapor Pressure (Torr)

Solubility (mg/L)

Org. Carbon Sorption Coeff (KoC) (mL/g)

Volatilization Half-Life (hrs)

Molecular Weight (g/mol)

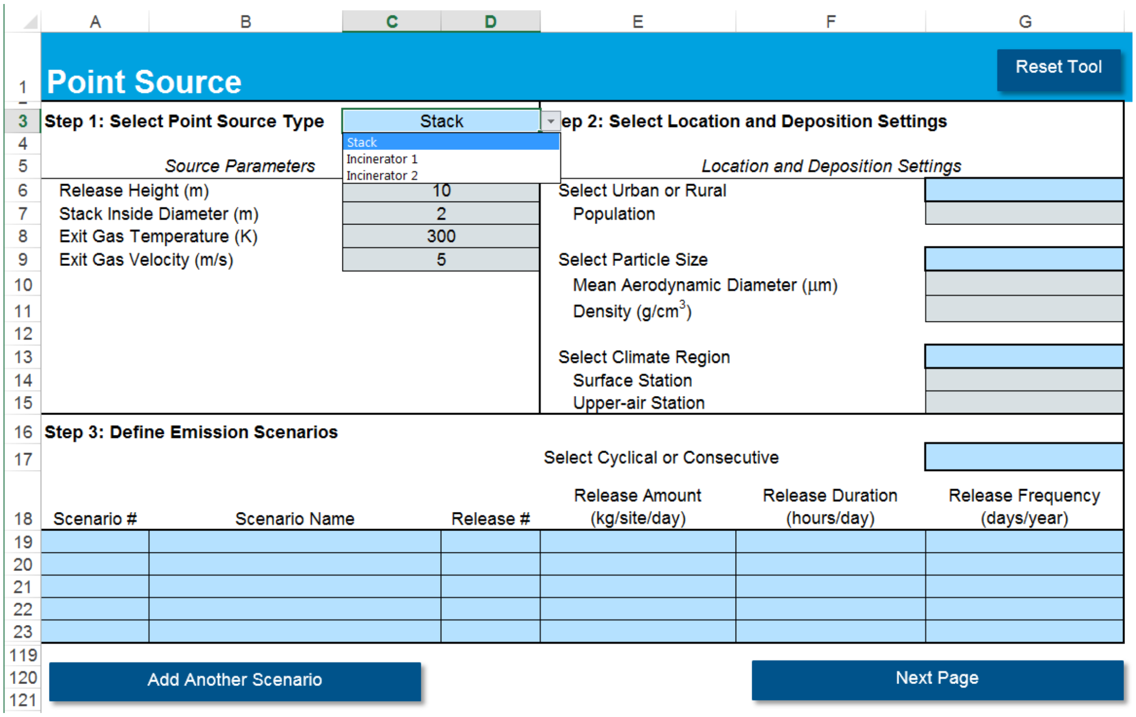
Figure 4. Chemical-specific properties required by IIOAC for area water sources.

## 4.5 Source Inputs Tab

IIOAC has a **Source Inputs Tab** for each source type, which varies slightly depending on the source type. In general, the **Source Inputs Tab** consists of three steps: (1) entering source parameters; (2) selecting location and deposition settings; and (3) defining emission scenarios. See Table 12 and Table 13 in Section 5 for full details on source parameters and location and deposition settings.

In step 1, the user is required to enter source parameters. Depending on the source type, these source parameters include area of source, and for area water sources, the surface area, depth of water, and flowrate. For point sources, if the user did not import an inputs file, the user must select the point source type (stack, incinerator 1, incinerator 2) from the drop-down menu, which will auto-populate the source parameters (see Figure 5).

For area water sources, the user can differentiate between batch and continuous-flow sources by specifying a flowrate value of zero for batch sources and a non-zero flowrate value for continuous-flow sources. The question mark next to the flowrate in IIOAC reminds the user of this differentiation (see Figure 6).



Point Source

Step 1: Select Point Source Type: Stack

Step 2: Select Location and Deposition Settings

| Source Parameters | |
|---|---|
| Release Height (m) | 10 |
| Stack Inside Diameter (m) | 2 |
| Exit Gas Temperature (K) | 300 |
| Exit Gas Velocity (m/s) | 5 |

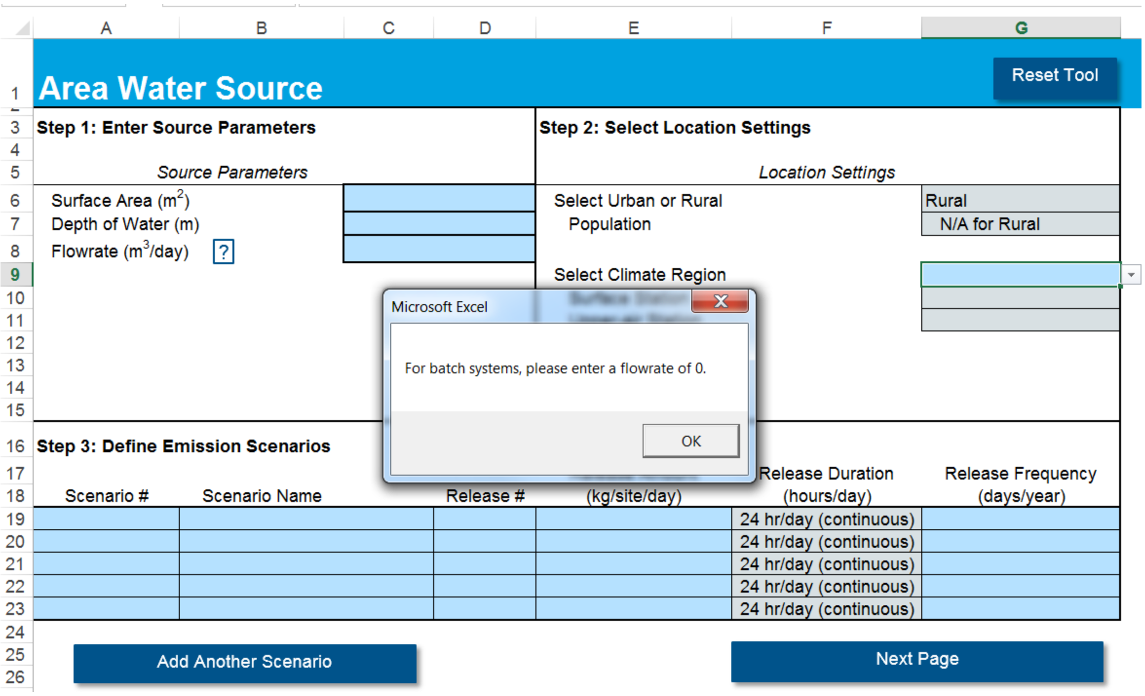
| Location and Deposition Settings | |
|---|---|
| Select Urban or Rural | |
| Population | |
| Select Particle Size | |
| Mean Aerodynamic Diameter (μm) | |
| Density (g/cm$^3$) | |
| Select Climate Region | |
| Surface Station | |
| Upper-air Station | |

Step 3: Define Emission Scenarios

Select Cyclical or Consecutive

| Scenario # | Scenario Name | Release # | Release Amount (kg/site/day) | Release Duration (hours/day) | Release Frequency (days/year) |
|---|---|---|---|---|---|
| | | | | | |
| | | | | | |
| | | | | | |
| | | | | | |
| | | | | | |

Figure 5. Example Source Inputs Tab for point sources when an input file is not imported.



Area Water Source

Step 1: Enter Source Parameters

Step 2: Select Location Settings

| Source Parameters | |
|---|---|
| Surface Area (m$^2$) | |
| Depth of Water (m) | |
| Flowrate (m$^3$/day) | |

| Location Settings | |
|---|---|
| Select Urban or Rural | Rural |
| Population | N/A for Rural |
| Select Climate Region | |

For batch systems, please enter a flowrate of 0.

Step 3: Define Emission Scenarios

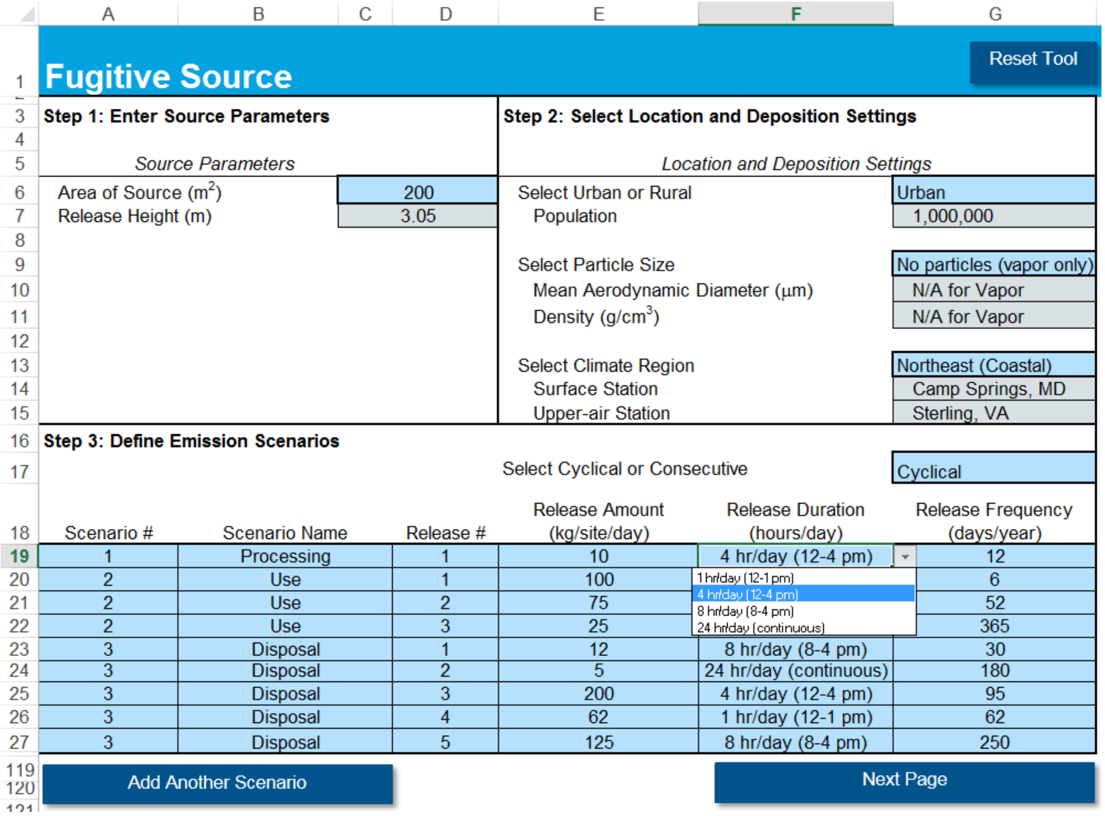
| Scenario # | Scenario Name | Release # | (kg/site/day) | Release Duration (hours/day) | Release Frequency (days/year) |
|---|---|---|---|---|---|
| | | | | 24 hr/day (continuous) | |
| | | | | 24 hr/day (continuous) | |
| | | | | 24 hr/day (continuous) | |
| | | | | 24 hr/day (continuous) | |
| | | | | 24 hr/day (continuous) | |

Figure 6. Information button for area water sources specifying that the user can define a batch system by entering a flowrate of zero.

In step 2, the user defines the location and deposition settings through a series of drop-down menus for population scenario (urban or rural), particle size (fine, coarse, or no particles), and climate region (14 possibilities). The choices offered in IIOAC for location and deposition settings are explained in further detail in Section 5. Blue boxes define what the user must select and the grey boxes are auto-populated based on the user's selection. Depending on what the user selects in this step, the tool will access the corresponding pre-run AERMOD results of air concentration and particle deposition from the zip file and import these results into the tool.

In step 3, defining emission scenarios, if the user imported an input file, the table in step 3 will already be auto-populated with a default release duration of 24 hours/day. The user can also manually change the release duration for point and fugitive sources (see Figure 7). If an input file was not imported, the user must manually enter the information. Additional scenarios can be added using the **Add Another Scenario** button, up to a total of 100 scenarios for each source type. For point and fugitive sources, step 3 has an additional feature of asking the user to select whether the releases in a scenario are cyclical (i.e., evenly spaced out over 365 days) or consecutive releases (i.e., consecutive days of release).

Note the default release duration is 24 hours for all source types. However, the user has the option of selecting release durations of 1, 4, and 8 hours for point (stack, incinerators) and fugitive sources.



Fugitive Source

Step 1: Enter Source Parameters

*Source Parameters*

Area of Source ($m^2$): 200
Release Height (m): 3.05

Step 2: Select Location and Deposition Settings

*Location and Deposition Settings*

Select Urban or Rural: Urban
Population: 1,000,000
Select Particle Size: No particles (vapor only)
Mean Aerodynamic Diameter (µm): N/A for Vapor
Density ($g/cm^3$): N/A for Vapor
Select Climate Region: Northeast (Coastal)
Surface Station: Camp Springs, MD
Upper-air Station: Sterling, VA

Step 3: Define Emission Scenarios

Select Cyclical or Consecutive: Cyclical

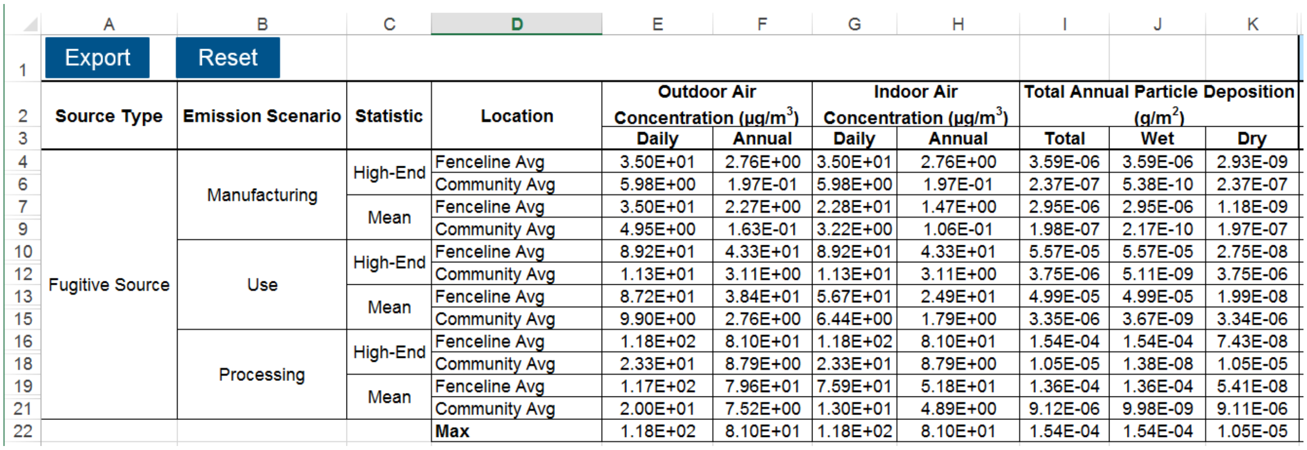
| Scenario # | Scenario Name | Release # | Release Amount (kg/site/day) | Release Duration (hours/day) | Release Frequency (days/year) |
|---|---|---|---|---|---|
| 1 | Processing | 1 | 10 | 4 hr/day (12-4 pm) | 12 |
| 2 | Use | 1 | 100 | | 6 |
| 2 | Use | 2 | 75 | | 52 |
| 2 | Use | 3 | 25 | | 365 |
| 3 | Disposal | 1 | 12 | 8 hr/day (8-4 pm) | 30 |
| 3 | Disposal | 2 | 5 | 24 hr/day (continuous) | 180 |
| 3 | Disposal | 3 | 200 | 4 hr/day (12-4 pm) | 95 |
| 3 | Disposal | 4 | 62 | 1 hr/day (12-1 pm) | 62 |
| 3 | Disposal | 5 | 125 | 8 hr/day (8-4 pm) | 250 |

Figure 7. Release duration options for point and fugitive sources.

For users that do not have specific source and/or location and deposition settings in mind, the default settings recommended to provide the conservative estimates for a given scenario (i.e., generally the largest values of air concentration or deposition amounts) are point (specifically stack) sources, urban settings, coarse particles, and climate region corresponding to Idaho Falls (East North Central). Further detail of default settings are provided in Section 5.7.

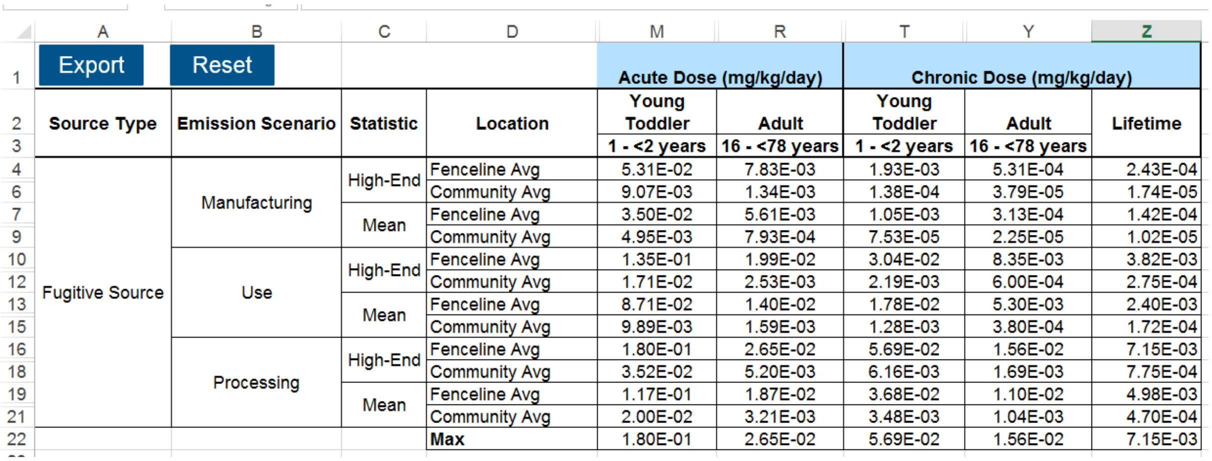
## 4.6 Output Tab

The **Output Tab** provides the outdoor, indoor, total annual particle deposition, and acute and chronic exposure doses (see Figure 8 and Figure 9) for each of the emission scenarios provided by the user. High-end and mean results are provided by receptor group (inner ring or fenceline receptors and near-facility community receptors). For area soil and area water sources, the particle deposition columns will be empty as these sources do not emit fine or coarse particles.



| Source Type | Emission Scenario | Statistic | Location | Outdoor Air Concentration (μg/m$^3$) | | Indoor Air Concentration (μg/m$^3$) | | Total Annual Particle Deposition (g/m$^2$) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | Daily | Annual | Daily | Annual | Total | Wet | Dry |
| Fugitive Source | Manufacturing | High-End | Fenceline Avg | 3.50E+01 | 2.76E+00 | 3.50E+01 | 2.76E+00 | 3.59E-06 | 3.59E-06 | 2.93E-09 |
| | | | Community Avg | 5.98E+00 | 1.97E-01 | 5.98E+00 | 1.97E-01 | 2.37E-07 | 5.38E-10 | 2.37E-07 |
| | | Mean | Fenceline Avg | 3.50E+01 | 2.27E+00 | 2.28E+01 | 1.47E+00 | 2.95E-06 | 2.95E-06 | 1.18E-09 |
| | | | Community Avg | 4.95E+00 | 1.63E-01 | 3.22E+00 | 1.06E-01 | 1.98E-07 | 2.17E-10 | 1.97E-07 |
| | Use | High-End | Fenceline Avg | 8.92E+01 | 4.33E+01 | 8.92E+01 | 4.33E+01 | 5.57E-05 | 5.57E-05 | 2.75E-08 |
| | | | Community Avg | 1.13E+01 | 3.11E+00 | 1.13E+01 | 3.11E+00 | 3.75E-06 | 5.11E-09 | 3.75E-06 |
| | | Mean | Fenceline Avg | 8.72E+01 | 3.84E+01 | 5.67E+01 | 2.49E+01 | 4.99E-05 | 4.99E-05 | 1.99E-08 |
| | | | Community Avg | 9.90E+00 | 2.76E+00 | 6.44E+00 | 1.79E+00 | 3.35E-06 | 3.67E-09 | 3.34E-06 |
| | Processing | High-End | Fenceline Avg | 1.18E+02 | 8.10E+01 | 1.18E+02 | 8.10E+01 | 1.54E-04 | 1.54E-04 | 7.43E-08 |
| | | | Community Avg | 2.33E+01 | 8.79E+00 | 2.33E+01 | 8.79E+00 | 1.05E-05 | 1.38E-08 | 1.05E-05 |
| | | Mean | Fenceline Avg | 1.17E+02 | 7.96E+01 | 7.59E+01 | 5.18E+01 | 1.36E-04 | 1.36E-04 | 5.41E-08 |
| | | | Community Avg | 2.00E+01 | 7.52E+00 | 1.30E+01 | 4.89E+00 | 9.12E-06 | 9.98E-09 | 9.11E-06 |
| | | | **Max** | 1.18E+02 | 8.10E+01 | 1.18E+02 | 8.10E+01 | 1.54E-04 | 1.54E-04 | 1.05E-05 |

