6.0 Air Module

6.1 Purpose and Scope

The Air Module estimates the annual average air concentration of dispersed constituents and the annual deposition rates of vapors and particles at various receptor points in the area of interest (AOI). This module simulates the transport and diffusion of constituents in the form of volatilized gases or fugitive dust emitted from area sources into the air. The predicted air concentrations are used to estimate biouptake into plants, and human exposures due to direct inhalation. The predicted deposition rates are used to determine constituent loadings to farm crops and soils, watershed soils, and surface waterbodies. Figure 6-1 shows the relationship and information flow between the Air Module and the 3MRA modeling system.

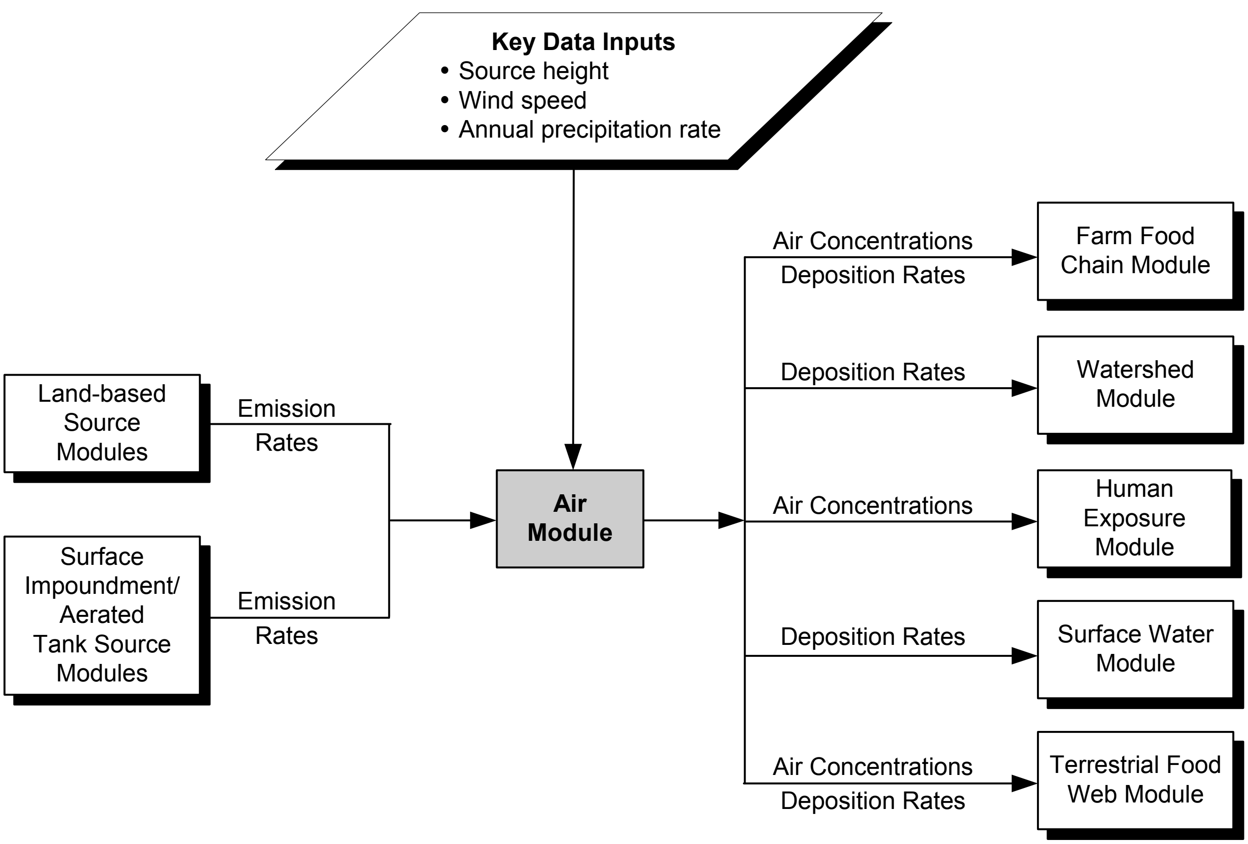

Figure 6-1. Information flow for the Air Module in the 3MRA modeling system.

