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Air

USER'S GUIDE FOR THE ASSESSMENT SYSTEM FOR POPULATION EXPOSURE NATIONWIDE (ASPEN, VERSION 1.1) MODEL

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CONTENTS

FIGURES

Figure Page

TABLES

PREFACE

This user's guide provides documentation for the Assessment System for Population Exposure Nationwide (ASPEN, Version 1.1), referred to hereafter as ASPEN. It includes a technical description of the ASPEN algorithms, instructions for running the individual modules and a tutorial for getting started.

Version 1.0 of the ASPEN model was used in the EPA's Office of Policy's Cumulative Exposure Project. The changes to ASPEN in version 1.1, were to make file handling more flexible and easier. None of the technical algorithms were modified. Therefore, given the same input data, the results from versions 1.0 and versions 1.1 should be identical, although the output files are formatted somewhat differently.

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1.0 INTRODUCTION

The User's Guide for the Assessment System for Population Exposure Nationwide (ASPEN) provides the technical description of the ASPEN algorithms. It includes an overview of ASPEN, a discussion of its features, instructions for running the individual modules, and a tutorial for getting started.

1.1 BACKGROUND

The **A**ssessment **S**ystem for **P**opulation **E**xposure **N**ationwide (**ASPEN**), a new version of the **H**uman **E**xposure **M**odel (**HEM**), was developed as part of the Cumulative Exposure Project, sponsored by the US Environmental Protection Agency's Office of Policy, Planning, and Evaluation. The Cumulative Exposure Project report (Rosenbaum et al., 1998) includes sensitivity analysis of the features of ASPEN. ASPEN was designed to efficiently estimate outdoor concentrations and depositions of multiple pollutants emitted from a large number of sources at a large scale (e.g., national), while reporting results at the spatial resolution of census tracts. The number of emission sources, HAPs, and census tracts included in an analysis are specified by the user.

As part of the ASPEN development, a number of enhancements were made to HEM. These include:

- Modification of plume rise and dispersion parameters and formulations to assure consistency with those in the Industrial Source Complex - Long Term Model, Version 2 (ISCLT2; EPA, 1992);
- Expansion of HEM's reactive decay options;
- Incorporation of simple treatment of secondary formation of HAPs;
- Improvement of HEM's dry deposition algorithm;
- Addition of a wet deposition algorithm;
- Modification of the treatment of locations near point sources;
- Modification of the treatment of area and mobile sources; and
- Improvement of computational procedures to reduce run times.

1.2 OVERVIEW OF THE ASPEN MODEL

The Assessment System for Population Exposure Nationwide (ASPEN) model consists of two modules, ASPENA and ASPENB, and a series of post-processing programs. ASPENA is a dispersion module that estimates ambient concentration increments at a set of fixed receptor locations in the vicinity of an emission source (i.e., the receptor grid). ASPENB is a mapping module that interpolates ambient concentration increment estimates from the grid receptors to census tract centroids, and sums contributions from all modeled sources. The post-processing programs:

- distribute background HAP concentrations by census tract (BCKGRND program),
- generate the secondary compound concentrations and combine the concentrations of the primary and secondary compounds (SEC_DAT program),
- calculate the total pollution concentration from all source categories for each HAP from the ASPENB output files (MRG_DAT program),
- calculate the annual average HAP concentration (AVG_DAT program), and
- convert the concentration data files from binary to ASCII format (EXTR_DAT program).

Together, the ASPEN programs estimate annual average air toxics concentrations (in $\mu g/m^3$) at each census tract for each of eight 3-hour time blocks for each HAP/source category combination. The major processes of the two modules are illustrated in the flow diagram shown in Figure 1-1.