Figure 8. IIOAC output metrics of outdoor air concentration, indoor air concentration, and total particle deposition.



| Source Type | Emission Scenario | Statistic | Location | Acute Dose (mg/kg/day) | | Chronic Dose (mg/kg/day) | | |
|---|---|---|---|---|---|---|---|---|
| | | | | Young Toddler 1 - <2 years | Adult 16 - <78 years | Young Toddler 1 - <2 years | Adult 16 - <78 years | Lifetime |
| Fugitive Source | Manufacturing | High-End | Fenceline Avg | 5.31E-02 | 7.83E-03 | 1.93E-03 | 5.31E-04 | 2.43E-04 |
| | | | Community Avg | 9.07E-03 | 1.34E-03 | 1.38E-04 | 3.79E-05 | 1.74E-05 |
| | | Mean | Fenceline Avg | 3.50E-02 | 5.61E-03 | 1.05E-03 | 3.13E-04 | 1.42E-04 |
| | | | Community Avg | 4.95E-03 | 7.93E-04 | 7.53E-05 | 2.25E-05 | 1.02E-05 |
| | Use | High-End | Fenceline Avg | 1.35E-01 | 1.99E-02 | 3.04E-02 | 8.35E-03 | 3.82E-03 |
| | | | Community Avg | 1.71E-02 | 2.53E-03 | 2.19E-03 | 6.00E-04 | 2.75E-04 |
| | | Mean | Fenceline Avg | 8.71E-02 | 1.40E-02 | 1.78E-02 | 5.30E-03 | 2.40E-03 |
| | | | Community Avg | 9.89E-03 | 1.59E-03 | 1.28E-03 | 3.80E-04 | 1.72E-04 |
| | Processing | High-End | Fenceline Avg | 1.80E-01 | 2.65E-02 | 5.69E-02 | 1.56E-02 | 7.15E-03 |
| | | | Community Avg | 3.52E-02 | 5.20E-03 | 6.16E-03 | 1.69E-03 | 7.75E-04 |
| | | Mean | Fenceline Avg | 1.17E-01 | 1.87E-02 | 3.68E-02 | 1.10E-02 | 4.98E-03 |
| | | | Community Avg | 2.00E-02 | 3.21E-03 | 3.48E-03 | 1.04E-03 | 4.70E-04 |
| | | | **Max** | 1.80E-01 | 2.65E-02 | 5.69E-02 | 1.56E-02 | 7.15E-03 |

Figure 9. IIOAC output metrics of acute exposure dose by age groups.

## 4.7 Export and Reset Features

IIOAC offers the user the ability to export the Inputs file, **Source Inputs Tab** and **Output Tab** into a separate Excel workbook. Throughout the use of the tool, the user can also click on **Reset** to clear all data entered into the tool and restart the tool.

# 5 Selection of AERMOD Inputs

## 5.1 Overview

IIOAC uses pre-run AERMOD results to calculate the output metrics listed in Section 4.6. Within IIOAC, the pre-run AERMOD results are scaled according to the user-specified release amount and, for fugitive and area water/soil sources, area size (see Sections 5.9 and 9).

Point sources release emissions from a one-dimensional point location, while fugitive and area sources have emission releases spread out across a two-dimensional area. A classic example of a point source is a chimney or other pipe/stack releasing emissions from a combustion activity. Fugitive sources may include loading docks, bag houses, and areas where a facility building is leaking or venting. Area sources in IIOAC are open-air soil or water sources where a chemical is first applied to the soil or water, and then the chemical volatilizes off the surface and into the air. Examples of area water sources are surface impoundments, lakes, and clarifiers in wastewater treatment processes, while area soil sources may include waste applied to fields.

This section describes the selected AERMOD scenarios that were pre-run in AERMOD version 16216r and the rationale for selection.

## 5.2 Source Characterization

### 5.2.1 Point Sources

Three point source scenarios, shown in Table 6, were developed to cover a range of release-point parameters that may exist at U.S. facilities.

Table 6. Point source configurations used in the pre-run AERMOD scenarios.

| Point Source Configuration | Release Height (m) | Exit Gas Temperature (K) | Inside Diameter (m) | Exit Gas Velocity (m/s) |
|---|---|---|---|---|
| Stack | 10 | 300 | 2 | 5 |
| Average Incinerator | 25 | 500 | 1 | 15 |
| High-temperature Incinerator | 50 | 1,200 | 2 | 15 |

***Stack Heights.*** The three release heights used (10, 25, and 50 m above ground) were considered representative of most U.S. point sources. According to the 2011 version of the U.S. EPA National-scale Air Toxics Assessment (NATA; this was the latest version available at the time of IIOAC development), about 80 percent of U.S. point sources have release heights between 5 and 75 m, with the majority being 5 to 15 m tall (EPA 2015a).

As a supplementary measure of representativeness, about 88 percent of individual types of point sources have default release heights within the range of 5–75 m, again with the majority being 5–15 m. These default point-source release parameters came from version 4.0 of the U.S. EPA SMOKE emissions model (UNC 2016; specifically, the PSTK file of point-source replacement stack parameters), which was used in the 2011 NATA for populating missing point-source parameters at individual facilities, based on Source Classification Code (SCC) (EPA 2015c). Note that these statistics using default SCC parameters weight each SCC equally, not accounting for the number of U.S. point sources that correspond to a given SCC.

***Exit Gas Temperatures*****.** The three exit gas temperatures used (300, 500, and 1,200 K) were considered broadly representative of most U.S. point sources. According to the 2011 NATA (EPA 2015a), about 78 percent of U.S. point sources have exit gas temperatures between 230 and 630 K (with the majority being below about 400 K), and the modeled 1,200 K value covers most of the higher temperatures as well. In addition, about 96 percent of point-source SCCs have default exit gas temperatures in the range of 230–630 K (UNC 2016).

***Inside Diameter*****.** The two inside diameters used (1 and 2 m) were considered representative of the majority of U.S. point sources. About 52 percent of U.S. point sources in the 2011 NATA had inside diameters between 0.5 and 2.5 m (especially near 1 m) (EPA 2015c). As a supplementary statistic, about 65 percent of point-source SCCs have default inside diameters in this range (UNC 2016).

***Exit Gas Velocities*****.** The two exit gas velocities (5 and 15 m/s) were considered representative of an approximate majority of U.S. point sources. About 48 percent of U.S. point sources in the 2011 NATA had exit gas velocities between 2.5 and 17.5 m/s, somewhat preferring smaller values (EPA 2015c). In addition, about 64 percent of point-source SCCs had default exit gas velocities in this range (UNC 2016).

***Combined Parameters*****.** The three combinations of these values (creating the stack, incinerator 1, and incinerator 2 point sources) were created so that together they would result in a wide range of air concentrations. As shown in Table B1 of Appendix B, the stack point source should generally result in the highest air-concentration and deposition values relative to the other point sources, due to its lower height and lower plume rise (due to lower buoyancy and momentum). The two incinerator point sources should generally result in much smaller air-concentration and deposition values relative to the stack source, due to their higher heights and plume rise values—the incinerator 2 in particular should often show reductions in air-concentration and deposition values of more than 90 percent relative to the stack source, at receptor locations both close to (100 m) and farther away (1,000 m) from the emission source.

### 5.2.2 Fugitive Sources

For fugitive sources, five scenarios for horizontal dimensions (shown in Table 7) were modeled in AERMOD to cover a wide range of values that OPPT may consider. Each of these are not available as source-configuration choices in IIOAC—rather, as discussed further in Section 5.9, they were used in the pre-run AERMOD scenarios to derive regressions associating changes in horizontal dimension with changes in air concentrations and deposition. These regressions use the 100 $m^2$ fugitive source as the baseline source upon which those regression associations are applied in IIOAC for a user-defined size of fugitive source. Iowa City, IA was the baseline meteorology station, as discussed in Section 5.4. The release height (3.05 m) is the default value used for fugitive sources in the 2011 NATA (EPA 2015c).

Table 7. Fugitive-source configurations used in the pre-run AERMOD scenarios.

| Area ($m^2$; equal length and height) | Release Height (m) |
|---|---|
| 25 | 3.05 |
| 50 | |
| 100 (default) | |
| 200 | |
| 500 | |

### 5.2.3 Area Sources

Similar to fugitive sources (see Section 5.2.2), five scenarios for horizontal dimensions (shown in Table 8) were modeled in AERMOD to cover a wide range of values that OPPT may consider. Each of these are not available as source-configuration choices in IIOAC—rather, as discussed further in Section 5.9, they were used in the pre-run AERMOD scenarios to derive regressions associating changes in horizontal dimension with changes in air concentrations. These regressions use the 50 acre area source as the baseline source upon which those regression associations are applied in IIOAC for a user-defined size of area source. Iowa City, IA was the baseline meteorology station, as discussed in Section 5.4. Because these area sources are used in the IIOAC as releases from soil or water surfaces, the release heights are at ground level.

Table 8. Area-source configurations used in the pre-run AERMOD scenarios.

| Area (acres; equal length and height) | Release Height (m) |
|---|---|
| 10 | 0 |
| 20 | |
| 50 (default) | |
| 200 | |
| 500 | |

## 5.3 Emission Characterization

For the pre-run AERMOD scenarios, each source emitted at a constant rate of 1 g/s. For sources modeled as areas (the fugitive and area sources described respectively in Sections 5.2.2 and 5.2.3), the 1 g emitted mass was spread evenly across the area. For example, a 25 $m^2$ fugitive area emitted 0.04 $g/s/m^2$.

These emission rates were specific to the phase of the emitted pollutant. Vapor phase pollutants will disperse more widely than particle phase pollutants. Smaller diameter particles will disperse more widely than larger diameter particles. Separate AERMOD runs, with separate outputs, allowed for the modeling of 1 g/s of particle phase pollutant with larger diameters, 1 g/s of particle phase pollutant with smaller diameters, and 1 g/s of vapor phase pollutant. All source types (point, fugitive, and area) were modeled to emit vapor phase pollutants (with deposition assumed to be negligible in the near-field), and point and fugitive sources additionally emitted particle phase pollutants (with deposition processes modeled).

Smaller diameter particles were modeled with mass-mean aerodynamic diameters of 2.5 µm (the upper limit of the typical definition of “fine” particles) and an assumed density of 1 $g/cm^3$. The same density was used for larger particles, which had mass-mean aerodynamic diameters of 10 µm (the upper limit of the typical definition of “coarse” particles). Larger particles will deposit closer to the emission source relative to smaller particles.

## 5.4 Meteorology and Land Cover

With the goal of providing stations that broadly represent meteorology conditions encountered throughout the U.S., 14 meteorological stations were used for surface meteorology in the pre-run AERMOD scenarios and were selected based on previous analyses for OPPT (US EPA, 2014b). These surface stations, and the upper-air stations they were paired with, are listed in Table 9 and shown in a map in Figure 10. Table 9 also contains information on the elevation above sea level of each surface station as well as a qualitative description of the land cover within 1 km and 10 km of the surface station (according to year-1992 land-cover data, which are the vintage of data used by EPA’s land-cover processor [AERSURFACE] for AERMOD; MRLC 2001).

In that previous analysis for OPPT, one station was initially selected for each of nine U.S. climate regions. The representativeness of a station relative to its region was determined using the ventilation factor, which is the product of wind speed and mixing height. The ventilation factor represents a measurement of the dispersion flux through an idealized box around a source of pollution, where larger ventilation factors represent larger mixing volumes and lower average concentrations. The representative station was selected whose distribution of hourly ventilation factors was most similar to that of the aggregate of all stations in the region.

For regions with coastlines, if the selected station (using the ventilation-factor method) was on the coast, then an inland station was added for the region; if the selected station was inland, then a coastal station was added. Relative to the stations initially selected above using the ventilation factor, these supplementary stations experienced significantly different wind patterns and were in different states in the region.

Meteorology data were used from the five most recent years available at the beginning of the project development (years 2011–2015), including one-minute processing of wind data at all but one station (the Camp Springs, MD station did not have one-minute wind data available). Corresponding period-average wind roses are shown in Figure 11. Meteorological processors and pre-processors included: AERMINUTE v15272, AERSURFACE v13016, and AERMET v16216. Hourly surface data, one-minute surface wind data, and twice-daily upper-air data were obtained from NOAA (2017b, 2017a, and 2017c, respectively), and land-cover data were obtained from MRLC (2001). Upper-air stations were selected based on proximity to the surface station (primary factor) and on having similar geography and meteorological characteristics relative to the surface station (secondary factor).

For the purposes of deriving micrometeorological parameters using AERSURFACE, several recent years of remotely-sensed vegetation data (specifically the Normalized Difference Vegetation Index as a measure of greenness; NASA 2017) were analyzed in the vicinity of each station. Qualitative assumptions were made about monthly vegetative-season assignments based on the greenness index (Table 10). Historical snow-cover data (NOAA 2012) were further used to identify whether the site typically has more than 30 days of snow on the ground, and in such cases the months identified as “after harvest or first frost” were identified as also having continuous snow cover. AERSURFACE was run assuming average surface-moisture conditions relative to climatology, with surface-roughness calculations conducted within a 1-km radius and within 12 30-degree sectors around the surface meteorological station.

All 14 meteorology datasets were modeled for all point-source AERMOD runs. For fugitive and area sources, where pre-run AERMOD scenarios were used to derive regressions associating changes in horizontal dimension with changes in air concentrations and deposition, the Iowa City, IA location was used as the baseline meteorology scenario to calculate those regressions. It was assumed that those regression relationships (relating source size and AERMOD outputs) derived using Iowa City, IA meteorology data would be roughly applicable to other meteorological conditions from the other 13 meteorology stations; that is, the user may select any of the 14 meteorological stations in IIOAC, but for fugitive and area sources the regression applied to the user-entered source size comes from modeling using the Iowa City station.

Iowa City was selected for the fugitive- and area-source regressions because it is reasonably representative of U.S. meteorological stations as a whole. The Iowa City station is located near the center of the country and does not experience substantial terrain or water-body/coastal influences. In order to gauge the representativeness of the Iowa City’s wind speeds, mixing heights, and precipitation amounts relative to overall U.S. conditions, a small comparison exercise was conducted using year-2016 meteorological data from over 800 stations across the U.S. Note that these are not the same years of data used in the modeling to support IIOAC—EPA OAQPS had already run these year-2016 data through AERMOD’s meteorology processor, and the pre-run meteorology data are available from EPA OAQPS's Human Exposure Model website (EPA 2017c). Using those year-2016 data, a comparison was made between the typical conditions at the non-coastal stations used in this tool and the typical conditions from all 800+ stations (which included coastal stations). According to that comparison, from among the non-coastal stations used in IIOAC, the Iowa City station ranked 3rd, 5th, and 3rd most representative of all U.S. stations for wind speed, mixing height, and precipitation, respectively; all other stations had at least one ranking of 6th or larger. Therefore, the Iowa City station was judged to be a reasonably representative station.

Table 9. Specifications of the meteorology stations used in the AERMOD runs.

| | Surface Station | | | | | Upper-air Station | | |
|---|---|---|---|---|---|---|---|---|
| **Climate Region** | **WBAN (Call Sign)** | **Location** | **Coastal or Inland (with approx. distances to water for coastal)** | **Lat.<br>Long.<br>Elev.** | **Qualitative Land-cover Description (1992)[a]** | **WBAN** | **Location** | **Lat.<br>Long.** |
| 1<br>(East North Central) | 14937<br>(KIOW) | Iowa City, IA | Inland | 41.633<br>-91.543<br>198 m | 1 km: Mostly developed, some farmland<br>10km: Half developed, half farmland, some forest | 94982 | Davenport, IA | 41.6<br>-90.57 |
| 2<br>(North-east) | 13705<br>(KADW) | Camp Springs, MD | Coastal (31 km from Chesapeake Bay, 60 km from Atl. Ocean) | 38.811<br>-76.867<br>86 m | 1 km: Developed<br>10 km: Mostly developed, some forest and farmland | 93734 | Sterling, VA | 38.98<br>-77.47 |
| | 14762<br>(KAGC) | Pittsburgh, PA | Inland | 40.355<br>-79.922<br>380 m | 1 km: Mostly developed, some forest<br>10 km: Mostly developed, some forest | 94823 | Township, PA | 40.53<br>-80.23 |
| 3<br>(North-west) | 24222<br>(KPAE) | Everett, WA | Coastal (4 km from Puget Sound, 50 km from Salish Sea, 180 km from Pac. Ocean) | 47.908<br>-122.28<br>184 m | 1 km: Developed<br>10 km: Developed, some open water | 24232 | Salem, OR | 44.92<br>-123.02 |
| | 24145<br>(KIDA) | Idaho Falls, ID | Inland | 43.516<br>-112.06<br>1,441 m | 1 km: Developed<br>10 km: Mostly farmland, some development | 24061 | Riverton, WY | 43.06<br>-108.47 |
| 4<br>(South) | 13920<br>(KFOE) | Topeka, KS | Inland | 38.95<br>-95.664<br>325 m | 1 km: Developed<br>10 km: Mostly farmland, some development | 13996 | Topeka, KS | 39.07<br>-95.62 |

| Climate Region | Surface Station |  |  |  |  | Upper-air Station |  |  |
|---|---|---|---|---|---|---|---|---|
|  | WBAN (Call Sign) | Location | Coastal or Inland (with approx. distances to water for coastal) | Lat. Long. Elev. | Qualitative Land-cover Description (1992)[a] | WBAN | Location | Lat. Long. |
|  | 03937 (KLCH) | Lake Charles, LA | Coastal (41 km from Gulf of Mexico) | 30.125<br>-93.228<br>3 m | 1 km: Half developed, half farmland<br>10 km: Mostly farmland, some development and open water | 03937 | Lake Charles, LA | 30.12<br>-93.22 |
| 5 (South-east) | 93727 (KNCA) | New River, NC | Coastal (20 km from Atl. Ocean) | 34.7<br>-77.433<br>8 m | 1 km: Mostly developed, some wetlands<br>10 km: Mix of wetlands, forest, farmland, open water, and development | 93768 | Morehead City, NC | 34.7<br>-76.8 |
|  | 13874 (KATL) | Atlanta, GA | Inland | 33.64<br>-84.427<br>308 m | Mostly developed | 53819 | Peachtree City, GA | 33.35<br>-84.56 |
| 6 (South-west) | 23066 (KGJT) | Grand Junction, CO | Inland | 39.134<br>-108.538<br>1,481 m | 1 km: Mix of shrubland (rough terrain) and development<br>10 km: Mostly shrubland (rough terrain) with some development and farmland | 23062 | Denver, CO | 39.77<br>-104.88 |
| 7 (West) | 93111 (KNTD) | Point Mugu, CA | Coastal (2 km from Pac. Ocean) | 34.117<br>-119.110<br>4 m | 1 km: Developed<br>10 km: Mix of shrubland, farmland, and open water, with some development | 93214 | Vandenberg AFB, CA | 34.75<br>-120.57 |

| Climate Region | Surface Station |  |  |  |  | Upper-air Station |  |  |
|---|---|---|---|---|---|---|---|---|
|  | WBAN (Call Sign) | Location | Coastal or Inland (with approx. distances to water for coastal) | Lat.<br>Long.<br>Elev. | Qualitative Land-cover Description (1992)[a] | WBAN | Location | Lat.<br>Long. |
|  | 23169 (KLAS) | Las Vegas, NV | Inland | 36.079<br>-115.155<br>665 m | 1 km: Developed<br>10 km: Mostly developed, some shrubland (desert) | 53103 | Flagstaff, AZ | 35.23<br>-111.82 |
| 8 (West North Central) | 14944 (KFSD) | Sioux Falls, SD | Inland | 43.577<br>-96.754<br>435 m | 1 km: Mostly developed<br>10 km: Mix of development and farmland | 94980 | Omaha, NE | 41.32<br>-96.37 |
| 9 (Central) | 94822 (KRFD) | Rockford, IL | Inland | 42.196<br>-89.093<br>223 m | 1 km: Developed<br>10 km: Mostly farmland, with some development and forest | 94982 | Davenport, IA | 41.6<br>-90.57 |