The Air Module performs four major functions, as follows:

1. **Characterize source-specific parameters.** For each AOI, the Air Module characterizes emission sources in terms of waste management unit (WMU) dimensions, emission rate, and the site-layout. As an option, the module can calculate the source-specific, long-term average particulate mass fraction distribution from the outputs of the Land-based Source Modules (Landfill, Waste Pile, or Land Application Unit [LAU] Module).

2. **Calculate receptor locations (polar grid or site specific).** The Air Module provides the option to model directly to all site-specific output coordinates needed by the 3MRA modeling system or to model to a set of polar coordinates and then use a two-dimensional (2-D) cubic spline method to interpolate from the polar set to the larger set of interest. The spline interpolation can be used to reduce the ISCST3 run time.

3. **Calculate receptor-specific contaminant concentration and deposition rates.** The Air Module calculates annual average air concentration and deposition rates for each receptor location specified. Concentrations and deposition rates calculated include

   – Air concentration of vapors,
   – Air concentration of particles,
   – Wet deposition rate for vapors and particles, and
   – Dry deposition rate for particles.

4. **Calculate constituent-specific annual average concentrations and deposition rates.** The Air Module converts the receptor-specific concentrations and deposition rates based on unit emission rates (e.g., 1 g/m^2-s) to constituent-specific estimates by multiplying the values by the constituent-specific emission rate for each year.

ISCST3 may be implemented by the 3MRA modeling system during a run, or it may be run outside of the 3MRA modeling system and the results called by the Air Module.

6.2 Conceptual Approach

Figure 6-2 illustrates the dispersion and subsequent deposition of vapors and particles from a WMU into the environment. Constituents are released to the air as vapors (by volatilization) or sorbed to particulates (by wind erosion and mechanical disturbances) and move through the air to locations around the AOI. The constituents can then deposit on soil and plant surfaces. The Air Module is used to estimate air concentrations and deposition rates for each contaminant/site/WMU combination.