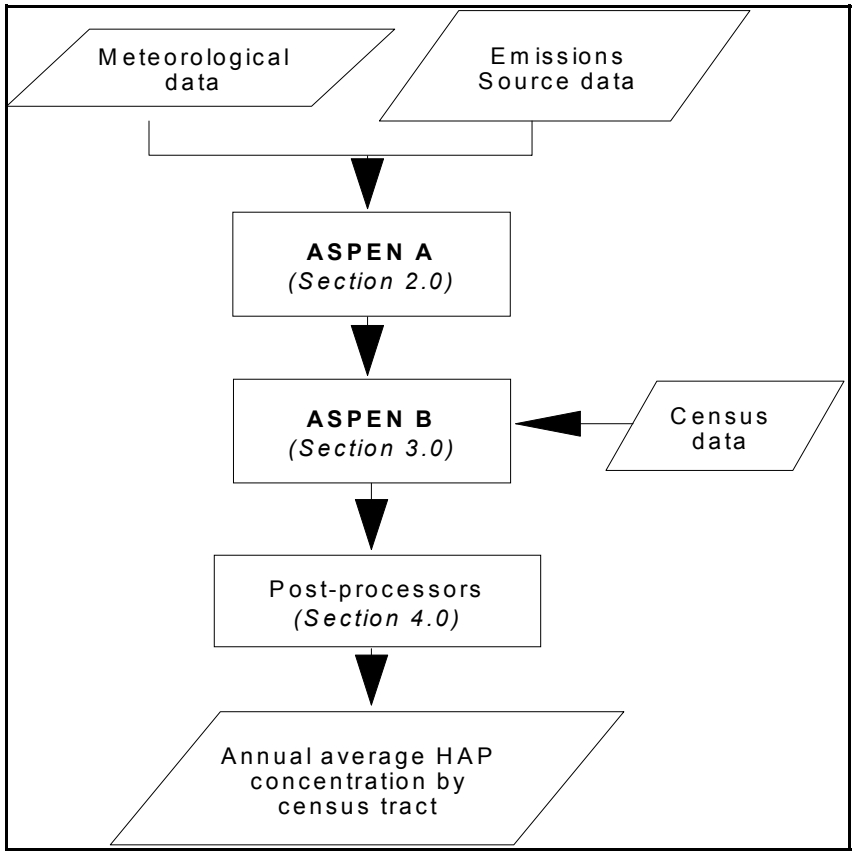

Figure 1-1 Flow diagram of the ASPEN modeling system

For ease in discussion and application, the ASPEN modeling system can be examined by its two main components: dispersion module (ASPENA) and mapping module (ASPENB).

ASPENA - Like its predecessors, the Human Exposure Model (HEM) and the South Coast Risk and Exposure Assessment Model - Version 2 (SCREAM2), ASPENA uses a Gaussian model formulation and climatological data to estimate long-term average pollution concentrations. For each source, the model calculates ground-level concentrations as a function of radial distance and direction from the source at a set of receptors laid out in a radial grid pattern. These concentrations represent the steady-state concentrations that would occur with constant emissions and meteorological parameters. For each grid receptor, concentrations are calculated for each of a standard set of stability class/wind speed/wind direction combinations. These concentrations are averaged together using the annual frequency of occurrence of each combination (i.e., the climatology) as weightings.

These meteorological frequency distributions are typically prepared for the entire simulation period, usually one or more years. For ASPEN, however, meteorological data are stratified by time of day into eight 3-hour time blocks, to preserve any characteristic diurnal patterns that might be important in subsequent estimation of population exposure. In addition to the climatology, other inputs to ASPEN that are specified by time block include emission rate, mixing height, and reactive decay rates. The resulting output of ASPENA is a grid of annual average concentration estimates for each source/pollutant combination by time block.

ASPENB - In ASPENB, the mapping module, annual average concentration estimates from ASPENA are interpolated from the grid receptors to census tract centroids, and contributions from all modeled sources are summed to give estimates of cumulative ambient concentration increments in each census tract. By accounting for all identified source categories (including background concentrations), the sum of the concentration increments should yield an estimate of the overall concentration of each HAP within each census tract. These estimates are designed to represent population-weighted concentration averages (each census tract represents approximately 4000 people).

1.2.1 Input Data Requirements

The three types of inputs needed to run the ASPEN models are the emission/control file, meteorological data files, and census tract data files.

- Emission/control file - contains the selected modeling options, source parameter data (including emission rates), and meteorological station assignments

- Meteorological data - includes the annual frequency of occurrence of each stability/wind speed/wind direction combination (by time block), temperatures (maximum, minimum and average), precipitation data, and mixing height (by time block) for meteorological stations within the modeling region

- Census tract data - contains the Federal Information Processing Standards (FIPS) code, location of the tract centroid, hypothetical radius, and urban/rural designation of each census tract within the modeling region

The emission control file and the meteorological data files are described in detail in Section 4.2 while the census tract data files are described in Section 5.1.