[a] MRLC (2001)

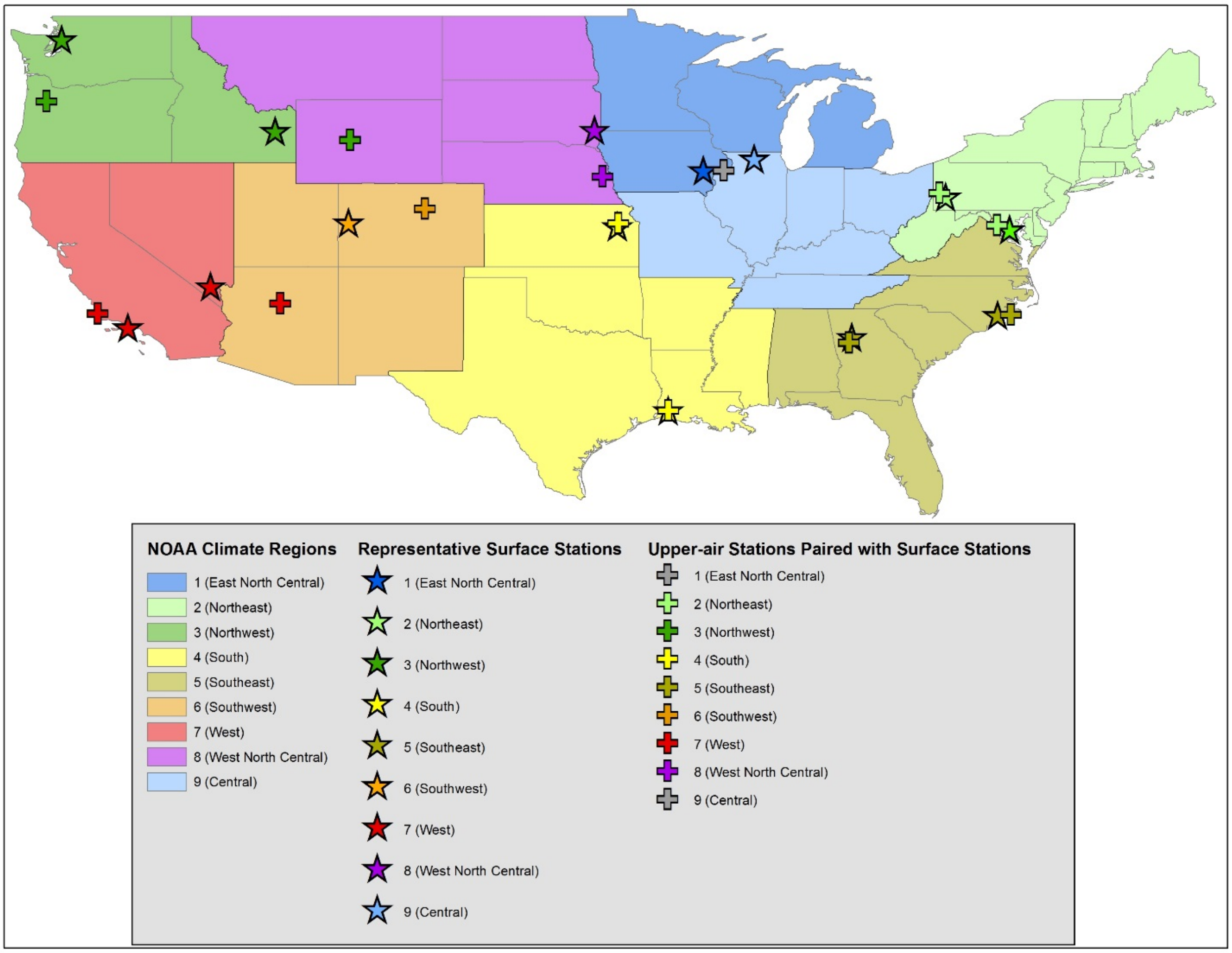


Figure 10. Map of the meteorology stations used in the AERMOD runs.

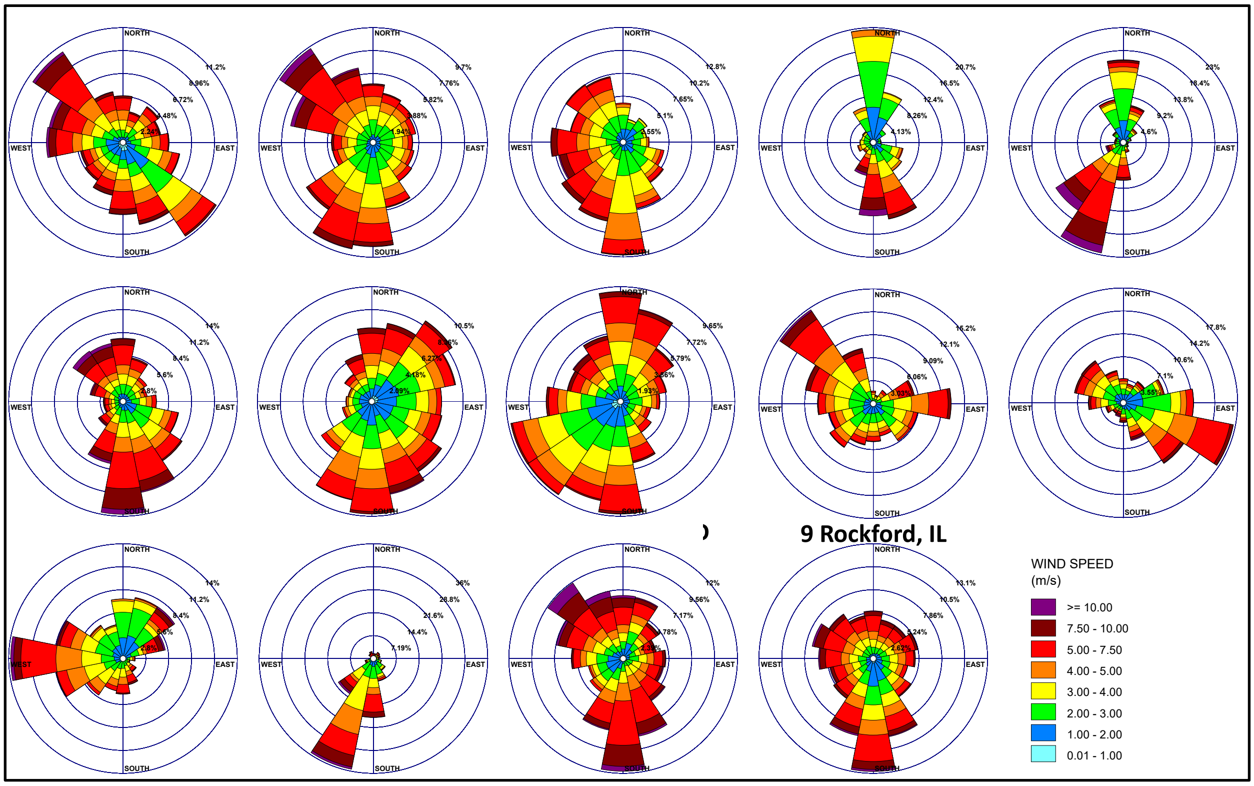


Figure 11. Wind roses for the meteorology stations used in the AERMOD runs.

Table 10. Season assignments (defined by vegetation and snow) for the meteorological stations used in the AERMOD runs.

| Climate Region | Location of Surface Station | Month and Season Assignment[a] | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Jan | Feb | Mar | Apr | May | Jun | Jul | Aug | Sep | Oct | Nov | Dec |
| 1<br>(East North Central) | Iowa City, IA | 1s | 1s | 2 | 2 | 2 | 3 | 3 | 3 | 4 | 4 | 4 | 1s |
| 2<br>(Northeast) | Camp Springs, MD | 1 | 1 | 2 | 2 | 2 | 3 | 3 | 3 | 4 | 4 | 4 | 1 |
| | Pittsburgh, PA | 1s | 1s | 1s | 2 | 2 | 3 | 3 | 3 | 4 | 4 | 4 | 1s |
| 3<br>(Northwest) | Everett, WA | 1 | 1 | 1 | 2 | 2 | 3 | 3 | 3 | 3 | 4 | 1 | 1 |
| | Idaho Falls, ID | 1s | 1s | 1s | 2 | 2 | 3 | 3 | 4 | 4 | 4 | 1s | 1s |
| 4<br>(South) | Topeka, KS | 1 | 1 | 1 | 2 | 2 | 3 | 3 | 3 | 4 | 4 | 4 | 1 |
| | Lake Charles, LA | 1 | 1 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 4 | 4 | 1 |
| 5<br>(Southeast) | New River, NC | 1 | 1 | 1 | 2 | 2 | 3 | 3 | 3 | 3 | 4 | 4 | 1 |
| | Atlanta, GA | 1 | 1 | 1 | 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 1 |
| 6<br>(Southwest) | Grand Junction, CO | 1 | 1 | 2 | 2 | 2 | 3 | 3 | 3 | 4 | 4 | 4 | 1 |
| 7<br>(West) | Point Mugu, CA | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| | Las Vegas, NV | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |

| Climate Region | Location of Surface Station | Month and Season Assignment[a] | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Jan | Feb | Mar | Apr | May | Jun | Jul | Aug | Sep | Oct | Nov | Dec |
| 8<br>(West North Central) | Sioux Falls, SD | 1s | 1s | 1s | 2 | 2 | 2 | 3 | 3 | 4 | 4 | 4 | 1s |
| 9<br>(Central) | Rockford, IL | 1s | 1s | 2 | 2 | 2 | 3 | 3 | 3 | 4 | 4 | 4 | 1s |

[a] 1 = after harvest or first frost, 1s = 1 with continuous snow cover, 2 = partial green coverage or short annuals, 3 = lush vegetation, 4 = autumn prior to harvest or first frost

## 5.5 Urban/Rural

Each point and fugitive source in the pre-run AERMOD scenarios was modeled once with the urban-effects setting turned on in AERMOD and once without it turned on. The urban setting in AERMOD modifies turbulence parameters to better account for the effect of the urban heat island on the nocturnal boundary layer and subsequent transition to the daytime boundary layer. AERMOD uses a population-count value to tailor its urban-heat-island calculations, and a value of 1 million people was used in the urban runs.

It was assumed that soil and water area sources would not be in urban areas. As such, area sources were not modeled with the urban setting.

## 5.6 Receptors

Output metrics are determined for two groups of receptors (fenceline and community) as indicated below:

- 16 inner ring or fenceline receptor-points: a polar-grid ring of receptor points 100 m from the point source (or approximately 100 m from the corners of the fugitive- or area-source square), spaced every 22.5 degrees (oriented north, north-northeast, northeast, east-northeast, etc. of the center of the source)
- 228–658 near-facility community receptor points: a Cartesian grid of receptor points filling the space between the fenceline receptors and an outer-ring receptors 1000 m from the source, with 100-m spacing between receptors. The number of community receptors varies by source type and area size (the area between the two rings of receptors grows as the source becomes bigger), as shown in Table 11.

Air-concentration metrics were obtained at a 1.8-m height above ground to coincide with typical breathing height (for all source types), and deposition metrics were obtained at ground level (only for point and fugitive sources).

Table 11. Number of receptor points modeled by source type and source size.

| Source Type | Number of Receptor Points | | |
|---|---|---|---|
| | Fenceline | Community | Total |
| Point | 16 | 228 | 244 |
| Fugitive (25 m$^2$) | 16 | 236 | 252 |
| Fugitive (50 m$^2$) | 16 | 236 | 252 |
| Fugitive (100 m$^2$) | 16 | 234 | 250 |
| Fugitive (200 m$^2$) | 16 | 236 | 252 |
| Fugitive (400 m$^2$) | 16 | 240 | 256 |
| Area (10 acres) | 16 | 296 | 312 |
| Area (20 acres) | 16 | 316 | 332 |
| Area (50 acres) | 16 | 366 | 382 |
| Area (200 acres) | 16 | 502 | 518 |
| Area (500 acres) | 16 | 658 | 674 |

## 5.7 Recommendation on Default Selections in IIOAC

The default scenarios recommended generally characterize central-tendency (mean) and high-end (95th percentile) exposures for a range of exposure scenarios based on the pre-run AERMOD results. Using these selections provides a central-tendency and high-end conservative estimate for air concentrations and exposure doses. In some cases, one scenario may lead to the highest air concentrations and deposition at the fenceline while not at the community receptors, or at one single point but not at another, and one scenario may lead to the highest air concentrations at a location but not the highest deposition amounts. The ranking of scenarios was determined based on the average air concentration and deposition values from five years of meteorological data (2011 through 2015) across all fenceline and community receptors within each scenario. For area and fugitive sources, only the base scenarios (i.e., those with an area of 50 acres and 100 m$^2$, respectively) were considered in the analysis. The default scenarios described below are recommended for first-tier assessment, and follow-up air modeling may be needed based on chemical and site specific conditions.

### 5.7.1 Default Source Scenarios

The fugitive source is more conservative relative to the point sources and and area sources.

For point sources, the stack source is considerably more conservative than the incinerator sources. For fugitive sources, smaller fugitive sources will generally provide the most conservative air concentrations and deposition amounts. For area sources, smaller area sources will generally provide the most conservative air concentrations (deposition amounts are not modeled for area sources).

### 5.7.2 Default Selection of Vapor or Particle

Vapor phase chemicals are the only option available for area sources.

For point sources, modeling with coarse particles will generally be the most conservative option overall. For fugitive sources, coarse particles will generally be the most conservative option for deposition amounts, while vapor-phase chemical will generally be the most conservative option for air concentrations.

### 5.7.3 Default Selection of Urban or Rural

Rural is the only option available for area sources.

For point sources, the urban selection will tend to lead to higher air concentrations and deposition amounts, while for fugitive sources the rural selection will. However, the magnitude of the effect of the urban setting is dependent on the selected meteorology station and the distance between the source and the receptor.

### 5.7.4 Default Selection of Meteorology

The Lake Charles, LA station (South, Coastal) is a good choice for conservative air concentration results as it has the highest average air concentration from among the 14 station options; however it has the 8th highest deposition rank. The Pittsburgh, PA (Northeast, Inland) station is a good choice for conservative particle deposition results, as it has the highest deposition values from among the 14 station options; however it has the lowest air concentration values. If both air concentration and particle deposition are considered, the Iowa City, IA station (East North Central) is a good choice for conservative results, as it has the 3rd and 5th highest air concentration and deposition ranks, respectively, among 14 station options.

For central tendency results, the Sioux Falls, SD station (West North Central) would be a good selection when considering either air concentration or particle deposition, as it exhibits the 6th and 9th highest average air concentration and deposition values, respectively, out of the 14 station options.

## 5.8 Summary of AERMOD Runs for Point Sources

The pre-run point source scenarios are outlined in Table 12. These scenarios were defined to represent a range of possible site conditions across the U.S. In total, there were 252 pre-run AERMOD scenarios for point sources: 3 source type scenarios × 2 population scenarios × 3 particle/vapor scenarios × 14 meteorology scenarios.

Point sources include stack and incinerator sources that release emissions directly to the air, with source specifications (heights, diameters, temperatures, and velocities) that differ among the three source types. AERMOD runs for point sources were performed using 1 g/s emission rates that were constant in time, with 1 g/s of vapor phase emissions modeled separately from

1 g/s fine particle phase emissions and 1 g/s coarse particle phase emissions. User-specified variations on emission rates are accounted for in IIOAC itself.

Point source runs included 14 meteorological stations (years 2011–2015) covering a wide range of climatological, geographic, and land-cover characteristics. Each point source run included an urban option that modified turbulence parameters to better represent the urban heat island (as well as runs without the urban option). Each run included 16 fenceline polar-grid receptors and 228-658 community Cartesian-grid receptors, with air concentrations estimated at 1.8-m above ground and deposition estimated at ground level.

Table 12. AERMOD scenarios for point sources.

| Parameter | Options | Comments |
|---|---|---|
| Source Type | Stack<br>h=10 m, d=2 m, t=300 K, v=5 m/s | Concentrations from stack emissions should generally be larger than those from the other point sources, and concentrations from the high-temperature incinerator's emissions should generally be lower than those from the other point sources |
| | Incinerator 1<br>h=20 m, d=1 m, t=500 K, v=15 m/s | |
| | Incinerator 2<br>h=50 m, d=2 m, t=1,200 K, v=15 m/s | |
| Population | Not urban | |
| | Urban (1 million people) | |
| Constant Emission Duration | 1 hour once per day (12-1)pm | Run AERMOD under constant emission, extract relevant data for each emission duration using post-processing code |
| | 4 continuous h/d (12–4pm) | |
| | 8 continuous h/d (8–4pm) | |
| | Constant | |
| Particle/Vapor | Vapor (no deposition) | Vapor phase pollutants and finer-sized particles will disperse more widely than larger-sized particles, which deposit closer to the source |
| | Fine particles ($PM_{2.5}$, 2.5 µm) | |
| | Coarse particles ($PM_{10}$, 10 µm) | |
| Meteorology and Land Cover | Iowa City, IA | Use meteorological data from years 2011–2015, land-cover data from year 1992, average wetness for Bowen ratio calculations, and local determinations of arid/non-arid and vegetative seasons |
| | Camp Springs, MD | |
| | Pittsburgh, PA | |
| | Everett, WA | |
| | Idaho Falls, ID | |
| | Topeka, KS | |
| | Lake Charles, LA | |
| | New River, NC | |
| | Atlanta, GA | |
| | Grand Junction, CO | |
| | Point Mugu, CA | |
| | Las Vegas, NV | |
| | Sioux Falls, SD | |
| | Rockford, IL | |

Note: h = height, d = inside diameter, t = exit gas temperature, v = exit gas velocity, m = meters, K = Kelvin, m/s = meters per second, h/d = hours per day

## 5.9 Summary of AERMOD Runs for Fugitive and Area Sources

The pre-run fugitive and area source scenarios are outlined in Table 13. Like point sources, fugitive and area sources release emissions to the air; unlike point sources, fugitive and area releases are spread out evenly across a two-dimensional area. All were modeled using 1 g/s emission rates that were constant in time (identical to point sources). Area sources emitted only vapor phase pollutant, as emissions are due to volatilization of chemicals to the air from the soil and water. Fugitive sources had 1 g/s of vapor phase emissions modeled separately from 1 g/s fine particle phase emissions and 1 g/s coarse particle phase emissions. These emission rates were then spread evenly around the two-dimensional area, so that a 25 $m^2$ fugitive source emitted at a rate of 0.04 $g/s/m^2$, for example. User-specified variations on emission rates are accounted for in IIOAC itself. All fugitive sources emitted at 3.05 m above ground (the default value used for fugitive sources in the 2011 NATA), while all area sources emitted at ground level.

The sizes modeled in AERMOD for the two-dimensional areas were selected to be representative of the range of sources OPPT is likely to consider for each type of source. However, IIOAC is designed to estimate pollutant outputs for user-customized sizes. Test modeling showed an approximate linear relationship between the sizes of larger sources and the AERMOD results. A number of smaller sources were also included because the test modeling showed more variability in their AERMOD results, introduced by the surface geometry. In total, 30 AERMOD scenarios were run to derive the regression relationship between the size of a fugitive source and outputs of air concentrations and deposition—2 population scenarios × 3 particle/vapor scenarios × 5 source sizes (using the Iowa City, IA meteorology scenario). Similarly, five AERMOD scenarios were run to derive the regression relationship between the size of an area source and outputs of air concentrations, corresponding to five source sizes (using the Iowa City, IA meteorology scenario). A baseline fugitive-source size of 100 $m^2$ is used in IIOAC, upon which the regression is applied to relate the outputs of the baseline source size to those of the user-entered source size—84 fugitive-source AERMOD scenarios were run with the baseline size (2 population scenarios × 3 particle/vapor scenarios × 14 meteorology scenarios). A baseline area source size of 50 acres is used in IIOAC, upon which the regression is applied to relate the outputs of the baseline source size to the user-entered source size—14 area source AERMOD scenarios were run with the baseline size (corresponding to the 14 meteorology stations). See Section 1 on scaling factors for fugitive and area sources, and see Section 5.4 for a discussion on using the Iowa City, IA station as a representative U.S. station.