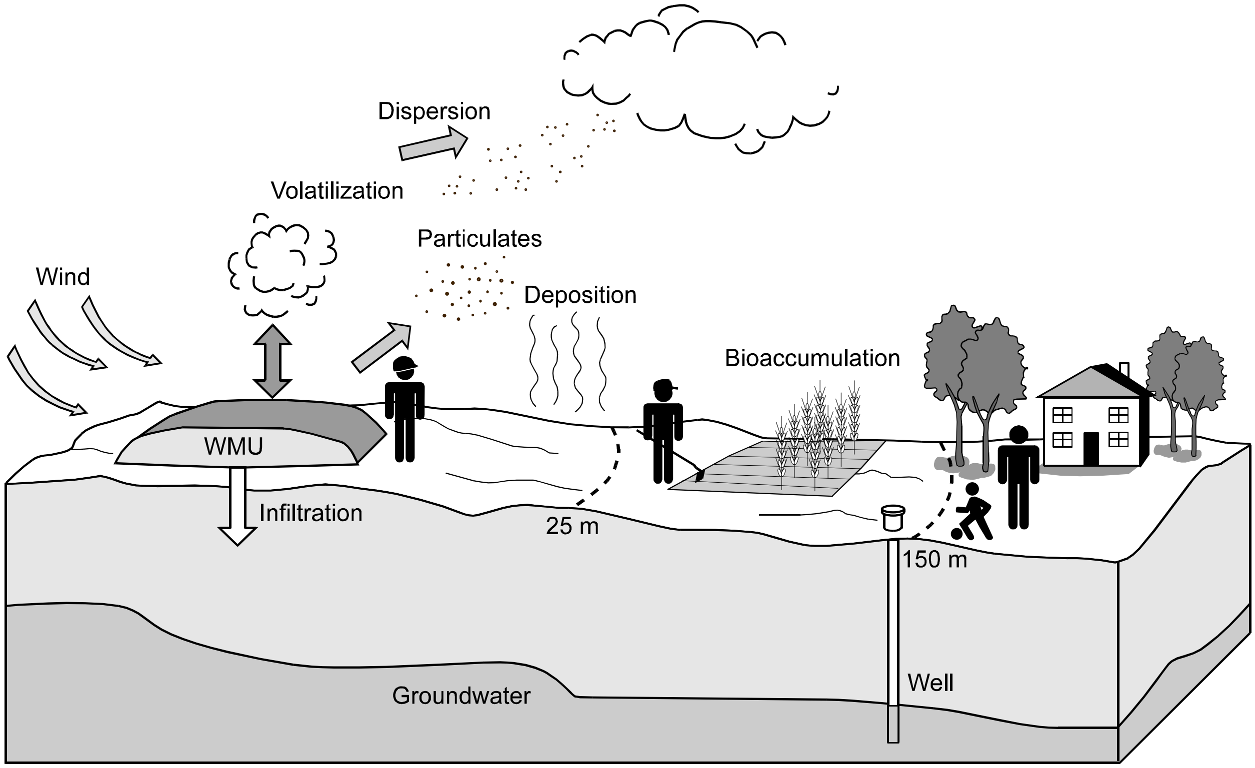

Figure 6-2. Conceptual diagram of dispersion and deposition.

The Air Module is based on EPA's legacy model Industrial Source Complex Short-Term Model, Version 3 (ISCST3), which has been used extensively by EPA in regulatory applications. ISCST3 was extended for use in the Air Module through the development of pre- and postprocessors that serve as an interface between the ISCST3 model and the rest of the 3MRA modeling system. The preprocessor reads initial settings from files generated by the 3MRA modeling system. Next, the preprocessor determines if the core model needs to be run or if results from previous runs can be reused. If the ISCST3 model needs to be run, the preprocessor builds an input file that controls the ISCST3 run. The ISCST3 model is run using unit constituent emissions to produce receptor-specific annual average air concentrations and deposition rates normalized to emission rate. The postprocessor converts these normalized concentration and deposition estimates to constituent-specific annual averages by multiplying the values by the constituent-specific emission rates for the WMU for each year. The resulting annual averages are written to files that are read by other modules. A summary of the ISCST3 model—the science and the computational core of the Air Module—is presented in the accompanying text box. The full capabilities of the ISCST3 model are explained in U.S. EPA (1995).

Summary of ISCST3

ISCST3 (U.S. EPA, 1999a,b), a recommended dispersion model in EPA's *Guideline on Air Quality Models* (U.S. EPA, 1999c), is a steady-state, Gaussian plume dispersion model. A steady-state model is one in which the model inputs and outputs are constant with respect to time. The term "Gaussian plume" refers to the kind of mathematical solution used to solve the air dispersion equations. It essentially means that the constituent concentration is dispersed within the plume laterally and vertically according to a Gaussian distribution, which is similar to a normal distribution. These assumptions and solutions hold for each hour modeled. The results for each hour are then processed to provide values for different averaging times depending on the user's needs (e.g., annual average).

ISCST3 is capable of simulating dispersion of pollutants from a variety of sources, including point, area, volume, and line sources. ISCST3 can account for both long- and short-term air concentration of particles and vapor, and wet and dry deposition of particles and vapor. In addition to deposition, wet and dry plume depletion can be selected to account for removal of matter by deposition processes and to maintain mass balance. Receptor locations can be specified in polar or cartesian arrays or can be set to discrete points as needed. Flat or rolling terrain can be modeled, but only flat terrain can be used for area sources. ISCST3 considers effects of the environmental setting on dispersion by allowing the user to set urban or rural dispersion parameters. Dispersion around the centerline of the constituent plume is estimated by empirically derived dispersion coefficients that account for horizontal and vertical movement of constituents. In addition, constituent movement from the atmosphere to the ground is also modeled to account for deposition processes driven by gravitational settling and removal by precipitation.