1.2.2 Computer Hardware Requirements

The computer resources required to run an ASPEN application are contingent upon the number of emission sources and HAPs to be processed. The disk storage requirement to run a simulation on a UNIX workstation (Sun Ultra Sparc 2 / Solaris 2.5.1), using the emissions from one source category (on-road mobile), one reactivity class (reactivity class 2 including emissions from 11 HAPs) in a single EPA region (EPA region 9) is approximately 1.3 Mbytes for ASPENA, and 2.7 Mbytes for ASPENB. It takes approximately 6 CPU hours to run both ASPENA and ASPENB for this simulation run.

1.3 HOW TO USE THE ASPEN MODEL

1.3.1 Novice Users

Novice users are those that are new to the ASPEN model and have limited dispersion modeling experience. These users should begin with Section 1.2 to gain a conceptual overview of the model. Section 8 provides a brief tutorial on setting up simple input files under two example scenarios. Once users have a basic understanding of the model, they will want to review the ASPENA and ASPENB user's instructions, respectively, in Sections 4 and 5. Section 2 provides a complete descriptions of the ASPENA dispersion module. Section 3 provides a detailed description of the ASPENB mapping module. Section 6 includes a discussion of the software used to post-process the ASPEN model output. Also, the tutorial provided will help them learn the structure of the input files and how to review the modeling results.

1.3.2 Experienced Modelers

Modelers that are unfamiliar with the ASPEN models but experienced using dispersion models in a variety of situations will also benefit from first reviewing the content of Section 1.2 to gain a basic orientation to the ASPEN model. Sections 4, 5 and 6 can be used as a reference for learning the overall capabilities of the modeling system's main components. Finally, the Appendices provide details of the formats for the ASPEN input and output files. Experienced modelers may also be interested in reviewing sections 2 and 3, which describe the technical details of ASPENA and ASPENB.

1.3.3 Management/Decision Makers

Those involved in air quality management or decision-making capacities related to dispersion modeling will benefit most from an overview of the model, and a general introduction to the input data needs and computer hardware requirements for running the model (Section 1.2). Upon review of this section, managers will understand the basic capabilities of the model well enough to judge the suitability of the model for particular applications.

1.3.4 Programmers/Systems Analysts

Programmers and systems analysts, specifically those in charge of maintaining the code or those involved with installing the ASPEN model code on other computer systems should review Section 7. Section 7 discusses the minimum hardware requirements to run the model, and how to port the model to various hardware environments. They may also wish to review Section 1.2 in order to have a basic understanding of the nature and overall capabilities of the model.

2.0 ASPENA DISPERSION MODULE DESCRIPTION

The ASPEN dispersion module estimates the ambient concentration increments at a set of fixed receptor locations within the vicinity of the emission source. The steady-state Gaussian plume equation is used in conjunction with diurnally stratified climatological data, including wind speed, wind direction, and atmospheric stability, to estimate long-term average ground-level concentrations at receptor grid locations resulting from elevated point emission sources. The specific formulation and equations used are described in the following subsections. Unless otherwise noted, all equations are identical to those in the **I**ndustrial **S**ource **C**omplex – **L**ong **T**erm **2** (ISCLT2) model.

2.1 POINT SOURCE EMISSIONS

2.1.1 The Gaussian Sector Average Equation

The ASPEN modeling system uses the steady-state Gaussian plume equation in order to simulate elevated point sources with continuous emissions. To reduce computing requirements, ASPEN utilizes a climatological modeling approach. As with other climatological models (e.g., the **E**nvironmental **P**rotection **A**gency's (EPA) Climatological Dispersion Model (CDM) and ISCLT), the dispersion module is supplied with a **ST**ability **AR**ray (STAR) joint probability matrix. A STAR matrix describes the joint frequency distribution of hourly meteorological measurements sorted into classes, or bins, by wind speed, wind direction, and atmospheric stability. The long-term concentration is calculated by simulating the average concentration for each meteorological bin and summing the averages across bins, weighting each by its frequency of occurrence.

Normally, a single STAR matrix is prepared for the entire simulation period, usually one or more years. For ASPEN, meteorological data were prepared in 3-hour time blocks. For example, there is a STAR matrix for the time period from 3 a.m. to 6 a.m., reflecting the relative long-term frequency of each meteorological condition for that time of day.