Fugitive and area source runs included 14 meteorological stations (years 2011–2015) covering a wide range of climatological, geographic, and land-cover characteristics. Area sources were run without the urban option in AERMOD (assuming soil and water sources are not located in urbanized areas), while fugitive sources, like point sources, included runs with and without the urban option (the urban option modifies turbulence parameters to better represent the urban heat island). As with the point-source runs, each fugitive and area source run included 16 fenceline polar-grid receptors and hundreds of community Cartesian-grid receptors at a spacing of 100 m. Air concentrations were estimated at 1.8-m above ground and, for fugitive sources only, deposition values were estimated at ground level.

Table 13. AERMOD scenarios for fugitive and area (water and soil) sources.

| Parameter | Fugitive Source Options | Area Source Options | Comments |
|---|---|---|---|
| Area Size and Release Height | 25 $m^2$<br>l=5 m, w=5 m, h=3.05 m | 10 acres<br>l=201 m, w=201 m, h=0 m | |
| | 50 $m^2$<br>l=7.1 m, w=7.1 m, h=3.05 m | 20 acres<br>l=284 m, w=284 m, h=0 m | |
| | 100 $m^2$ (default)<br>l=10 m, w=10 m, h=3.05 m | 50 acres (default)<br>l=450 m, w=450 m, h=0 m | |
| | 200 $m^2$<br>l=14.1 m, w=14.1 m, h=3.05 m | 200 acres<br>l=900 m, w=900 m, h=0 m | |
| | 400 $m^2$<br>l=20 m, w=20 m, h=3.05 m | 500 acres<br>l=1,422 m, w=1,422 m, h=0 m | |
| Population | Not urban | Not urban | |
| | Urban (1 million people) | | |
| Constant Emission Duration | 1 hour once per day (12-1)pm | Constant | For Fugitive sources run AERMOD under constant emission, extract relevant data for each emission duration using post-processing code |
| | 4 continuous h/d (12-4pm) | | |
| | 8 continuous h/d (8-4pm) | | |
| | Constant | | |
| Particle/ Vapor | Vapor (no deposition) | Vapor (no deposition) | Vapor phase pollutants and finer-sized particles will disperse more widely than larger-sized particles, which deposit closer to the source |
| | Fine particles ($PM_{2.5}$, 2.5 µm) | | |
| | Coarse particles ($PM_{10}$, 10 µm) | | |
| Meteor-ology and Land Cover | Iowa City, IA | Iowa City, IA | Use meteorological data from years 2011–2015, land-cover data from year 1992, average wetness for Bowen ratio calculations, and local determinations of arid/non-arid and vegetative seasons |
| | Camp Springs, MD | Camp Springs, MD | |
| | Pittsburgh, PA | Pittsburgh, PA | |
| | Everett, WA | Everett, WA | |
| | Idaho Falls, ID | Idaho Falls, ID | |
| | Topeka, KS | Topeka, KS | |
| | Lake Charles, LA | Lake Charles, LA | |
| | New River, NC | New River, NC | |
| | Atlanta, GA | Atlanta, GA | |

| Parameter | Fugitive Source Options | Area Source Options | Comments |
|---|---|---|---|
| | Grand Junction, CO | Grand Junction, CO | |
| | Point Mugu, CA | Point Mugu, CA | |
| | Las Vegas, NV | Las Vegas, NV | |
| | Sioux Falls, SD | Sioux Falls, SD | |
| | Rockford, IL | Rockford, IL | |

Note: l = length, w = width, h = height, m = meters, h/d = hours per day

# 6 Modeling Approach for Facility Sources

## 6.1 Overview and Assumptions

IIOAC calculates outdoor air concentration based on post-processed AERMOD results for unit emission and adjusts these values by the user-specified release duration and days of release per year. Indoor air concentrations are calculated by multiplying the outdoor air concentration by the indoor-outdoor ratio.

Releases from facility sources (i.e., point or fugitive) emit directly to outdoor air and are assumed to follow either a pattern of consecutive or cyclical (evenly spaced) release days. Once an emission stops, air concentrations fall to zero instantaneously, which is a property of AERMOD. Because AERMOD calculates dispersion, air concentrations, and deposition in hourly time steps, IIOAC uses hourly emissions and hourly meteorological data. For the IIOAC tool, AERMOD was run with a unit emission rate of 1 g/s for all scenarios. The hourly model outputs were then post-processed to calculate daily-and annual-averaged outdoor air concentrations. For fugitive sources, AERMOD runs were set up using an area size of 100 $m^2$.

## 6.2 Post-Processing of AERMOD Hourly Air Concentrations

All AERMOD emission scenarios were run with constant emission for five years, based on EPA regulatory guidance (US EPA, 2017d). However, within IIOAC, users can select from release durations of 1, 4, 8, or 24 hours per day, which correspond to emission times of 12-1pm, 12-4pm, 8am-4pm, and all day, respectively. For release durations that are 1, 4, and 8 hours, AERMOD data for hours when the emission is not occurring were set to zero, as shown in the table (Table 14) for one day.

Table 14. Example of hourly concentrations set to zero when there is no emission for a 1, 4, and 8 hour release duration.

| **Pre-processed Hourly AERMOD Outputs** | | | **Post-processed Hourly AERMOD Outputs** | | |
|---|---|---|---|---|---|
| **Continuous Emission, 1 g/s** | | | **Air Concentration (μg/$m^3$) – Set to Zero When No Emission** | | |
| Day | Time | Air Concentration (μg/m3) | 1 hr Duration | 4 hrs Duration | 8 hrs Duration |
| 1-Jan | 0:00 | 0.06 | 0 | 0 | 0 |
| 1-Jan | 1:00 | 0.51 | 0 | 0 | 0 |
| 1-Jan | 2:00 | 0.52 | 0 | 0 | 0 |
| 1-Jan | 3:00 | 0.00 | 0 | 0 | 0 |
| 1-Jan | 4:00 | 0.60 | 0 | 0 | 0 |
| 1-Jan | 5:00 | 0.37 | 0 | 0 | 0 |

|  |  |  |  |  |  |
|---|---|---|---|---|---|
| 1-Jan | 6:00 | 0.59 | 0 | 0 | 0 |
| 1-Jan | 7:00 | 0.60 | 0 | 0 | 0 |
| 1-Jan | 8:00 | 0.79 | 0 | 0 | 0 |
| 1-Jan | 9:00 | 0.51 | 0 | 0 | 0.51 |
| 1-Jan | 10:00 | 0.43 | 0 | 0 | 0.43 |
| 1-Jan | 11:00 | 0.49 | 0 | 0 | 0.49 |
| 1-Jan | 12:00 | 0.31 | 0 | 0 | 0.31 |
| 1-Jan | 13:00 | 0.71 | 0.71 | 0.71 | 0.71 |
| 1-Jan | 14:00 | 0.04 | 0 | 0.04 | 0.04 |
| 1-Jan | 15:00 | 0.86 | 0 | 0.86 | 0.86 |
| 1-Jan | 16:00 | 0.16 | 0 | 0.16 | 0.16 |
| 1-Jan | 17:00 | 0.34 | 0 | 0 | 0 |
| 1-Jan | 18:00 | 0.15 | 0 | 0 | 0 |
| 1-Jan | 19:00 | 0.60 | 0 | 0 | 0 |
| 1-Jan | 20:00 | 0.87 | 0 | 0 | 0 |
| 1-Jan | 21:00 | 0.05 | 0 | 0 | 0 |
| 1-Jan | 22:00 | 0.24 | 0 | 0 | 0 |
| 1-Jan | 23:00 | 0.96 | 0 | 0 | 0 |

For each receptor group and AERMOD emission scenario (e.g., fugitive, urban setting, fine particles, Northeast climate region), all five years of the AERMOD hourly outputs were post-processed to determine the mean and high-end (defined as the 95th percentile) daily-averaged and annual-averaged concentrations. This was done for all release days (i.e., 1 through 365) per year. For the first four years of data, the annual-averaged concentrations start with the first day of release and extends for a one year period. For year 5, the annual-averaged concentration is simply the year 5 average in order to have 365 days to average over. The post-processing results are organized in Excel lookup tables like the example shown in Table 15.

Table 15. Example lookup table for one AERMOD emission scenario and receptor group.

| **Exposure Metric** | **Release Duration (hrs/day)** | **Number of Release Days** |  |  |  |  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
|  |  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** | **…** | **365** |
| Mean Daily Average | 1 | Filled in with post-processed AERMOD results in μg/m$^3$ |  |  |  |  |  |  |  |  |  |  |  |
|  | 4 |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 8 |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 24 |  |  |  |  |  |  |  |  |  |  |  |  |
| High-End Daily Average | 1 |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 4 |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 8 |  |  |  |  |  |  |  |  |  |  |  |  |

|  |  |  |
|---|---|---|
|  | 24 |  |
| Mean Annual Average | 1<br>4<br>8<br>24 |  |
| High-End Annual Average | 1<br>4<br>8<br>24 |  |

## 6.3 Calculating Outdoor Air Concentration and Particle Deposition Estimates

IIOAC calculates outdoor air concentration and particle deposition based on the release duration and number of days of release per year entered by the user (e.g., release occurs 4 hrs/day for 52 days in a year). An adjusted emission rate is first calculated, as shown in Equation 1, to take into account the release duration and convert the user-defined mass released per day into g/s.

$$ER_{adj} = \frac{ER}{h} \cdot 0.2778 \tag{1}$$

where $ER_{adj}$ = adjusted emission rate [g/s]
$ER$ = user-defined mass released per day [kg/day]
$h$ = emission duration [hrs/day]
$0.2778$ = conversion factor from kg/hr to g/s

Air concentrations are calculated in Equation 2 by scaling the post-processed AERMOD result, obtained based on an emission of 1 g/s, by the adjusted emission rate. For fugitive sources, scaling by just the adjusted emission rate gives an air concentration corresponding to an area size of 100 m$^2$, the same as that used in the AERMOD runs. To account for a different area size, an area size scaling factor, $SF_j$, is applied. Further details on the area size scaling factor is described in Section 9.2.

$$C_{outdoor} = \frac{ER_{adj}}{1\ g/s} \cdot SF_j \cdot Postprocessed\ AERMOD\ result \tag{2}$$

where $C_{outdoor}$ = outdoor air concentration [μg/m$^3$]
$ER_{adj}$ = adjusted emission rate [g/s]
$SF_j$ = scaling factor for fugitive area size *j* [–]; set to 1 for point sources

For point and fugitive sources, three particle size scenarios are available:

- Fine particles (with a mass-mean aerodynamic diameter of 2.5 µm),
- Coarse particles (with a mass-mean aerodynamic diameter of 10 µm), and
- Vapor (no particles).

All calculated air concentrations of fine and coarse particles are capped by an upper limit equal to the National Ambient Air Quality Standards (NAAQS) for particulate matter (PM) (US EPA 2016b). These limits are 35 and 150 µm/m$^3$ for fine and coarse particles (i.e., the NAAQS for $PM_{2.5}$ and $PM_{10}$), respectively. For vapors, the chemical is released in gaseous form and therefore there is no transfer from one phase to another. IIOAC currently does not set an upper limit for point and fugitive sources in vapor form.

When there are multiple releases at a single site, the air concentrations estimates are totaled for the site. Concentrations of particulates are capped by the upper-limit before totaling.

## 6.4 Aggregation of Stack and Incinerator Sources into Single Point Source

In the case where an input file is imported into IIOAC and all sources are selected, the tool aggregates the outputs of stack and incinerator sources into a single point source output. As an example, if an emission scenario has both a stack and incinerator source, the aggregated point source output at a specific receptor is calculated as:

$$High\text{-}end\ daily\text{-}averaged\ air\ conc_{stack} = 4\ \frac{\mu g}{m^3}$$

$$High\text{-}end\ daily\text{-}averaged\ air\ conc_{incinerator} = 2.9\ \frac{\mu g}{m^3}$$

$$High\text{-}end\ daily\text{-}averaged\ air\ conc_{point} = 4 + 2.9 = 6.9\ \frac{\mu g}{m^3}$$

Appendix C provides an example calculation using a hypothetical site with three releases of varying release amounts, frequencies, and durations.

# 7 Modeling Approach for Area Soil Sources

## 7.1 Overview and Assumptions

Area soil sources are modeled as a batch system, as shown in Figure 12, using the following assumptions:

(i) The chemical only leaves the soil through volatilization.
(ii) Releases are evenly applied across the entire surface area of the soil.
(iii) Releases are applied immediately at the start of each day.
(iv) The first day of all releases is January 1st.

(v) Releases are evenly timed throughout the year.
(vi) The time scale of emissions from area soil sources is much longer (hours to days) than the time scale of emissions directly to air (i.e., point and fugitive sources), allowing short-term impacts of meteorology to be excluded.

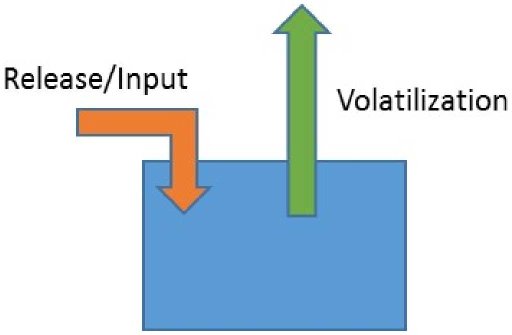


Figure 12. Schematic of area soil source, modeled as a batch system.

For area sources, AERMOD outputs are based on an emission rate of 1 g/s and an area of 50 acres. To calculate the chemical concentration in air as a result of volatilization from the soil, IIOAC must first calculate the mass flux from the soil to air. The mass flux is dependent on both the physicochemical properties, the area of the source, and the mass of chemical on the soil. Depending on the chemical, the mass flux can differ greatly, for example, a 100 kg/m$^2$ release over an area of 200,000 m$^2$ results in a flux of $1.48 \times 10^{-4}$ and 0.29 kg/m$^2$/day for Aldicarb and hexachloroethane, respectively. As such, a mass balance must be performed each day to determine the mass on the soil at the start of each day, which is then used to calculate the corresponding emission rate.

## 7.2 Equations to Calculate Daily-Averaged Air Concentrations

All daily-averaged air concentrations are calculated within IIOAC using the equations described in this section.

IIOAC uses a modified version of the Woodrow and Sieber equation (1997) to calculate the mass flux, $J$, due to volatilization from soil. The original study developed empirical natural logarithm correlations between flux for pesticides and known physicochemical properties. EPA later modified and used the equation in the Volatilization Screening Tool (US EPA, 2014a) developed by EPA to estimate screening-level air concentrations downwind of fields treated with semi-volatile pesticides. The modified equation used in Volatilization Screening Tool is given by Equation 3, with $R$ defined in Equation 4.

$$J = \frac{\exp(0.8688 \cdot R + 21.535)}{3600} \cdot (8.64 \times 10^{-5}) \quad (3)$$

and

$$R = \ln\left(\frac{VP \cdot AR}{Sol \cdot K_{oc}}\right) \tag{4}$$

where $J$ = mass flux from soil to air [kg/m$^2$/day]
$VP$ = vapor pressure [Pa]
$AR$ = mass of chemical per area [kg/ha]
$Sol$ = solubility in water [mg/L]
$K_{oc}$ = organic carbon sorption coefficient [mL/g]
0.8688 = regression coefficient (US EPA, 2014a)
21.535 = regression coefficient (US EPA, 2014a)
$8.64 \times 10^{-5}$ = conversion factor from μg/m$^2$/s to kg/m$^2$/day

Note that the equation above was developed using data points for $-16 < R < 0$. Users that enter chemical properties resulting in $R$ values outside this range will receive a warning message within IIOAC indicating that the calculated results are potentially outside the scope of applicability.

To determine the outdoor air concentration, the AERMOD results are scaled up as shown in Equation 5. For each flux value calculated, an emission rate in kg/day is determined by multiplying the flux with the user-specified area size. The AERMOD results are then scaled up by the calculated emission rate and by an area size scaling factor, $SF_j$. The area size scaling factor, $SF_j$, accounts for different area sizes and is further described in Section 9.2. As short-term impacts of meteorology can be excluded (see assumptions above), an hourly concentration averaged over the day was used as the AERMOD result to be scaled up.

$$C_{outdoor,i} = \frac{J_i \cdot A}{1\ g/s} \cdot 0.01157 \cdot SF_j \cdot Postprocessed\ AERMOD\ result_i \tag{5}$$

where $C_{outdoor,i}$ = air concentration for day *i* [μg/m$^3$]
$J_i$ = mass flux from soil to air for day *i* [kg/m$^2$/day]
$A$ = area of the source, as defined by the user [m$^2$]
$0.01157$ = conversion factor from [kg/day to g/s]
$SF_j$ = scaling factor for area size *j* [–]

All calculated air concentrations are compared to the saturation air concentration, which is the concentration at which exchange between the gas and liquid phases of the chemical are at equilibrium, and is calculated as shown in Equation 6.

$$C_{sat} = \frac{(1.33 \times 10^5) \cdot VP \cdot MW}{R \cdot T} \tag{6}$$

where $C_{sat}$ = saturation air concentration [μg/m$^3$]
$VP$ = vapor pressure [Torr]
$MW$ = molecular weight [g/mol]
$R$ = universal gas constant, 8.314 J/mol-K

$T$ = absolute temperature, set to 298 [K]
$1.33\times10^5$ = conversion factor from Torr to Pa and from g to μg

Calculated air concentrations may not be greater than the saturation air concentration. In the case when a calculated mass flux results in an air concentration above the saturated air concentration, IIOAC replaces the calculated air concentration for that day with the saturation air concentration. IIOAC returns any chemical mass above the saturation air concentration to the area soil source to be used in the calculation for the next day. IIOAC uses concentrations at the inner receptors to determine the excess concentration and corresponding mass to be returned to the soil.

For each day, to calculate $J_i$, the $AR$ value is calculated as shown in Equation 7.

$$AR_i = \frac{M_i}{A} \tag{7}$$

where $AR_i$ = mass of chemical per area [kg/ha]
$M_i$ = mass of chemical on the soil at the start of day *i* [kg]
$A$ = area of the source [$m^2$]

To determine the mass of chemical on the soil at the start of day *i*, a mass balance must be performed as follows:

$$\Delta M = M_i - M_{i-1} = TR_{add,i} \cdot \Delta t - M_{vol,i-1} \tag{8}$$

where $\Delta M$ = change in mass between the start of day *i* and the start of day *i-1* [kg]
$M_i$ = mass of chemical on the soil at the start of day *i* [kg]
$M_{i-1}$ = mass of chemical on the soil at the start of day *i-1* [kg]
$TR_{add,i}$ = total mass added to soil at the start of day *i* from all releases [kg/day]
$\Delta t$ = change in time [days]
$M_{vol,i-1}$ = mass volatilized in day *i-1* [kg]

The mass volatilized is calculated in Equation 9 as the mass flux multiplied by the surface area of the source.

$$M_{vol,i-1} = J_{i-1} \cdot A \cdot \Delta t \tag{9}$$

where $M_{vol,i-1}$ = mass volatilized in day *i-1* [kg]
$J_{i-1}$ = mass flux from soil to air in day *i-1* [$kg/m^2/day$]
$A$ = area of the source [$m^2$]
$\Delta t$ = change in time [days]

For day *i* and $\Delta t$ of 1 day, the mass on the soil at the start of the day is given by Equation 10.

$$M_i = M_{i-1} + (TR_{add,i} - J_{i-1} \cdot A) \cdot (1\ day) \tag{10}$$

where $M_i$ = mass of chemical on the soil at the start of day *i* [kg]
$M_{i-1}$ = mass of chemical on soil at the start of the previous day *i* [kg]
$TR_{add,i}$ = total mass added to soil at the start of day *i* from all releases [kg/day]
$J_{i-1}$ = mass flux on day *i*-1 [kg/m$^2$/day]
$A$ = area of the source [m$^2$]

Using a hypothetical site with three releases with varying release amounts and release frequencies, Table 16 shows how daily air concentrations are calculated using the equations presented above. Step-by-step details of the calculations are presented in Appendix D.

Once daily air concentrations are determined for the 5-year period (2011-2015), the high-end and mean values, from all the daily-averaged values over the 5-year period, can be calculated. A high-end and mean annual-averaged concentration can also be determined for each of receptor group.