For area sources, the general equation for ground-level concentration at a receptor is given by a double integral in the upwind (x) and crosswind (y) directions:

$$\chi = \frac{Q_A K}{2\pi u_s} \int_x \frac{VD}{\sigma_y \sigma_z} \left(\int_y \exp\left[-0.5 \left(\frac{y}{\sigma_y} \right)^2 \right] dy \right) dx \qquad (6\text{-}1)$$

where

χ	=	concentration at x, y (mass per volume)
Q_A	=	area source emission rate (mass per unit area per unit time)
K	=	scaling coefficient to convert calculated concentrations to desired units (default value of 1×10^6 for Q in g/s and concentration in $\mu g/m^3$)
x	=	distance from source in wind direction (positive is downwind) (m)
y	=	distance from centerline of plume across the wind direction (m)
z	=	vertical distance from ground (m)
V	=	vertical term accounting for vertical distribution of the plume (includes effects of source elevation, receptor elevation, plume rise, limited mixing in the vertical direction, and gravitational settling and dry deposition of particulates)
D	=	decay term accounting for pollutant removal by physical or chemical processes
σ_y, σ_z	=	standard deviation of lateral and vertical concentration distribution (m)
u_s	=	mean wind speed at release height (m/s).

Key meteorological data required for the ISCST3 model include

- **Wind Direction:** Determines the direction of the greatest impacts.
- **Windspeed:** Affects ground-level air concentration. The lower the windspeed, the higher the concentration.
- **Stability Class:** Affects rate of lateral and vertical diffusion. The more unstable the air, the greater the diffusion.
- **Mixing Height:** Determines the height to which constituents can be diffused vertically.
- **Deposition Parameters:** Additional site-specific meteorological parameters are required to make estimates of dry and/or wet deposition. These parameters vary based on land-use types and seasons.

6.2.1 Characterize Source-specific Parameters

For each site, ISCST3 input files can be created that contain source-specific information such as WMU type, dimensions, location, and source variables for settling, removal, and deposition. Values for most of these data are obtained from other modules or the 3MRA modeling system databases.

The WMU types modeled by the 3MRA modeling system include surface impoundments, aerated tanks, landfills, waste piles, and LAUs. All of these unit types except for aerated tanks and waste piles are modeled as ground-level area sources. Aerated tanks and waste piles are modeled as elevated area sources.

For the 201 sites in the representative national data set, the location and the size of the sources is determined from the 3MRA modeling system site-based database. The sources for these data are the 1985 Screening Survey for Industrial Subtitle D Establishments (Westat, 1987) and the 1986 Survey of Hazardous Waste Treatment, Storage, and Disposal Facilities (U.S. EPA, 1987). Neither of these data sources includes data on height; therefore, the waste pile heights were calculated based on volume of waste and area of the pile, and tank height was randomly selected. These heights are stored in the representative national data set.

When modeling particulates, ISCST3 requires a long-term average particle size distribution. As an option, the Air Module can calculate the source-specific mass fraction distribution. The Land-based Source Modules (i.e., the Landfill, Waste Pile, and LAU Modules) generate a time series of particle size distributions (i.e., one distribution per year), as well as a time series of particulate mass fluxes for particles less than or equal to 30 µm in diameter. From these inputs, the Air Module estimates the long-term average particle size distribution.

Other source-specific information included in the ISCST3 input file include specification of rural versus urban setting and meteorological dataset information.

Rural vs. Urban. The rural vs. urban setting in ISCST3 allows the user to account for differences between rural and urban environments. In urban environments, the built environment (e.g., buildings, roads, and parking lots) alters the dispersion character of the atmosphere, particularly at night as a result of building-induced turbulence and reduced nighttime cooling. Thus, there is greater nighttime mixing of constituents in urban areas compared with rural areas. For the purposes of ISCST3 modeling, the urban classification applies mainly to large cities; even small cities and suburban areas are more appropriately classified as rural.

Meteorological data. The 3MRA modeling system database contains meteorological data collected at regional meteorological stations. Each of the 201 sites contained in the 3MRA modeling system representative national data set was assigned to the nearest station with similar weather conditions and adequate data. In making these assignments, EPA considered all available data from 218 meteorological stations across the United States to find the best data for each site. Each of the meteorological data sets included in the 3MRA modeling system database contains a minimum of 10 years of data.

6.2.2 Calculate Receptor Locations (polar-grid or site-specific)

The user has the option of specifying receptor locations for all cartesian coordinates as requested by the 3MRA modeling system, or for a set of polar grid coordinates. If the second option is chosen, a two-dimensional cubic spline method (discussed below) is applied to interpolate from the polar grid coordinates to the larger receptor location set requested by the 3MRA modeling system.