Table 16. Summary of mass flux and air concentrations due to emissions from soil at a hypothetical site with three releases.

| **Day** | **Release #1 (kg/day)** | **Release #2 (kg/day)** | **Release #3 (kg/day)** | **Total Mass Added to Soil from all Releases, $TR_{add}$ (kg/day)** | **Mass on Soil at Start of Day, M (kg)** | **Mass per Area, AR (kg/ha)** | **Mass Flux, J (kg/m$^2$/day)** | **Mass Volatilized from Soil, $M_{vol}$ (kg/ha)** | **AERMOD Unit Value[a] (ug/m$^3$)** | **Air Conc (ug/m$^3$)** |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 100 | 75 | 25 | 200.00 | 200.00 | 10.00 | 2.70E-04 | | 5.43 | 3.41[b] |
| 2 | 0 | 0 | 25 | 25.00 | 212.88 | 10.64 | 2.85E-04 | | 19.1 | 12.7[b] |
| 3 | 0 | 0 | 25 | 25.00 | 234.45 | 11.72 | 3.10E-04 | | 34.6 | 24.9[b] |
| 4 | 0 | 0 | 25 | 25.00 | 257.55 | 12.88 | 3.36E-04 | | 16.5 | 12.9[b] |
| 5 | 0 | 0 | 25 | 25.00 | 278.55 | 13.93 | 3.60E-04 | | 12.5 | 10.4[b] |
| 6 | 100 | 0 | 25 | 125.00 | 398.27 | 19.91 | 4.91E-04 | | 30.9 | 35.3[b] |
| 7 | 0 | 0 | 25 | 25.00 | 421.14 | 21.06 | 5.15E-04 | | 29.1 | 34.9[b] |
| 8 | 0 | 75 | 25 | 100.00 | 518.88 | 25.94 | 6.17E-04 | | 16.9 | 24.3[b] |
| 9 | 0 | 0 | 25 | 25.00 | 540.00 | 27.00 | 6.39E-04 | | 3.96 | 5.90[b] |
| 10 | 0 | 0 | 25 | 25.00 | 548.40 | 27.42 | 6.48E-04 | | 6.79 | 10.3[b] |
| … | continue until *M* or *J* falls below a threshold level of $10^{-7}$ | | | | | | | | | |

[a] AERMOD Unit Value based on 1 g/s of emission

[b] Indicates calculated air concentration exceeds saturation air concentration

# 8 Modeling Approach for Area Water Sources

## 8.1 Overview and Assumptions

The approach for area water sources estimates chemical volatilization from water into air, and is can be used to model releases from wastewater treatment plants or standing bodies of water such as bays, estuaries, or impoundments, or holding ponds. Area water sources are modeled as either a batch or continuous flow-through system, as shown below in Figure 13. The difference between the two systems is the extra chemical loss term for a flow-through system, due to the continuous flow of water into and out of the system.

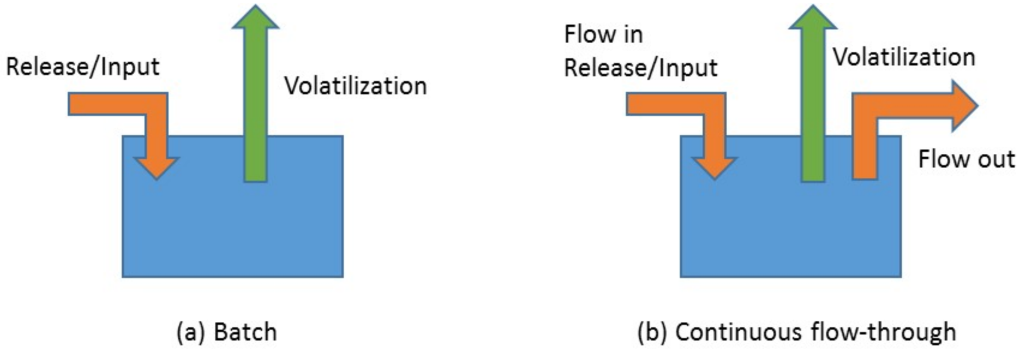


Figure 13. Schematic of area water source, modeled as (a) batch and (b) continuous flow-through system.

The following assumptions are made for area water sources:

- (i) The chemical only leaves the water through volatilization and/or continuous flow out of the system (chemical removal through biodegradation and adsorption to sludge are not considered).
- (ii) Instantaneous mixing occurs.
- (iii) Steady state conditions reached immediately.
- (iv) Releases are applied immediately at the start of each day.
- (v) The first day of all releases is January 1st.
- (vi) Releases are evenly timed throughout the year.
- (vii) The time scale of emissions from area water sources is much longer (hours to days) than the time scale of emissions directly to air (i.e., point and fugitive sources), allowing short-term impacts of meteorology to be excluded.

Like the approach for area soil sources (Section 7), the approach for area water sources uses air concentration results from AERMOD with an emission rate of 1 g/s and an area of 50 acres. To calculate the chemical concentration in air from the area water source, IIOAC uses mass balance calculations to estimate the mass volatilized each day.

## 8.2 Equations to Calculate Daily-Averaged Air Concentrations

All daily-averaged air concentrations are calculated within IIOAC using the equations described in this section. The equations in this section were developed for a flow-through system with a flowrate in and out of the system. For batch systems, the same equations apply; however, the flowrate would be set to zero.

As shown in Equation 11, outdoor air concentrations from area water sources are calculated by multiplying the mass volatilized each day by the unit emission AERMOD result (i.e., in μg/m$^3$) and an area size scaling factor, $SF_j$. The area size scaling factor, $SF_j$, accounts for the size of the area water source and is described in detail in Section 9.2. As short-term meteorological effects can be excluded (see assumptions above), the area water source calculations uses daily-averaged AERMOD results.

$$C_{outdoor,i} = \frac{M_{vol,i}\ /\ day}{1\ g/s} \cdot 0.01157 \cdot SF_j \cdot Postprocessed\ AERMOD\ result_i \tag{11}$$

where $C_{outdoor,i}$ = air concentration for day *i* [μg/m$^3$]
$M_{vol,i}$ = mass volatilized on day *i* [kg]
$0.01157$ = conversion factor from kg/day to g/s
$SF_j$ = scaling factor for area size *j* [–]

All calculated air concentrations are capped at chemical specific saturation air concentrations (Equation 6). If a calculated air concentration is above the saturated air concentration, IIOAC replaces the calculated air concentration for that day with the saturation air concentration. For mass balance purposes, IIOAC returns the chemical mass in excess of the saturation air concentration to the area water source. IIOAC uses concentrations at the inner receptors to determine the excess concentration and corresponding mass to be returned to the water.

For each day, the mass volatilized on day *i* is calculated with Equation 12.

$$M_{vol,i} = k_{vol} \cdot C_i \cdot V \cdot (1\ day) \tag{12}$$

where $M_{vol,i}$ = mass volatilized on day *i* [kg]
$k_{vol}$ = volatilization rate constant [1/day]
$C_i$ = chemical concentration in water on day *i* [kg/m$^3$]
$V$ = volume of the water source [m$^3$]

The volatilization rate constant, $k_{vol}$, is calculated as shown in Equation 13.

$$k_{vol} = \frac{\ln(2)}{t_{1/2} \cdot \frac{1}{24}} \tag{13}$$

where $k_{vol}$ = volatilization rate constant [1/day]

$t_{1/2}$ = half-life of volatilization from water [hrs]
$\frac{1}{24}$ = conversion factor from hrs to days

The volume of the water source is calculated using Equation 14.

$$V = A \cdot d \tag{14}$$

where $V$ = volume of the water source [m$^3$]
$A$ = area of water source [m$^2$]
$d$ = depth of the water source [m]

The half-life of volatilization from water, $t_{1/2}$, is calculated in EPA's Estimation Programs Interface (EPI) Suite screening-level tool (US EPA, 2017b) based on depth of water, water velocity, and wind velocity. EPI Suite uses a two-film concept described in Thomas (1990) to estimate mass flux across the air-water interface, and corresponding volatilization half-lives. In addition to estimating parameters for chemicals with existing CAS numbers, this program also estimates parameters of new chemicals based on their structure.

The mass volatilized on day *i* is dependent on the initial mass in water at the start of the day and is calculated by performing a mass balance on a control volume as shown below (Equations 15 and 16). The concentration of chemical in the water source is assumed to be the same as the concentration exiting the system.

$$\begin{aligned} &change\ in\ mass \\ &\quad = mass\ flow\ in - mass\ flow\ out + total\ mass\ from\ releases - mass\ volatilized \end{aligned} \tag{15}$$

which is calculated as:

$$\Delta M = M_i - M_{i-1} = (Q \cdot C_{in} \cdot \Delta t) - (\, Q \cdot C_{i-1} \cdot \Delta t) + (TR_i \cdot \Delta t) - (k_{vol} \cdot C_{i-1} \cdot V \cdot \Delta t) \tag{16}$$

where $\Delta M$ = change in mass between the start of day *i* and the start of day *i-1* [kg]
$M_i$ = mass of chemical in water at the start of day *i* [kg]
$M_{i-1}$ = mass of chemical in water at the start of day *i-1* [kg]
$Q$ = water flow rate of the system [m$^3$/day]
$C_{in}$ = concentration of chemical in the flow rate into the system [kg/m$^3$]
$C_{i-1}$ = concentration of chemical in the system on day *i-1* [kg/m$^3$]
$\Delta t$ = change in time [days]
$TR_i$ = total mass added at the start of day *i* from all releases [kg]
$k_{vol}$ = volatilization rate constant [1/day]
$V$ = volume of the water area source [m$^3$]

Substituting $C$ for $\frac{M}{V}$, and setting $C_{in}$ to zero because there is no continuous mass flow into the system gives Equation 17.

$$\Delta M = -\frac{Q}{V} \cdot M_{i-1} \cdot \Delta t + TR_i \cdot \Delta t - k_{vol} \cdot M_{i-1} \cdot \Delta t \qquad (17)$$

For day *i* and $\Delta t$ of 1 day, the mass in water at the start of the day is given by Equation 18.

$$M_i = M_{i-1} + \left(TR_i - \left(\frac{Q}{V} + k_{vol}\right) \cdot M_{i-1}\right) \times (1\ day) \qquad (18)$$

Using a hypothetical site with three releases with varying release amounts and release frequencies, Table 17 shows how daily air concentrations are calculated using the equations presented above. Step-by-step details of the calculations are presented in Appendix E.

Once daily air concentrations are determined for the 5-year period (2011-2015), the high-end and mean values, from all the daily-averaged values over the 5-year period, can be calculated. A high-end and mean annual-averaged concentration can also be determined for each of receptor group.

Table 17. Summary of mass volatilized and air concentrations due to emissions from water at a hypothetical site with three releases.

| Day | Release #1 (kg/day) | Release #2 (kg/day) | Release #3 (kg/day) | Total Mass Added to Water from All Releases, $TR_{add}$ (kg/day) | Mass in Water at Start of Day, M (kg/m$^3$) | Mass Volatilized from Water, $M_{vol}$ (kg) | AERMOD Unit Value[a] (ug/m$^3$) | Air Conc (ug/m$^3$) |
|---|---|---|---|---|---|---|---|---|
| 1 | 100 | 75 | 25 | 200 | 200 | 30.1 | 3.42 | 2.67 |
| 2 | 0 | 0 | 25 | 25 | 194.6 | 29.4 | 33.3 | 25.3 |
| 3 | 0 | 0 | 25 | 25 | 190.5 | 28.7 | 63.8 | 47.4 |
| 4 | 0 | 0 | 25 | 25 | 187.4 | 28.1 | 37.8 | 27.6 |
| 5 | 0 | 0 | 25 | 25 | 184.3 | 27.7 | 36.0 | 25.8 |
| 6 | 100 | 0 | 25 | 125 | 281.6 | 42.3 | 11.5 | 12.6 |
| 7 | 0 | 0 | 25 | 25 | 264.3 | 39.7 | 16.5 | 16.9 |
| 8 | 0 | 75 | 25 | 100 | 324.6 | 48.8 | 19.7 | 24.8 |
| 9 | 0 | 0 | 25 | 25 | 300.8 | 45.2 | 34.2 | 40.0 |
| 10 | 0 | 0 | 25 | 25 | 280.6 | 42.1 | 7.00 | 7.63 |
| … | continue until *M* or mass flux[b] falls below a threshold level of $10^{-7}$ | | | | | | | |

[a] AERMOD Unit Value based on 1 g/s of emission

[b] For threshold level, a mass flux was calculated for each day

# 9 Scaling Factors for Fugitive and Area Water/Soil Sources

## 9.1 Overview

For fugitive and area water/soil sources, IIOAC calculates the outdoor air concentration, indoor air concentration, and acute and chronic doses for a user-specified area size and release amount. For fugitive sources, particle deposition is also calculated. However, as the tool uses pre-run AERMOD results with a fixed area size and release amount, scaling factors must be used to scale the AERMOD results according to the area size and the release amount. The application of scaling factors is automatically performed in IIOAC and has been incorporated in the equations in the previous sections to calculate air concentration. This section provides further detail on the scaling factors calculated and used in IIOAC to adjust for both area size and release amount.

## 9.2 Scaling Factor for Different Area Sizes

For fugitive sources and area water/soil sources, AERMOD runs were performed using set area sizes of 100 $m^2$ and 202,343 $m^2$, respectively, the latter which corresponds to 50 acres.

To determine the scaling factor for various area sizes, five area sizes were run in AERMOD using meteorological data for the Iowa City station. It is assumed that the remaining 13 met locations follow the same relationship between area size and air concentration. The rationale for selecting Iowa City to represent all met stations is provided in Section 5.4. A regression equation was fit to the AERMOD outputs to determine the relationship between air concentration and area size for the inner ring and community receptor groups. Using the regression equation, IIOAC estimate air concentrations for area sizes within the range of 25-500 $m^2$ for Fugitive sources and 40,468-2,023,000 $m^2$ (or 10-500 acres) for area Water/Soil sources.

Table 18 provides example data used to determine the regression coefficients. Note that five different area sizes need to be run separately for fugitive and for area water/soil sources due to the difference in release height (3.05 m for fugitive sources and 0 m for area water/soil sources). For the purposes of the example below, the same AERMOD results are used for both fugitive and area water/soil sources. All regression coefficients for fugitive and area sources are provided in Appendix A.

Table 18. Example data of air concentration as a function of area size.

| Area | | Average Concentration in 2011-2015 (μg/m³) | |
|---|---|---|---|
| (acre) | (m²) | Inner Ring | Community |
| 10 | 40,468.6 | 47.75 | 9.37 |
| 20 | 80,937.2 | 35.13 | 8.30 |
| 50 | 202,343 | 21.91 | 6.25 |
| 200 | 809,372 | 9.45 | 3.06 |
| 500 | 2,023,430 | 5.07 | 1.84 |

Using inner ring as an illustrative example, the regression equation is obtained from Figure 14.

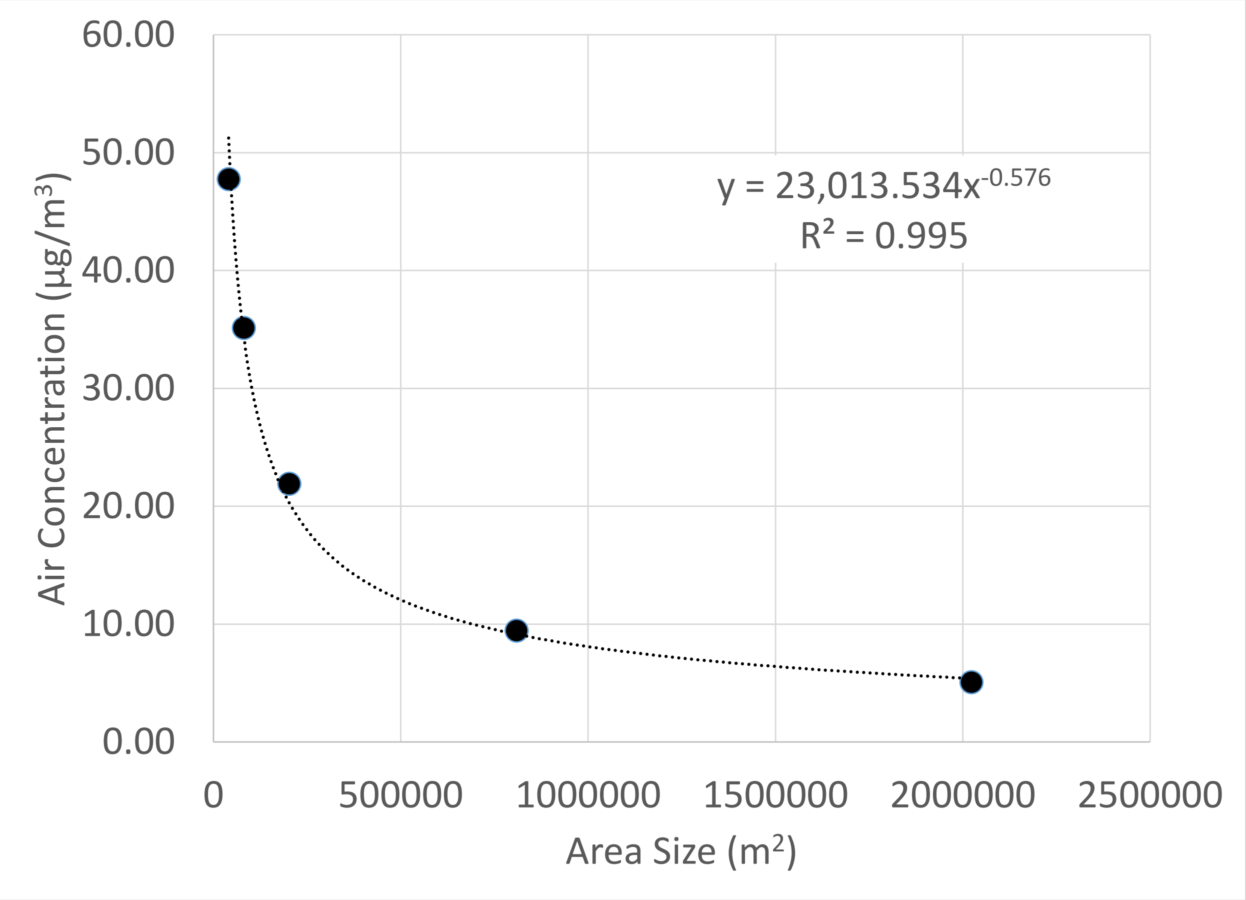


Figure 14. Outdoor air concentration as a function of area size for inner ring receptors.

The regression equation has the form:

$$C = a \cdot A^b \tag{19}$$

where $C$ = air concentration [μg/m³]
$A$ = area size [m²]
$a$ = regression coefficient [–]
$b$ = regression coefficient [–]

Using the example above, for inner ring, the regression coefficients are:

$a$ = 23,013
$b$ = -0.5757

The general equation to calculate a scaling factor for any area, *j*, is given by Equation 20.

$$SF_j = \frac{C_j}{C_{base}} \tag{20}$$

where $SF_j$ = scaling factor for area *j* [–]
$C_j$ = air concentration for area *j* [μg/m³]
$C_{base}$ = air concentration for base area [μg/m³]

For area water/soil sources, where the base area used in the AERMOD runs is 202,343 m², a scaling factor can be calculated for any area, *j*, as shown in Equation 21.

$$SF_j = \frac{a \cdot j^b}{a \cdot A^b} = \frac{j^b}{202{,}343^b} \tag{21}$$

For example, if the user enters an area of 200,000 m² for an area soil/water source, the scaling factor would be 1.01.

For fugitive sources, the base area used in the AERMOD runs is 100 m², which leads to a scaling factor of 0.013 for an area of 200,000 m².

## 9.3 Scaling Factor for Different Emissions

In addition to accounting for different area sizes, a scaling factor is also used to obtain air concentration values corresponding to the user-defined emission rate. AERMOD runs were performed using 1 g/s emission over each area size. For area soil/water sources, the unit emission rate is released over an area of 202,343 m² (50 acres), while for fugitive sources, AERMOD runs were performed using an area of 100 m². When determining the scaling factor to adjust for different emission rates, the area size is assumed to be that used in the AERMOD runs.

The general equation to calculate a scaling factor for different emissions is given by Equation 22.

$$SF_k = \frac{ER_{adj}}{1\ g/s} \tag{22}$$

where $SF_k$ = scaling factor for different emissions [–]
$ER_{adj}$ = adjusted user-defined emission rate [g/s/m$^2$]

The corresponding air concentration is then calculated as:

$$C_k = C_{aermod} \cdot SF_k \tag{23}$$

where $C_k$ = air concentration [μg/m$^3$]
$C_{aermod}$ = air concentration from AERMOD output [μg/m$^3$]
$SF_k$ = scaling factor for different emissions [–]

## 9.4 Overall Calculation of Air Concentration

Combining the two scaling factors above, the air concentration for fugitive and area water/soil is calculated using Equation 24.

$$C_{j,k} = C_{aermod} \cdot SF_j \cdot SF_k \tag{24}$$

where $C_{j,k}$ = air concentration corresponding to user-defined parameters [μg/m$^3$]
$C_{aermod}$ = air concentration from AERMOD output [μg/m$^3$]
$SF_j$ = scaling factor for area *j* [–]
$SF_k$ = scaling factor for different emissions [–]

## 9.5 Illustrative Example to Calculate Scaling Factors

Assume for a fugitive source, the air concentration from the pre-run AERMOD results (corresponding to 100 m$^2$) is 50 μg/m$^3$ for a specific receptor. Using the regression coefficients obtained from Figure 14, where $b$ = -0.5757, a user defined emission of 0.07 g/s, and an area of 650 m$^2$, the air concentration is calculated as:

$$C_{air} = 50\ \frac{\mu g}{m^3} \cdot \frac{650^{-0.5757}}{100^{-0.5757}} \cdot \frac{0.07}{1} = 1.19\ \frac{\mu g}{m^3}$$

# 10 Indoor: Outdoor Ratio

## 10.1 Overview

The indoor-outdoor ratio is a metric that is used to describe the relationship between the concentration of a chemical indoors to the concentration of that chemical outdoors according to Equation 25.

$$C_{indoor} = IO \cdot C_{outdoor} \tag{25}$$

where $C_{indoor}$ = outdoor air concentration [μg/m$^3$]
$C_{outdoor}$ = indoor air concentration [μg/m$^3$]
$IO$ = indoor-outdoor ratio [-]

The indoor-outdoor ratio is influenced by many factors including the characteristics of the building, the meteorological conditions, interior sources or sinks, and the physical form of the chemical substance (particulate or gas). Within IIOAC, indoor air concentrations are calculated by multiplying the modeled ambient air concentrations by an indoor-outdoor ratio.

IIOAC calculates a mean and high-end indoor air concentration based on the outdoor/ambient air concentration and mean and high-end indoor-outdoor ratios. In many screening models, the indoor-outdoor ratio is set to a value of 1, which represents the upper bound of this ratio if there are no indoor sources. In IIOAC, indoor-outdoor ratios of 0.65 and 1 are used for the mean and high-end ratios, respectively. The indoor-outdoor ratio of 0.65 is used to calculate indoor air concentrations corresponding to the mean outdoor air concentration for each receptor group. The indoor-outdoor ratio of 1 is used to calculate the indoor air concentration corresponding to the 95th percentile of outdoor air concentration of each receptor group as shown below in Table 19.

Table 19. Use of indoor-outdoor ratios to calculate indoor air concentration.

| Source Type | Emission Scenario | Statistic | Location | Outdoor Air Concentration (μg/m$^3$) | | Indoor Air Concentration (μg/m$^3$) | |
|---|---|---|---|---|---|---|---|
| | | | | **Daily** | **Annual** | **Daily** | **Annual** |
| Point | Manufacturing | High-End | Fenceline | 9.27 | 0.31 | 9.27 | 0.31 |
| | | | Community | 0.23 | 0.0075 | 0.23 | 0.0075 |
| | | Mean | Fenceline | 6.93 | 0.23 | 4.50 | 0.15 |
| | | | Community | 0.15 | 0.0050 | 0.099 | 0.0033 |

The process used to define the indoor-outdoor ratios used in IIOAC are described in the following sections and include a literature search to identify potential data sources of indoor-outdoor ratios, followed by analysis of these data. As IIOAC focuses on chemicals with exterior sources only, studies where interior sources dominated (and indoor-outdoor ratios are above 1) were not the focus of the search and were eliminated to the extent possible, as explained below.

## 10.2 Literature Search and Screening

To determine the appropriate values for use in the tool, an open literature search was conducted. The goal of the search was to identify potential data sources for all chemicals; then, based on the scope of the information found, a subset of those sources were used to determine refined indoor-outdoor ratios; the search and screening was not intended to collect data from all possible sources in a comprehensive fashion. The search was performed using Web of Science with the search strategy shown in Table 20.

Table 20. Search strategy used to identify potential indoor-outdoor ratio papers.

| Database | Keywords and Web of Science Categories | Date of Search | Number of Returned Studies |
|---|---|---|---|
| Web of Science | TOPIC: (air OR concentration OR concentrations)<br>AND TOPIC:<br>((indoor OR interior OR indoors) AND (outdoor OR outdoors OR ambient OR exterior))<br>*Refined by: WEB OF SCIENCE CATEGORIES: ( ENVIRONMENTAL SCIENCES OR PUBLIC ENVIRONMENTAL OCCUPATIONAL HEALTH OR ENGINEERING ENVIRONMENTAL )*<br>*Timespan: 2000-2017. Indexes: SCI-EXPANDED, SSCI.* | May 26, 2017 | 4,047 |

From the 4,047 results returned using the search strategy outlined above, title/abstract screening and full text screening were used to identify data for inclusion in the analysis. A diagram summarizing the overall screening process is shown in Figure 15 and is discussed below. A subset of titles/abstracts were screened for relevance, where relevance was determined using the acceptance criteria shown in Table 21. An initial batch of 1,525 titles and abstracts were reviewed to find a set of relevant articles that spanned multiple chemicals and conditions. Of these, 526 were marked as relevant using the acceptance criteria. This was termed the “Round 1” screening.

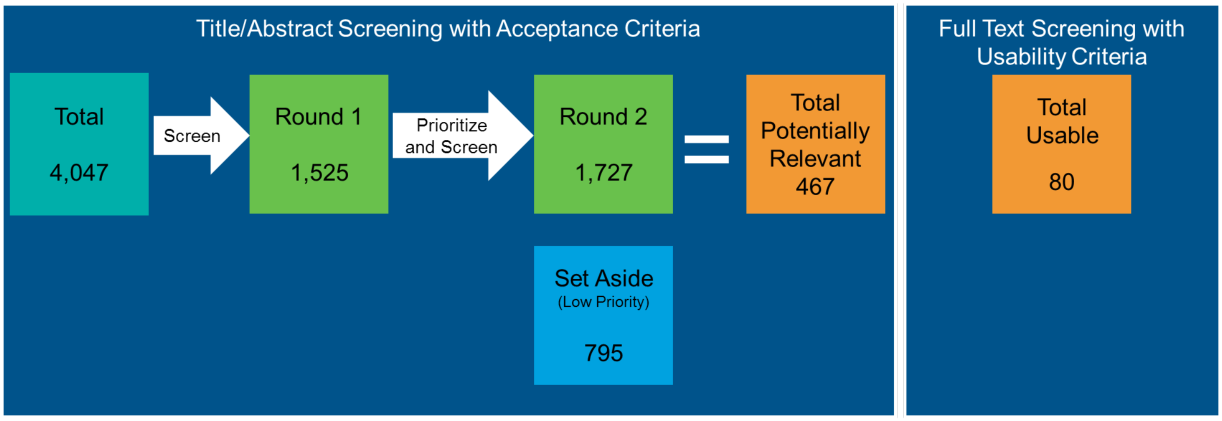


Figure 15. Summary of title/abstract and full text screening.

Table 21. Acceptance criteria applied in title/abstract screening.

| Quality Criterion | Acceptance Specification |
|---|---|
| Currency | • 2000 to present |
| Geographic Scope | • North America and Europe |
| Accuracy/Reliability | • Publication in peer-reviewed journal and is a primary source<br>• Source has documented qualifications/ credentials to discuss particular topic<br>• The chemical measured is clearly noted in the text |
| Unbiased | • Objective of the information is clear<br>• Methodology is designed to answer a specific question and is clearly described |
| Comparability | • Range of ratios is comparable to other studies of a similar chemical |
| Representativeness | • Sample size (in terms of number of buildings sampled or number of time points sampled) is greater than or equal to five |

Full review of all 4,047 references was not feasible with available resources and was not necessary to meet the project objectives, so prioritization techniques were used to select the full set of studies to be screened. For prioritization, text analytic algorithms (K-means and Non-negative matrix factorization, Varghese et al., 2017) were used to find studies whose titles and abstracts were similar to the relevant studies in the initial search, as shown in Figure 16. These algorithms create a user-defined number of study clusters based on keyword similarities in the title and abstract, and each algorithm is broadly-accepted in the text analytics scientific field. For this analysis, each of the algorithms was used to bin the studies into 10, 20, or 30 clusters, for a total of six different cluster analyses (six large circles in the figure). A random sample of sixty of the studies identified as relevant during Round 1 was included in the full body of literature that was clustered and served as “tracer” studies (pink circles in the figure). The tracer method involves following these relevant studies and determining the clusters the majority occur in; these clusters are then deemed more likely to contain other (as-yet unidentified) relevant studies.

To identify these high-priority clusters, the clusters containing up to 75% of the Round 1 relevant tracer studies were collected for each of the six analyses. These were termed the “high concentration of tracer” clusters. All non-tracer studies in those high-concentration clusters were then marked as “positive” for that analysis. Across the six analyses, studies were retained as sufficiently similar to the Round 1 relevant studies if they were “positive” in two or more analyses; studies that clustered with the Round 1 relevant studies in zero or one analysis were set aside from further screening. This ensemble method is used to increase confidence in the selection of prioritized studies by mitigating uncertainty from each individual analysis. After the prioritization, of the remaining 2,522 studies, 1,727 were identified as similar to the relevant tracer studies and their titles and abstracts were screened in Round 2.

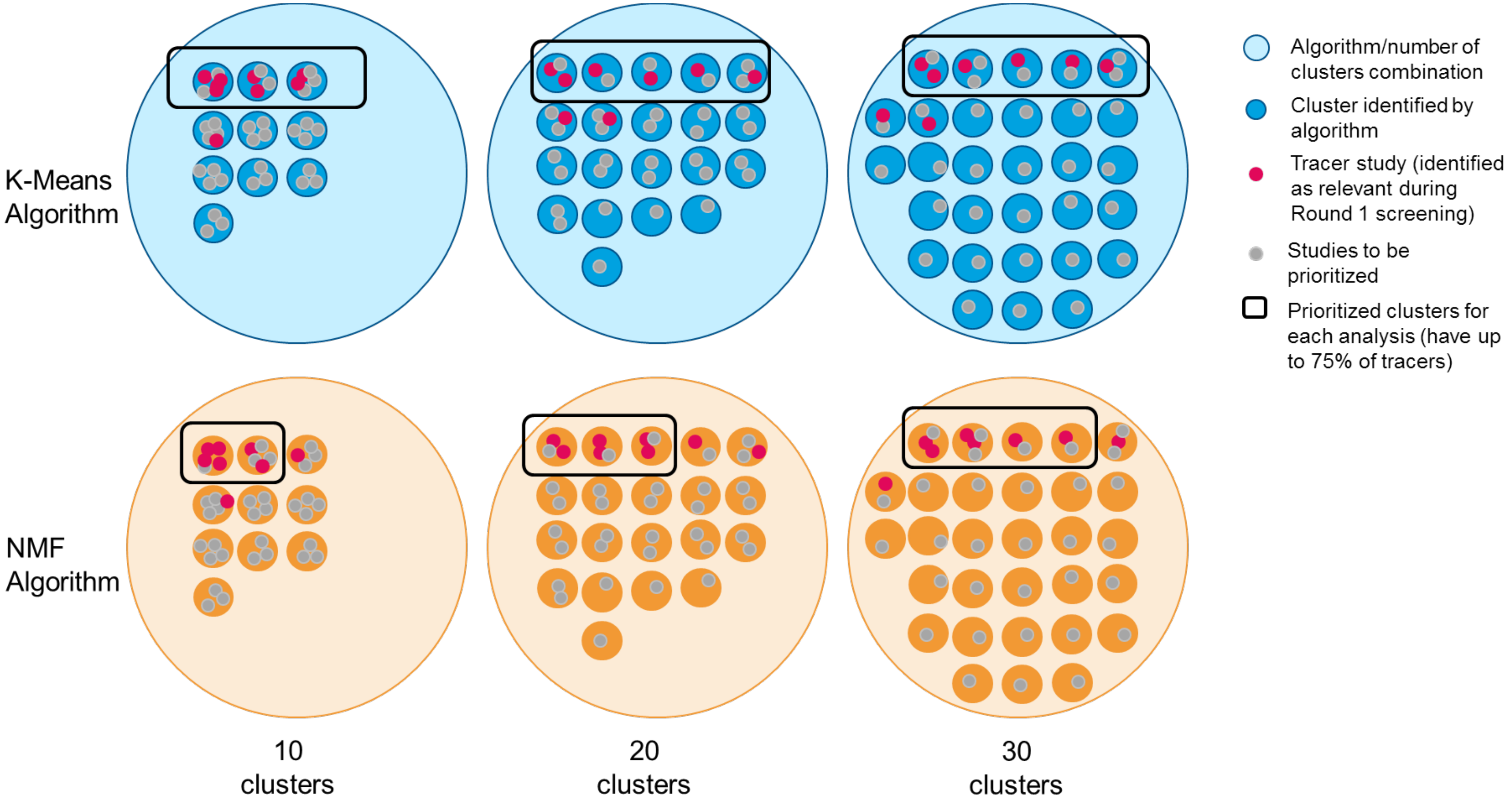


Figure 16. Ensemble text analytics method for prioritizing studies for screening.

After the completion of Round 1 and 2 title/abstract screening, 467 studies were identified as potentially relevant based on the title and abstract. Full text screening was then implemented for those studies with additional usability criteria (Table 22). These criteria focused on the practicality of extracting information from the study and on limiting the impact of indoor sources.

With regard to limiting indoor source effects, note that IIOAC is intended for use to estimate exposure from ambient sources for a wide variety of chemicals. The indoor sources of each chemical is likely unknown and is being excluded from consideration at this time. Thus, the indoor-outdoor ratio should not reflect ratios where indoor sources played a large role in the overall indoor concentration. Figure 17 illustrates how indoor sources might contribute to the overall indoor-outdoor ratio, where strong indoor sources might lead to ratios either above one (left) or less than one (middle). Ideally, we want to capture the indoor-outdoor ratio when no indoor sources are present (right). However, practically speaking, it is impossible to exclude studies with strong indoor sources without explicit information about the relative contribution from the study authors. Because this information is not typically available, the screening focused on studies where the indoor-outdoor ratio mean is less than one; this method provides a simple way to limit the impact of indoor sources (excludes studies where the mean measurement resembles the left side of Figure 17), although it does not completely eliminate the impact (includes studies where the mean measurement may resemble the center of Figure 17). Studies with means greater than one were handled differently in two different cases:

- **Study provided individual measurements**: if the study provided individual measurements, the measurements greater than one were excluded and the mean was recalculated by the screener; this occurred in 23 of the 404 total measurements used in the final analysis. This recalculation was intended to refocus the calculation on the study buildings without strong indoor sources.
- **Study did not provide individual measurements**: if the study did not provide individual measurements, the study was excluded as not usable.

In this round, 80 studies were identified as both relevant and usable.

Table 22. Usability criterion applied in full text screening.

| Quality Criterion | Usability Specification |
|---|---|
| Usability | • PDF of article is available<br>• At least one measurement of indoor-outdoor ratio in the study is less than one and the mean indoor-outdoor ratio is not greater than one. If measurements greater than one from the original study can be excluded and a new mean calculated, this calculation was performed and the resulting mean was flagged.<br>• Ratios are summarized in tables (no figures were digitized) |

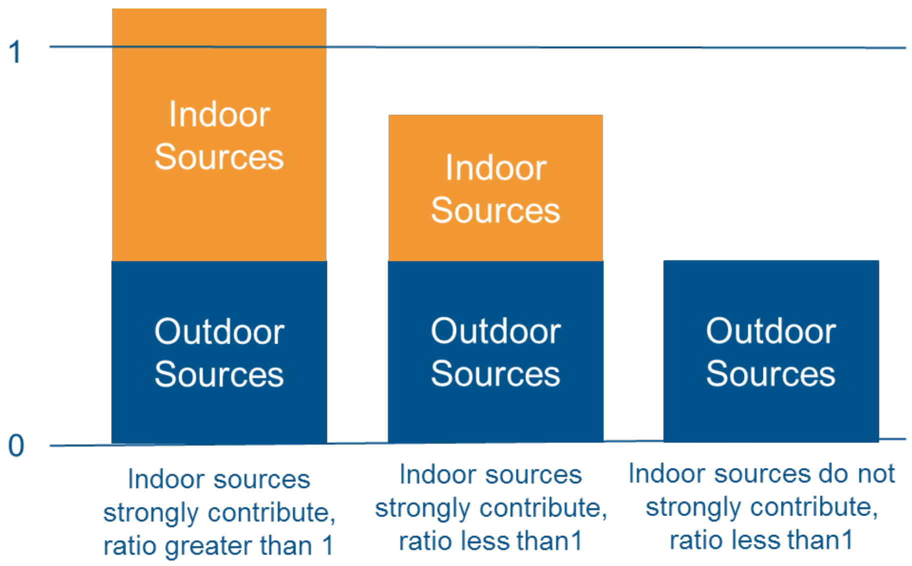


Figure 17. Diagram illustrating indoor-outdoor ratios with different fractional indoor source contributions.