The run time for ISCST3 can be long, particularly for large area sources with many receptor locations. As an option to minimize run time of ISCST3 in the Air Module, a 2-D cubic spline interpolation algorithm was developed. Under this option, run-time savings can be achieved by using ISCST3 to model directly to a smaller number of points than the total number of receptor locations for the site. In general, the points making up the spline data set are not a subset of the points representing the receptor locations; rather, they are uniformly distributed across the AOI. A requirement of the spline algorithm is that the data provided to the spline must be "complete" in the sense that, no matter how the underlying 2-D grid is configured (e.g., cartesian, polar), data must be provided at each intersection of the two dimensions. A polar grid is used as the basis for the spline because, under the "complete" data set requirement of the spline algorithm, a polar grid can achieve a higher resolution in the region of steepest output gradients (near the WMU) with fewer total points than can a cartesian grid.

The spline method can only interpolate values. Consequently, value estimates cannot be made for any points located outside of the outermost grid circle.

6.2.3 Calculate Receptor-specific Concentration and Deposition Rates

Both vapors and particles are modeled for landfills, waste piles, and LAUs; only vapors are modeled for surface impoundments and aerated tanks. The type of model output selected depends on the WMU being modeled. Concentration, dry deposition rate, and wet deposition rate are calculated for landfills, waste piles, and LAUs. Only concentration and wet deposition rate are calculated for surface impoundments and aerated tanks because the pollutants are only emitted in vapor phase. Dry deposition of vapors is not modeled in the Air Module. Consequently, dry deposition of vapors is calculated as part of the Farm Food Chain Module (see Section 10.2.1) and Terrestrial Food Web Module (see Section 11.2.1). These modules estimate the dry deposition rate of vapors based on the vapor-phase concentration in air and a vapor-phase dry deposition velocity (default value of 1 cm/s).

The Air Module calculates the following concentrations and deposition rates:

- *Air concentration of particles and vapors.* ISCST3 estimates air concentrations of particles and vapors, accounting for downwind movement of the plume. It also accounts for dispersion of vapors and particles around the centerline of the plume as the plume travels in a downwind direction. Removal of constituent mass from the plume occurs as a result of wet and dry deposition.

- *Wet deposition of particles and vapors.* Wet deposition is the loss of material from a plume onto a surface as a result of precipitation. A scavenging ratio approach is used to model the deposition of gases and particles through wet removal. The amount of material removed from the plume by wet deposition is a function of the scavenging rate coefficient, which is based on particle size (U.S. EPA, 1995) for particles. For vapors, ISCTS3 is typically run with constituent-specific scavenging coefficients. These scavenging coefficients are read in by the Air Module. When multiple constituents are run, this method proportionately increases the number of runs that need to be made. As an alternative to applying constituent-specific coefficients, a single set of gas scavenging coefficients stored in the representative national data set can be applied. These coefficients are based on approximating the gases as very small particles.

- *Dry deposition of particles*. Dry deposition refers to the loss of material from a plume that has been deposited onto a surface (e.g., ground, vegetation) as a result of processes such as gravitational settling, turbulent diffusion, and molecular diffusion. Dry deposition of particles is calculated as the product of air concentration and dry deposition velocity.

To reduce the computational burden on the 3MRA modeling system, several new features were added to ISCST3 to create the Air Module. A complete description of the technical algorithms for these features is provided in U.S. EPA (1999b). Operational instructions are provided in U.S. EPA (1999a).

- **Revised Plume Depletion Scheme.** The version of ISCST3 distributed by EPA's Office of Air Quality Planning and Standards contains the Horst (1983) plume depletion algorithm. This algorithm was found to be computationally intensive. A new plume depletion and settling algorithm developed by Venkatram (1998) was implemented for the Air Module, resulting in a faster, more robust approach. This approach is based on depleting material in a surface-based internal boundary layer that grows with distance from the source. In conjunction with this change, the deposition velocity algorithm was also modified by removing the inertial impaction term. The inclusion of this term appears to provide deposition velocity estimates that are too high for some particle sizes.