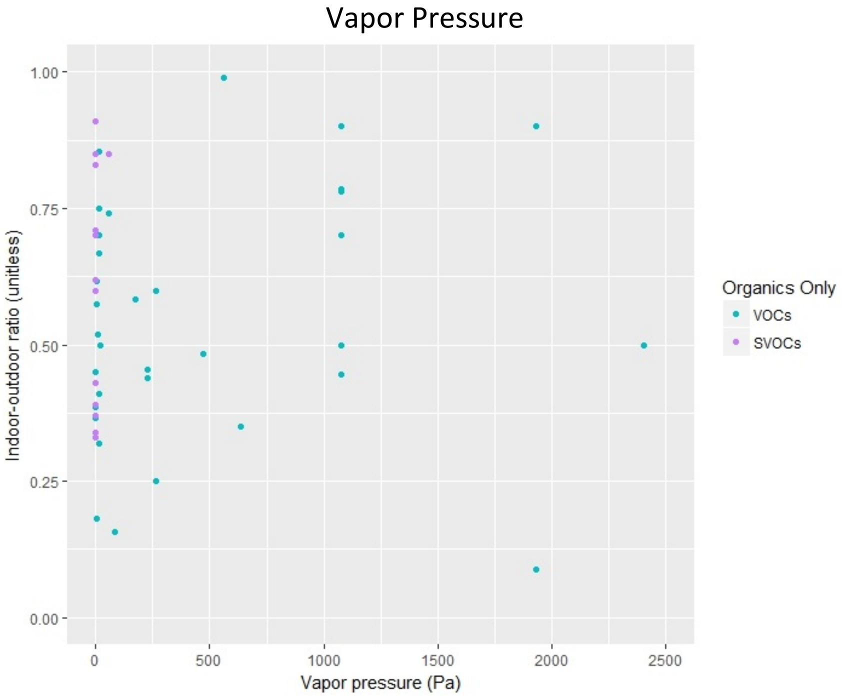
As full text screening identified relevant and usable studies, key study attributes for those studies were extracted into an Excel spreadsheet. Attributes were selected based on the knowledge of what might affect the indoor-outdoor ratio. These included:

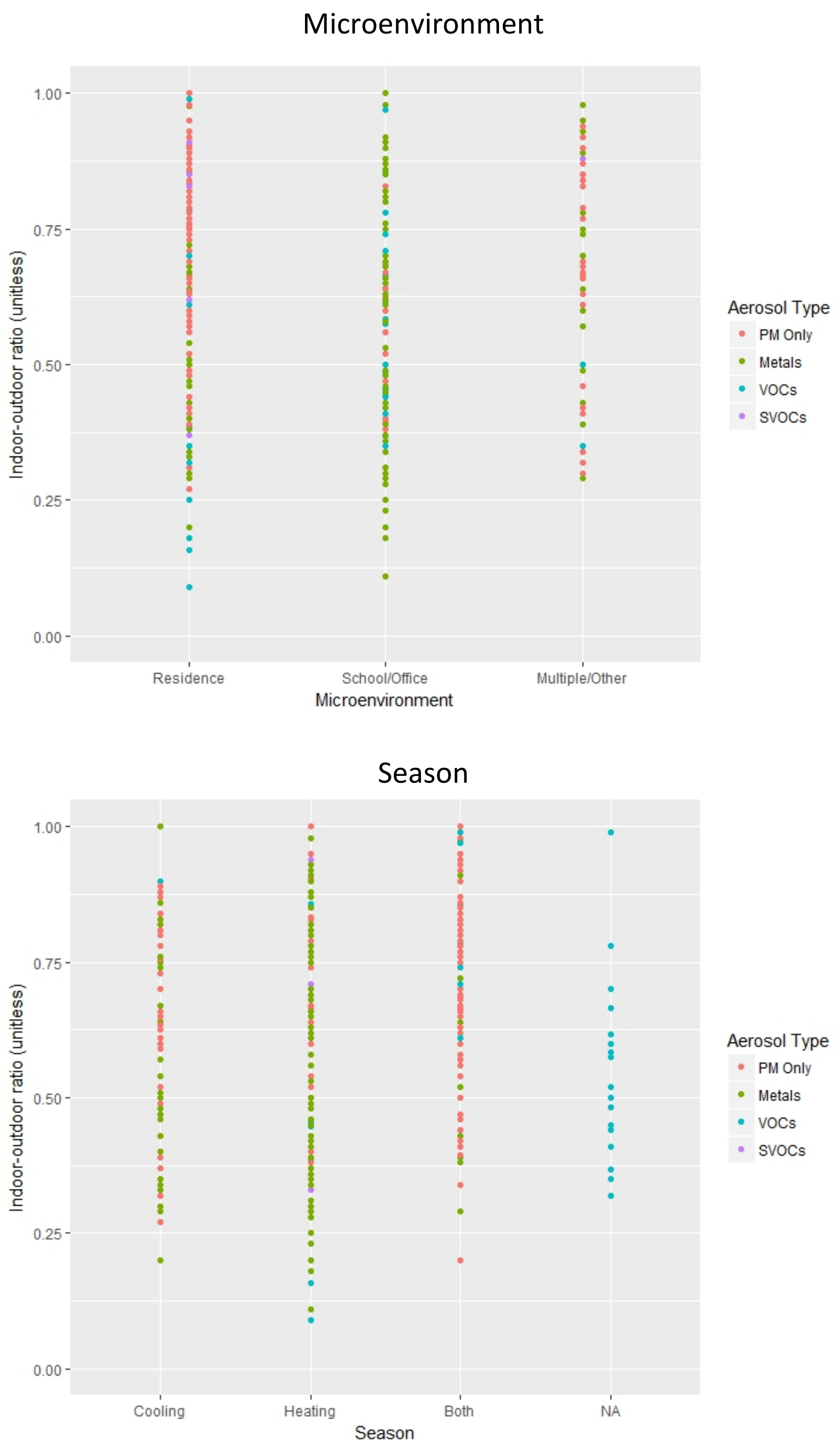
- Chemical/Particle type
    - Particulate matter
        - Particulate matter only
        - Organics on particulate matter
        - Metals on particulate matter
    - Vapor Phase
        - Free organics
            - Semi volatile organic compounds (SVOCs)
            - Volatile organic compounds (VOCs)
        - Free Metals
- Chemical Name, with CAS number and vapor pressure
- Particle size range (for particulate only)
- Microenvironment type
- Location
- Season
- Number of sites/measurements
- Indoor-outdoor ratio minimum
- Indoor-outdoor ratio maximum
- Indoor-outdoor ratio mean or median
- Indication of whether ratio was calculated by screener

In cases where paired concentrations (indoor and outdoor) at the same location were provided but the actual indoor-ratio was not calculated in the paper, these ratios were calculated and flagged as “ratio calculated by screener”.

## 10.3 Data Analysis

Next the data were examined by the different attributes collected to determine trends by chemical/particle type, microenvironment, and season. Figure 18 below shows the graph of central tendency (mean or median depending on the individual study) indoor-outdoor ratio by vapor pressure, by microenvironment, and by season. In general, the figures do not indicate a trend by any of these variables; instead, the values are spread between zero and one somewhat uniformly across the different variable values. This suggests the variation in individual building parameters and local conditions may affect the indoor-outdoor ratio more strongly than the chemical properties, microenvironment type, or season.




Microenvironment

Season

Figure 18. Central tendencies of indoor-outdoor ratios grouped by vapor pressure, microenvironment, and season.

Because numerical trends were not observed in the individual means, the data were compiled by finding the mean across usable data for a variety of different chemical types as shown in Table 23  and Figure 19. Table 23 has a) the mean calculation restricted to studies that provided means and b) the mean calculation including studies that provided either a mean or median. A comparison between the two sets of columns indicates inclusion of the medians does not strongly affect the overall mean for each chemical category. Table 23 also stratifies the data in different ways to determine any overall trend for different particulate matter (PM) types or different aggregation of organics (e.g., SVOCs versus VOCs, free SVOCs versus SVOCs on particulate matter, etc.). Aside from SVOCs on PM (which uses only two studies), all the different categories indicate mean ratios between 0.55 and 0.7 with standard deviations of approximately 0.2. In addition, the SVOCs on PM differences from the overall mean is not statistically significant. The consistency of mean values across different chemical types and in a variety of different study designs suggests this value of 0.65 with a standard deviation of 0.2 (the “overall” value) is representative of an expected value for an indoor-outdoor ratio for a variety of chemicals/microenvironments/seasons. A corresponding “high” value could be the central tendency plus two standard deviations, but in this case 0.65 + 0.4 is greater than one; thus, an upper value of one is used. These final values are shown in Table 24.

Table 23. Summary of means and standard deviations of indoor-outdoor ratios by chemical type.

| Category | Aerosol | No. of central tendencies (Unique studies) | Means only | | All central tendencies | |
|---|---|---|---|---|---|---|
| | | | Mean | Std Dev | Mean | Std Dev |
| **Overall** | | **367 (80)** | **0.65** | **0.22** | **0.65** | **0.21** |
| **PM** | **PM (All)**[a] | **305 (66)** | **0.65** | **0.20** | **0.66** | **0.20** |
| | PM Only | 164 (59) | 0.69 | 0.17 | 0.69 | 0.18 |
| | Organics (SVOCs) on PM | 3 (2) | 0.81 | 0.18 | 0.81 | 0.18 |
| | Metals on PM | 138 (15) | 0.61 | 0.22 | 0.62 | 0.22 |
| **Organics** | **Organics (All)**[b] | **64 (17)** | **0.59** | **0.23** | **0.61** | **0.23** |
| | **Free VOCs and SVOCs** | **61 (15)** | **0.57** | **0.23** | **0.60** | **0.23** |
| | Free VOCs | 45 (11) | 0.58 | 0.23 | 0.61 | 0.24 |
| | Free SVOCs | 16 (4) | 0.57 | 0.21 | 0.57 | 0.21 |
| | SVOCs on PM | 3 (2) | 0.81 | 0.18 | 0.81 | 0.18 |
| | SVOCs (All)[c] | 19 (6) | 0.60 | 0.22 | 0.60 | 0.22 |

[a] : Organics on PM and Free SVOCs

[b]: Organics on PM, Free SVOCs, and Free VOCs

[c] : PM Only, Organics on PM, and Metals on PM

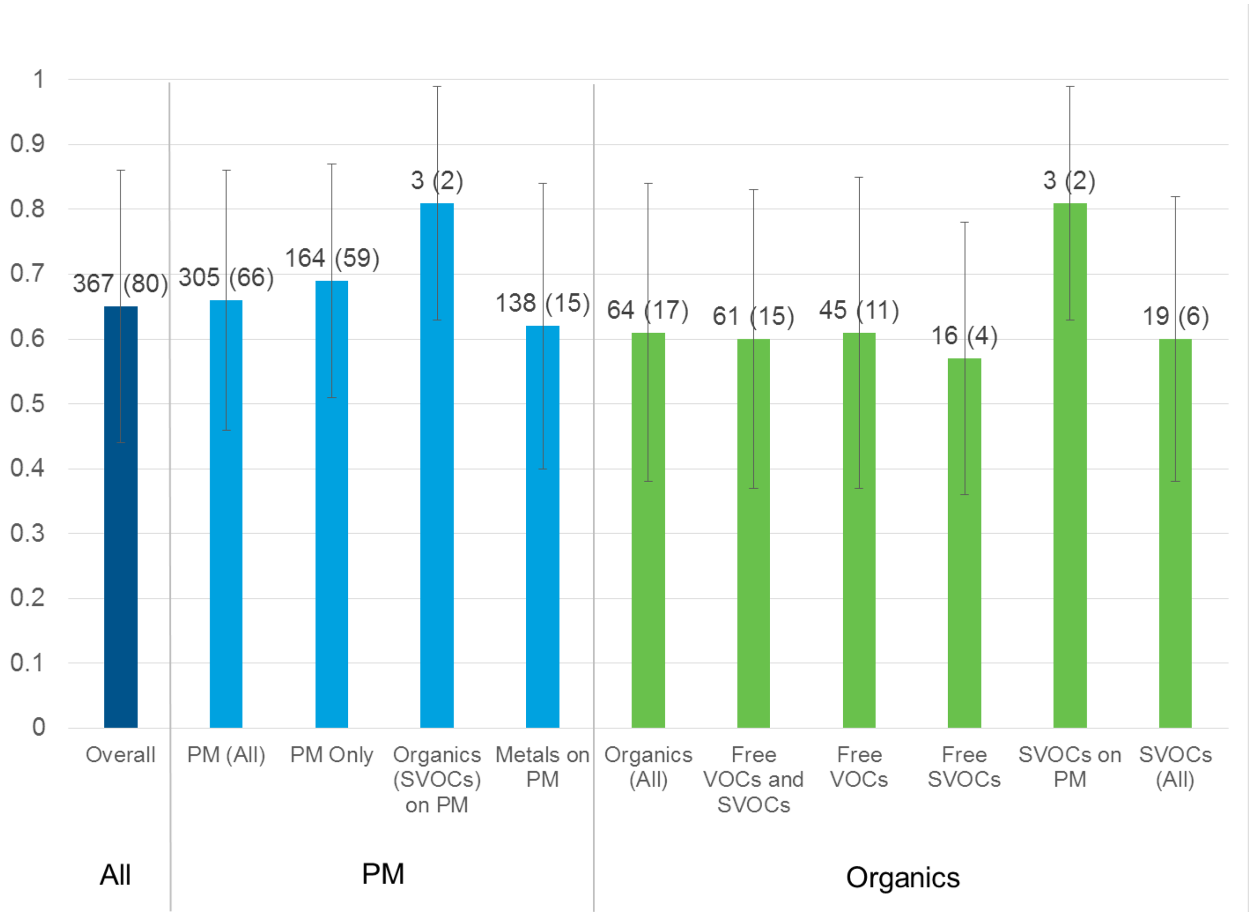


Figure 19. Summary of indoor-outdoor ratio means and standard deviations for different chemical types. Number labels are the number of measurements (number of studies); error bars are the standard deviations.

Table 24. Final summary of indoor-outdoor ratios.

| | Central Tendency | High |
|---|---|---|
| **Indoor/outdoor ratio** | **0.65** | **1.00** |

## 10.4 Illustrative Example to Calculate Indoor Air Concentration

Assume IIOAC calculates an outdoor air concentration of 75 $\mu g/m^3$ for a specific receptor. The corresponding high-end and mean indoor air concentrations are calculated as follows:

$$C_{indoor,high} = C_{outdoor} = 75\ \frac{\mu g}{m^3}$$

$$C_{indoor,mean} = 0.65 \times C_{outdoor} = 48.75\ \frac{\mu g}{m^3}$$

# 11 Dose Calculations

Acute and chronic dose rates by age group are calculated for the two receptor categories as given by Equations 26 and 27 (Versar, Inc., 2007).

$$ADR_{POT} = \frac{AC_{24} \cdot InhR \cdot ED \cdot CF_1}{BW \cdot AT} \tag{26}$$

$$LADD_{POT} = \frac{AC_{yr} \cdot InhR \cdot ED \cdot CF_1}{BW \cdot AT} \tag{27}$$

where $ADR_{POT}$ = potential acute dose rate [mg/kg/day]
$LADD_{POT}$ = potential chronic average daily dose [mg/kg/day]
$AC_{24}$ = weighted daily-averaged air concentration [µg/m$^3$]
$AC_{yr}$ = weighted annual-averaged average air concentration [µg/m$^3$]
$InhR$ = inhalation rate, in m$^3$/day for LADD$_{POT}$, and in m$^3$/hr for ADR$_{POT}$
$ED$ = exposure duration, in years for LADD$_{POT}$, and in days for ADR$_{POT}$
$BW$ = body weight [kg]
$AT$ = averaging time, in years for LADD$_{POT}$, and in days for ADR$_{POT}$
$CF_1$ = conversion factor from mg to µg, and is equal to 10$^{-3}$ mg/µg

The weighted daily-averaged and annual-averaged air concentrations are calculated using the outdoor and indoor air concentrations, and the daily activity patterns that specify the time spent outdoors and indoors:

$$AC = \left(\frac{t_{out}}{t_{in}+t_{out}}\right) \cdot C_{outdoor} + \left(\frac{t_{in}}{t_{in}+t_{out}}\right) \cdot C_{indoor} \tag{28}$$

where $AC$ = weighted daily-averaged or annual-averaged air concentration [µg/m$^3$]
$t_{out}$ = total time spent outdoors in one day [min]
$t_{in}$ = total time spent indoors in one day [min]
$C_{outdoor}$ = outdoor air concentration calculated in IIOAC [µg/m$^3$]
$C_{indoor}$ = indoor air concentration calculated using *IO* ratio [µg/m$^3$]

Parameters for inhalation rates, body weights, exposure durations, and activity patterns by age group are obtained from the Exposure Factors Handbook (US EPA, 2011) and the E-FAST documentation manual (Versar Inc., 2007) and are presented in Table 25-Table 28 below.

Table 25. Mean body weights by age group (taken from Table 8-1 in US EPA, 2011).

| Age Range | Mean Body Weight (kg) |
|---|---|
| Birth to 1 month | 4.8 |
| 1 to <3 months | 5.9 |
| 3 to <6 months | 7.4 |
| 6 to <12 months | 9.2 |

| | |
|---|---|
| 1 to <2 years | 11.4 |
| 2 to <3 years | 13.8 |
| 3 to <6 years | 18.6 |
| 6 to <11 years | 31.8 |
| 11 to <16 years | 56.8 |
| 16 to <21 years | 71.6 |
| Adults | 80.0 |

Table 26. Average inhalation rates for light intensity by age group (taken from Tables 6-1 and 6-2 in US EPA, 2011).

| Age Range | Average Inhalation Rate ($m^3$/day) (chronic) | Average Inhalation Rate ($m^3$/hr) (acute) |
|---|---|---|
| Birth to 1 month | 3.6 | |
| 1 to <3 months | 3.5 | |
| 3 to <6 months | 4.1 | |
| 6 to <12 months | 5.4 | |
| Birth to <1 year | 5.4 | 0.456 |
| 1 to <2 years | 8.0 | 0.72 |
| 2 to <3 years | 8.9 | 0.72 |
| 3 to <6 years | 10.1 | 0.66 |
| 6 to <11 years | 12.0 | 0.66 |
| 11 to <16 years | 15.2 | 0.78 |
| 16 to <21 years | 16.3 | 0.72 |
| 21 to <31 years | 15.7 | 0.72 |
| 31 to < 41 years | 16.0 | 0.72 |
| 41 to <51 years | 16.0 | 0.78 |
| 51 to <61 years | 15.7 | 0.78 |
| 61 to <71 years | 14.2 | 0.72 |
| 71 to <81 years | 12.9 | 0.72 |
| > 81 years | 12.1 | 0.72 |

Table 27. Exposure duration for acute and chronic exposures by age group (taken from Table 3-2 in Versar, Inc. 2007). Exposure duration for adults was modified from 30 to 33 years.

| Age range | Exposure Duration |
|---|---|
| Birth to <1 year | 1 day (acute) |
| 1 to <2 years | 1 day (acute) |
| 2 to 5 years | 1 day (acute) |
| 6 to 12 years | 1 day (acute) |
| 13 to 19 years | 1 day (acute) |
| Adult | 1 day (acute) |
| Adult | 33 years (chronic) |

Table 28. Recommended values for activity patterns by age group (taken from Table16-1 in US EPA, 2011).

| Age Range | Total Time Indoors (min) | Total Time Outdoors (min) |
|---|---|---|
| Birth to <1 month | 1,440 | 0 |
| 1 to <3 months | 1,432 | 8 |
| 3 to <6 months | 1,414 | 26 |
| 6 to <12 months | 1,301 | 139 |
| 1 to <2 years | 1,353 | 36 |
| 2 to <3 years | 1,316 | 76 |
| 3 to <6 years | 1,278 | 107 |
| 6 to <11 years | 1,244 | 132 |
| 11 to <16 years | 1,260 | 100 |
| 16 to <21 years | 1,248 | 102 |
| 18 to <65 years | 1,159 | 281 |
| ≥65 years | 1,142 | 298 |

IIOAC calculates acute and chronic exposure doses for the three age groups listed below using an age of 78 years to define the upper bound of adults. If necessary, a weighted body weight and inhalation rate is calculated for these age groups using the values listed in Table 25 and Table 26:

- Young toddler (1- <2 years),
- Adult (16- <78 years), and
- Lifetime (0- <78 years) – calculated for chronic exposure doses only.

For acute dose, IIOAC outputs only the exposure doses for the Young toddler and Adult age groups. For chronic dose, the Young Toddler, Adult, and Lifetime groups are displayed. Only selected age groups are output because preliminary analysis of IIOAC results indicated the maximum exposure doses always occurred in the Young toddler group. Exposure doses for the additional age groups listed below can be calculated using equations 26-28:

- Infant (<1 year),
- Young toddler (1- <2 years),
- Toddler (2- <3 years),
- Small child (3- <6 years),
- Child (6- <11 years), and
- Teen (11- <16 years).

# 12 Example Application of IIOAC

In addition to calculating air concentration and particle deposition for various scenarios, the IIOAC tool or its results can be used in various applications. One potential application of IIOAC is to determine the emission rate for each source type that would result in a specific air concentration. For example, if the user is interested in an upper limit of 10 ug/m$^3$ for a daily-averaged air concentration or an upper limit of 0.1 ug/m$^3$ for the annual-averaged air concentration, IIOAC can be used to determine the corresponding emission rate.

The approach for determining the emission rate depends on the source type. For point and fugitive sources, AERMOD results were post-processed and placed in lookup tables. As a result, the user can select a scenario and use the values in the lookup table to calculate the emission rate corresponding to 10 ug/m$^3$ for a daily-averaged air concentration or 0.1 ug/m$^3$ for the annual-averaged air concentration as follows:

$$ER_{adj} = \frac{C_{outdoor} \cdot 1\ g/s}{SF_j \cdot Postprocessed\ AERMOD\ result} \tag{29}$$

$$ER = \frac{ER_{adj}}{0.2778} \cdot h \tag{30}$$

For area soil/water sources, calculations are performed in the tool itself and therefore, back-calculation of the emission rate from a target air concentration is not possible. The user needs to use a trial-and-error approach to determine the emission rate.

As an illustrative example, the emission rate for each source type was calculated below for Idaho Falls, ID station. To obtain the most conservative value, it is assumed that the release occurs on one day out of the year (and therefore the selection of cyclical versus consecutive release days does not affect the results). For point and fugitive sources, the release duration is 1 hr and as such, the emission rate is equal to the adjusted emission rate. Additional parameters selected are shown in the table below. For area soil/water sources, benzene is used as the example chemical (vapor pressure = 75 Torr; solubility = 1790 mg/L; Koc = 66.1; volatilization half-life = 1 hr; molecular weight = 78.1 g/mol). Note that area soil/water sources only allow for 24 hour release duration.

Table 29. Emission rates corresponding to target maximum air concentrations.

| | | **Emission Rate** | |
|---|---|---|---|
| **Source Type** | **Parameters** | **Maximum daily-averaged air concentration of 10 ug/m3** | **Maximum annual-averaged air concentration of 0.1 ug/m3** |
| Point | Stack, Urban, Vapor, Consecutive, 1 hr duration, 1 day/yr, Idaho Falls | 71 kg/day | 257 kg/day |
| Fugitive | Urban, Vapor, 100 $m^2$, Consecutive, 1 hr duration, 1 day/yr, Idaho Falls | 22 kg/day | 82 kg/day |
| Area Soil | Urban, Vapor, 10 acres, 1 day/yr, Idaho Falls | 0.05 mg/day | 0.25 mg/day |
| Area Water | Urban, Vapor, 10 acres, 1 day/yr, Idaho Falls, 100 $m^3$/day | 800 kg/day | 3000 kg/day |

# 13 Remaining Uncertainties and Potential Future Updates

In the development of IIOAC, several assumptions were made, leading to uncertainties in the outputs of IIOAC. Potential future updates can address the following issues:

- Use of generic parameters rather than facility specific parameters.
- Use of regional meteorological and land cover data as representative of site-specific meteorological and land cover.
- No chemical-specific properties were accounted for in the point and fugitive source outputs, thus atmospheric chemistry and degradation were not factored in and vapor deposition was not calculated as this requires chemical-specific properties.
- Assumption that the regression relationships (relating source size and AERMOD outputs) derived using Iowa City, IA meteorology data would be roughly applicable to other meteorological conditions from the other 13 meteorology stations.

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# Appendix A Regression Coefficients for Air Concentration versus Area Size

Regression coefficients for fugitive and area sources are provided below where the regression equation has the form:

$$C = a \cdot A^b$$

where $C$ = air concentration [μg/m$^3$]
$A$ = area size [m$^2$]
$a$ = regression coefficient [–]
$b$ = regression coefficient [–]

Table A1. Regression coefficients for fugitive and area sources.

| | | **Inner Ring** | **Community** |
|---|---|---|---|
| Fugitive, Coarse, Rural | a = | 154.47 | 9.12 |
| | b = | -0.05298 | -0.0205 |
| Fugitive, Coarse, Urban | a = | 109.95 | 5.29 |
| | b = | -0.06118 | -0.01674 |
| Fugitive, Fine, Rural | a = | 74.73 | 6.77 |
| | b = | -0.04418 | -0.01582 |
| Fugitive, Fine, Urban | a = | 43.97 | 2.58 |
| | b = | -0.05751 | -0.01669 |
| Fugitive, Vapor, Rural | a = | 142.91 | 13.21 |
| | b = | -0.04507 | -0.01585 |
| Fugitive, Vapor, Urban | a = | 83.76 | 4.95 |
| | b = | -0.05675 | -0.01659 |
| Area | a = | 7.18 | 0.0716 |
| | b = | 0.2092 | 0.3923 |

# Appendix B Comparison of AERMOD Results for Selected Point Sources

The three options for point source offered in IIOAC (the stack, incinerator 1, and incinerator 2 point sources) were created so that together they would result in a wide range of air concentrations. As shown below, the stack point source should generally result in the highest air-concentration and deposition values relative to the other point sources, due to its lower height and lower plume rise (due to lower buoyancy and momentum). The two incinerator point sources should generally result in much smaller air-concentration and deposition values relative to the stack source, due to their higher heights and plume rise values—the incinerator 2 in particular should often show reductions in air-concentration and deposition values of more than 90 percent relative to the stack source, at receptor locations both close to and farther away from the emission source. Comparisons of air concentrations were made at the inner ring or fenceline receptors and an outer ring, set to 1000 m from the source.

Table B1. Comparison of air concentration for the three point sources at the inner and outer ring from a test run.

| | **Stack** | **Incinerator 1** | **Incinerator 2** |
|---|---|---|---|
| Height (m) | 10 | 25 | 50 |
| Temperature (K) | 300 | 500 | 1200 |
| Diameter (m) | 2 | 1 | 2 |
| Velocity (m/s) | 5 | 15 | 15 |
| Example Run – Annual Average Unit Concentration at Inner Ring (0, 100 meters) (µg/m3) | | | |
| Value | 5.830E+00 | 5.150E-02 | 1.839E-03 |
| Reduction vs. Stack | -- | 99.12% | 99.97% |
| Example Run - Annual Average Unit Concentration at Outer Ring (0,1000 meters) (µg/m3) | | | |
| Value | 4.240E-01 | 1.250E-01 | 3.367E-02 |
| Reduction vs. Stack | -- | 70.52% | 92.06% |

# Appendix C Illustrative Example for Facility Sources

Assume the user inputs three point source releases that occur at the same site, selects fine particles, and enters release data according to the following:

Table C1. User inputs for example releases for a point source.

| User Input | | | |
|---|---|---|---|
| | kg/day/site | # days/year | # hours/day |
| Release #1 | 100 | 73 | 24 |
| Release #2 | 75 | 52 | 4 |
| Release #3 | 25 | 365 | 1 |

Using Equation 1, the adjusted emission rate for the three releases are calculated as follows:

$$ER_{adj,1} = \frac{100}{24} \cdot 0.2778 = 1.157\frac{g}{s}$$

$$ER_{adj,2} = \frac{75}{4} \cdot 0.2778 = 5.208\frac{g}{s}$$

$$ER_{adj,3} = \frac{25}{1} \cdot 0.2778 = 6.944\frac{g}{s}$$

Based on the number of days per year and the hours of release per day, IIOAC looks up the corresponding AERMOD post-processed result and outputs the mean and high-end daily-averaged and annual-averaged hourly concentrations. In Table C2 below, hypothetical data have been used to fill in the lookup table.

Table C2. Example AERMOD post-processed air concentration results corresponding to the number of release days and release duration for releases 1, 2, and 3.

| Air Concentration (µg/m$^3$) | Release Duration (hrs/day) | Number of Release Days | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | … | 51 | 52 | … | 72 | 73 | … | 365 |
| Mean Daily Average | 1 | | | | | | | | | | 1.1 |
| | 4 | | | | | 0.8 | | | | | |
| | 8 | | | | | | | | | | |
| | 24 | | | | | | | | 0.7 | | |
| High-End Daily Average | 1 | | | | | | | | | | 6.1 |
| | 4 | | | | | 1.4 | | | | | |
| | 8 | | | | | | | | | | |
| | 24 | | | | | | | | 1.2 | | |
| Mean Annual Average | 1 | | | | | | | | | | 0.6 |
| | 4 | | | | | 0.3 | | | | | |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | 8 | | | | | | | | | | |
| | 24 | | | | | | | | 0.4 | | |
| High-End Annual Average | 1 | | | | | | | | | | 1.0 |
| | 4 | | | | | 0.6 | | | | | |
| | 8 | | | | | | | | | | |
| | 24 | | | | | | | | 1.1 | | |

For point source releases 1, 2, and 3, the high-end daily-averaged air concentration is calculated as:

$$High\text{-}end\ daily\text{-}averaged\ air\ conc_{ER1} = 1.157 \cdot \frac{1.2}{1} = 1.39\ \frac{\mu g}{m^3}$$

$$High\text{-}end\ daily\text{-}averaged\ air\ conc_{ER2} = 5.208 \cdot \frac{1.4}{1} = 7.29\ \frac{\mu g}{m^3}$$

$$High\text{-}end\ daily\text{-}averaged\ air\ conc_{ER3} = 6.944 \cdot \frac{6.1}{1} = 42.4\ \frac{\mu g}{m^3}$$

For fine particles, an upper limit of 35 μg/m$^3$ is applied to each of the individual point source releases. In the example above, only the third point source release results in an air concentration greater than the upper limit. For the three releases, the high-end daily-averaged air concentration is then equal to the sum of the high-end daily-averaged air concentrations for each of the individual releases, or 43.7 μg/m$^3$

# Appendix D Illustrative Example for Area Soil Sources

Assume the user inputs three releases and the physicochemical properties of a chemical according to the following table:

Table D1. User inputs for example releases for an area soil source.

| User Input | | | Tool Conversion |
|---|---|---|---|
| | kg/day/site | # days/year | Release occurs |
| Release #1 | 100 | 73 | Every 5 days |
| Release #2 | 75 | 52 | Every 7 days |
| Release #3 | 25 | 365 | Every day |
| | | | |
| Chemical = | Aldicarb | | |
| MW = | 190.26 | g/mol | |
| VP = | 0.01 | Pa | |
| Sol = | 6030 | mg/L | |
| $K_{oc}$ = | 21 | mL/g | |
| Area = | 20 | ha | which gives $SF_j$ = 1.01 |
| | 200000 | $m^2$ | |

Using equations 3-10, the mass flux and air concentration for day 1 and 2 at the inner ring are calculated as follows, with results from days 1-10 shown in the table below:

- Day 1:

$$Total\ mass\ released\ on\ day\ 1 = TER_1 = 100 + 75 + 25 = 200\ kg$$

$$\begin{aligned} Mass\ at\ start\ of\ day\ 1 = M_1 &= M_0 + (TER_1 - J_0 \cdot A) \cdot (1\ day) \\ &= 0 + (200 + 0) \cdot (1\ day) = 200\ kg \end{aligned}$$

$$Mass\ per\ area\ for\ day\ 1 = AR_1 = \frac{M_1}{A} = \frac{200\ kg}{20\ ha} = 10\frac{kg}{ha}$$

$$\begin{aligned} Mass\ flux\ in\ day\ 1 = J_1 & \\ &= \frac{\exp\left(0.8688\ \cdot\ \ln\left(\frac{VP \cdot AR}{Sol \cdot K_{oc}}\right) + 21.535\right)}{3600} \cdot (8.64 \times 10^{-5}) \\ &= \frac{\exp\left(0.8688 \cdot \ln\left(\frac{0.01 \cdot 10}{6030 \cdot 21}\right) + 21.535\right)}{3600} \cdot (8.64 \times 10^{-5}) \\ &= 2.70 \times 10^{-4} \frac{kg}{m^2 \times day} \end{aligned}$$

$$C_{outdoor}\ for\ day\ 1 = \frac{J_1 \cdot 200{,}000}{1} \cdot 0.01157 \cdot 1.01 \cdot Postprocessed\ AERMOD\ result_1$$

If the post-processed AERMOD result is 5.43 µg/m$^3$, this gives $C_{outdoor}$ = 3.41 µg/m$^3$. For Aldicarb, the saturation air concentration is calculated using equation 6 to be 0.766 µg/m$^3$. As such, $C_{outdoor}$ is set to 0.766 µg/m$^3$.

The mass flux that corresponds to an air concentration of 0.766 µg/m$^3$ is calculated as:

$$0.766 = 5.43 \cdot \frac{J_{1,sat} \cdot 200{,}000}{1} \cdot 0.01157 \cdot 1.01$$

$$J_{1,sat} = 6.04 \times 10^{-5}\, \frac{kg}{m^2 \times day}$$

- Day 2:

$$Total\ mass\ released\ on\ day\ 2 = TER_2 = 25\ kg$$

$$\begin{aligned} Mass\ at\ start\ of\ day\ 2 = M_2 &= M_1 + (TER_2 - J_1 \cdot A) \cdot (1\ day) \\ &= 200 + [25 - (6.04 \times 10^{-5}) \cdot 200000] \cdot (1\ day) \\ &= 213\ kg \end{aligned}$$

$$Mass\ per\ area\ for\ day\ 2 = AR_2 = \frac{M_2}{A} = \frac{171\ kg}{20\ ha} = 10.6\,\frac{kg}{ha}$$

$$\begin{aligned} Mass\ flux\ in\ day\ 2 = J_2 &= \frac{\exp\left(0.8688 \cdot \ln\left(\frac{VP \cdot AR}{Sol \cdot K_{oc}}\right) + 21.535\right)}{3600} \cdot (8.64 \times 10^{-5}) \\ &= \frac{\exp\left(0.8688 \cdot \ln\left(\frac{0.01 \cdot 10.6}{6030 \cdot 21}\right) + 21.535\right)}{3600} \cdot (8.64 \times 10^{-5}) \\ &= 2.84 \times 10^{-4}\, \frac{kg}{m^2 \times day} \end{aligned}$$

$$C_{outdoor}\ for\ day\ 2 = \frac{J_2 \cdot 200{,}000}{1} \cdot 0.01157 \cdot 1.01 \cdot Postprocessed\ AERMOD\ result_2$$

The calculated air concentration is then compared to the saturation air concentration, similar to the previous day.

- Days 1-10:

Table D2. Summary of mass flux and air concentrations due to emissions from soil at a hypothetical site with three releases.

| Day | Release #1 (kg/day) | Release #2 (kg/day) | Release #3 (kg/day) | Total Mass Added to Soil from all Releases, $TR_{add}$ (kg/day) | Mass on Soil at Start of Day, M (kg) | Mass per Area, AR (kg/ha) | Mass Flux, J (kg/m$^2$/day) | Mass Volatilized from Soil, $M_{vol}$ (kg/ha) | AERMOD Unit Value[a] (ug/m$^3$) | Air Conc (ug/m$^3$) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 100 | 75 | 25 | 200.00 | 200.00 | 10.00 | 2.70E-04 | | 5.43 | 3.41[b] |
| 2 | 0 | 0 | 25 | 25.00 | 212.88 | 10.64 | 2.85E-04 | | 19.1 | 12.7[b] |
| 3 | 0 | 0 | 25 | 25.00 | 234.45 | 11.72 | 3.10E-04 | | 34.6 | 24.9[b] |
| 4 | 0 | 0 | 25 | 25.00 | 257.55 | 12.88 | 3.36E-04 | | 16.5 | 12.9[b] |
| 5 | 0 | 0 | 25 | 25.00 | 278.55 | 13.93 | 3.60E-04 | | 12.5 | 10.4[b] |
| 6 | 100 | 0 | 25 | 125.00 | 398.27 | 19.91 | 4.91E-04 | | 30.9 | 35.3[b] |
| 7 | 0 | 0 | 25 | 25.00 | 421.14 | 21.06 | 5.15E-04 | | 29.1 | 34.9[b] |
| 8 | 0 | 75 | 25 | 100.00 | 518.88 | 25.94 | 6.17E-04 | | 16.9 | 24.3[b] |
| 9 | 0 | 0 | 25 | 25.00 | 540.00 | 27.00 | 6.39E-04 | | 3.96 | 5.90[b] |
| 10 | 0 | 0 | 25 | 25.00 | 548.40 | 27.42 | 6.48E-04 | | 6.79 | 10.3[b] |
| … | continue until *M* or *J* falls below a threshold level of $10^{-7}$ | | | | | | | | | |

[a] AERMOD Unit Value based on 1 g/s of emission

[b] Indicates calculated air concentration exceeds saturation air concentration

# Appendix E Illustrative Example for Area Water Sources

Assume the user inputs three releases with the following profiles. The user obtains the volatilization half-life from EPI Suite, which requires that the user enter a water depth, water velocity, and wind velocity.

Table E1. User inputs for example releases for an area water source. Note the value for water depth was selected for illustrative purposes and is not the default value (1 m for both river and lake) used in EPI Suite to estimate volatilization half-life.

| | **User Input** | | **Tool Conversion** |
|---|---|---|---|
| | **kg/day/site** | **# days/year** | **Release occurs** |
| Release #1 | 100 | 73 | Every 5 days |
| Release #2 | 75 | 52 | Every 7 days |
| Release #3 | 25 | 365 | Every day |
| | | | |
| Chemical = | Naphthalene | | |
| MW = | 128.2 | g/mol | |
| VP = | 1140 | Pa | |
| Depth of water = | 5 | m | |
| Water velocity = | 1 | m/s | |
| Wind velocity = | 1 | m/s | |
| $t_{1/2}$ = | 110 | hrs | |
| Surface area = | 50,000 | m$^2$ | which gives $SF_j$ = 2.24 |
| Flowrate = | 50 | m$^3$/day | |

Using equations 11-18, the mass flux and air concentration for day 1 and 2 are calculated as follows, with results from days 1-20 shown in the table below:

- Day 1:

$$k_{vol} = \frac{\ln(2)}{t_{1/2}} = \frac{\ln(2)}{(110\text{ hrs}) \cdot \dfrac{1\ day}{24\ hrs}} = 0.15 \frac{1}{day}$$

$$V = A \cdot d = 50{,}000 \cdot 5 = 250{,}000\ m^3$$

$$Total\ mass\ released\ on\ day\ 1 = TER_1 = \ 100 + 75 + 25 = 200\ kg$$

$$Mass\ at\ start\ of\ day\ 1 = M_1 = \ M_0 + \left(TER_1 - \left(k_{vol} + \frac{Q}{V}\right) \cdot M_0\right) \cdot 1$$

$$= \ 0 + 200 - \left(0.15 + \frac{50}{250{,}000}\right) \cdot 0 = 200\ kg$$

$$Mass\ volatilized\ on\ day\ 1 = \ M_{1,vol} = k_{vol} \ \cdot M_1 \cdot (1\ day) = 0.15 \cdot 200$$

$$= 30\ kg$$

$$C_{outdoor,1} = \frac{M_{vol,1}/day}{1\frac{g}{s}} \cdot 0.01157 \cdot SF_j \cdot Postprocessed\ AERMOD\ result_1$$
$$= \frac{30}{1} \cdot 0.01157 \cdot 2.24 \cdot Postprocessed\ AERMOD\ result_1$$

If the AERMOD Unit Value is 3.42 μg/m$^3$, this gives $C_{outdoor}$ = 2.66 μg/m$^3$, which is below the saturation air concentration calculated using Equation 6.

- Day 2:

$$Total\ mass\ released\ on\ day\ 2 = TER_2 = 25\ kg$$

$$Mass\ at\ start\ of\ day\ 2 = M_2 = M_1 + \left(TER_2 - \left(k_{vol} + \frac{Q}{V}\right) \cdot M_1\right) \cdot 1$$
$$= 200 + 25 - \left(0.15 + \frac{50}{250{,}000}\right) \cdot 200$$
$$= 195\ kg$$

$$Mass\ volatilized\ on\ day\ 2 = M_{2,vol} = k_{vol} \cdot M_2 \cdot (1\ day)$$
$$= 0.15 \cdot 195 = 29.2\ kg$$

$$C_{outdoor,2} = \frac{M_{vol,2}/day}{1\frac{g}{s}} \cdot 0.01157 \cdot SF_j \cdot Postprocessed\ AERMOD\ result_2$$
$$= \frac{29.2}{1} \cdot 0.01157 \cdot 2.24 \cdot Postprocessed\ AERMOD\ result_2$$

The calculated air concentration is then compared to the saturation air concentration, similar to the previous day.

- Days 1-10:

Table E2. Summary of mass volatilized and air concentrations due to emissions from water at a hypothetical site with three releases.

| Day | Release #1 (kg/day) | Release #2 (kg/day) | Release #3 (kg/day) | Total Mass Added to Water from All Releases, $TR_{add}$ (kg/day) | Mass in Water at Start of Day, M (kg/m$^3$) | Mass Volatilized from Water, $M_{vol}$ (kg) | AERMOD Unit Value[a] (ug/m$^3$) | Air Conc (ug/m$^3$) |
|---|---|---|---|---|---|---|---|---|
| 1 | 100 | 75 | 25 | 200 | 200 | 30.1 | 3.42 | 2.67 |
| 2 | 0 | 0 | 25 | 25 | 194.6 | 29.4 | 33.3 | 25.3 |
| 3 | 0 | 0 | 25 | 25 | 190.5 | 28.7 | 63.8 | 47.4 |
| 4 | 0 | 0 | 25 | 25 | 187.4 | 28.1 | 37.8 | 27.6 |
| 5 | 0 | 0 | 25 | 25 | 184.3 | 27.7 | 36.0 | 25.8 |
| 6 | 100 | 0 | 25 | 125 | 281.6 | 42.3 | 11.5 | 12.6 |
| 7 | 0 | 0 | 25 | 25 | 264.3 | 39.7 | 16.5 | 16.9 |
| 8 | 0 | 75 | 25 | 100 | 324.6 | 48.8 | 19.7 | 24.8 |
| 9 | 0 | 0 | 25 | 25 | 300.8 | 45.2 | 34.2 | 40.0 |
| 10 | 0 | 0 | 25 | 25 | 280.6 | 42.1 | 7.00 | 7.63 |
| … | continue until *M* or mass flux[b] falls below a threshold level of $10^{-7}$ | | | | | | | |

[a] AERMOD Unit Value based on 1 g/s of emission

[b] For threshold level, a mass flux was calculated for each day