- **Sampled Chronological Input Model (SCIM).** To reduce model run time, an option was added to the Air Module to sample the long-term meteorological record at regular, user-specified intervals and scale the model results at the end of the run to produce annual average estimates. This method is called the Sampled Chronological Input Model (SCIM). An advantage of this method is that it uses hourly meteorological data that maintain the serial correlation between wet deposition rate and concentration. The user specifies two sampling intervals. Using the first interval, the meteorological data are sampled, ignoring any recorded precipitation, and the air concentration and dry deposition rate are calculated for each receptor location of interest. The second interval specifies the sampling rate for the hours of meteorological data during which precipitation was recorded. This latter sampling rate is used to determine the air concentration, dry deposition rate, and wet deposition rate. The estimates from these separate schemes are combined at the end of the model run using a weighted average based on the number of hours sampled in each interval.

- **Output by Particle Size.** The Human Risk Module requires air concentrations for pollutants with particle sizes ≤ 10 µm to calculate inhalation risks. ISCST3 does not output concentrations by particle size. Therefore, an option was added to output concentration and deposition rate by particle size.

6.2.4 Calculate Constituent-specific Annual Average Concentrations and Deposition Rates

To reduce the number of required runs, the ISCST3 model is executed using unit emissions. The output from the model is normalized receptor-specific annual average concentrations and deposition rates. These estimates are converted to constituent-specific annual average concentrations and deposition rates by multiplying the values by the yearly emissions provided as output from the source modules.

6.3 Module Discussion

6.3.1 Strengths and Advantages

The Air Module has the following strengths and advantages:

- **ISCST concentration algorithms.** The concentration algorithms have been extensively reviewed and evaluated. The model has a long history of use by the EPA for fine-scale modeling and has been promulgated in the Guideline on Air Quality Modeling (U.S. EPA, 1999c).

- **ISCST particle deposition algorithms.** The particle deposition algorithms were selected for inclusion based on an extensive comparison against other algorithms and field data.

- **10-year period of record for the meteorological data.** The 10-year period of record ensures that all conditions typical of a meteorological station are modeled. EPA guidance for air quality applications requires only 5 years of off-site meteorological data to establish representativeness.

- **Urban or rural conditions.** The Air Module is appropriate for urban or rural dispersion conditions, depending on the location of the source.

- **Flexible receptor locations.** Receptors may be placed anywhere in the area of interest.

- **Options for use of meteorological data.** The Air Module provides the flexibility to either model all hours of meteorological data or use SCIM to model only selected hours if runtime is a constraint, which decreases runtime considerably.

6.3.2 Uncertainty and Limitations

The Air Module includes the following limitations or uncertainties:

- **Meteorological data gaps.** A data quality review uncovered missing data within the various meteorological data time series required for the 3MRA modeling system. Programs were written to automatically find and correct these data gaps, within the technical constraints established by Atkinson and Lee (1992). Missing data were typically less than 2 percent of all hours, so this correction should have little effect on the results.

- **Lack of data on shapes and heights of WMU.** Currently, none of the national-level data sets contain data on the shape, height, or orientation of the sources. In the absence of these data, units can be characterized as a square, rectangle, or 20-sided polygon shaped to approximate a circle.

- **Wet deposition of vapors.** Modeling of wet deposition of vapors requires constituent-specific scavenging coefficients and separate runs for each constituent. When modeling multiple constituents, the number of runs, as well as, the availability of constituent-specific data may be an issue. As an alternative, a set of gas scavenging coefficients that can be used for all constituents is stored in the representative national data set. These coefficients are based on approximating the gases as very small particles. This approach may lead to underprediction of wet deposition for some gases and overprediction of others depending on the Henry's law coefficient for the gas.

- **Dry deposition of vapors.** The Air Module is not designed to allow modeling of dry deposition of vapors using ISCST3. Modeling of dry deposition of vapors requires input of several contaminant-specific variables, which would require separate runs for each chemical. Alternatively, dry deposition of vapors is estimated in the Farm Food Chain Module (see Section 10.2.1) based on vapor-phase concentration in air and a default vapor-phase dry deposition velocity. Because dry deposition is calculated external to ISCST3, the plume is not depleted within the model. However, the impact to the modeling results is not expected to be significant.

6.4 References

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