Classification of the wind directions for preparation of the STAR matrix requires partitioning of the area surrounding each source into sectors of equal angular widths. The mean annual concentration at each receptor resulting from emissions from a single stack is obtained by averaging over all wind directions, wind speeds and stability classes according to:

$$\chi = \frac{1}{\sqrt{2\pi}} \frac{K}{R\Delta\theta'} \sum_{i,j,k} \frac{QfVD}{u_s \sigma_z}$$

where :

χ	=	concentration ($\mu g/m^3$)
K	=	units scaling coefficient (10^6)
Q	=	pollutant emission rate (g/s)

f	=	frequency of occurrence of the i^{th} wind-speed, the j^{th} wind-direction, and the k^{th} stability category (unitless)
$\Delta\theta N$	=	the sector width (radians)
R	=	radial distance from the point source to receptor (m)
u_s	=	mean wind speed at stack height for the i^{th} wind-speed category and the k^{th} stability category. (m/s)
σ_z	=	standard deviation of the vertical concentration distribution for the k^{th} stability category (m)
V	=	Vertical Term for the i^{th} wind-speed and k^{th} stability category (unitless)
D	=	Decay Term for the i^{th} wind-speed and k^{th} stability category (unitless)

Each of the terms above are defined and discussed briefly in the following subsections.

2.1.2 Wind Speed Profile

The stack height wind speed, u_s (m/s), is obtained by adjusting the observed wind speed, u_{ref} (m/s), at a reference height, z_{ref} (m), to the stack height, h_s (m), through use of the wind power law. The equation has the form,

$$u_s = u_{ref}\left(\frac{h_s}{z_{ref}}\right)^p$$

Where p is the wind profile exponent which is dependent on both the stability category as well as whether the source is classified as urban or rural. The default values used in the ASPEN model are the same as those for the ISCLT2 model and are given below:

Stability Category	Rural Exponent	Urban Exponent
A	0.07	0.15
B	0.07	0.15
C	0.10	0.20
D	0.15	0.25
E	0.35	0.30
F	0.55	0.30

The stack height wind speed, u_s, has a minimum value of 1.0 m/s.

2.1.3 Plume Rise Formulas

The ASPEN model uses all plume rise calculations in the ISCL2 model (EPA, 1992). Prior to any plume rise calculations, the physical stack height is modified in order to account for stack-tip

downwash effects. This modified stack height, h_sN, is then used in place of the physical stack height for all subsequent plume rise calculations.

2.1.3.1 Stack-tip Downwash

The physical stack height is modified to account for stack-tip downwash effects following the treatment of Briggs (1974):

$$h'_s = h_s + 2d_s\left[\frac{v_s}{u_s} - 1.5\right] \qquad for \qquad v_s < 1.5u_s$$

or

$$h'_s = h_s \qquad for \qquad v_s \geq 1.5u_s$$

where h_s is the physical stack height (m), v_s is the stack gas exit velocity (m/s), and d_s is the stack tip diameter (m). When stack-tip downwash is not considered, h_sN = h_s.

2.1.3.2 Buoyancy and Momentum Fluxes

For most calculations involving plume rise, the buoyancy parameter, F_b (m^4/s^3), as well as the momentum flux parameter, F_m (m^4/s^2), are needed. These parameters are calculated as follows:

$$F_b = gv_s d_s^2\left(\frac{\Delta T}{4T_s}\right)$$

$$F_m = v_s^2 d_s^2\left(\frac{T_a}{4T_s}\right)$$

Where $\Delta T = T_s - T_a$, T_s is the stack gas temperature (K), and T_a is the ambient air temperature (K).

2.1.3.3 Unstable or Neutral – Crossover between Momentum and Buoyancy

The determination of whether the plume rise is dominated by momentum or buoyancy in the case where the stack gas temperature is greater than or equal to the ambient air temperature, follows the procedure of Briggs as outlined in the ISC Users' Guide, Section 1.1.4.3 (EPA, 1992). A crossover temperature difference is calculated using the following equations:

For $F_b < 55$,

$$(\Delta T)_c = 0.0297T_s\frac{v_s^{1/3}}{d_s^{2/3}}$$

And for F_b $ 55,

$$(\Delta T)_c = 0.00575 T_s \frac{v_s^{2/3}}{d_s^{1/3}}$$

If the difference between the stack gas and ambient temperature is greater than or equal to the crossover temperature difference, then the plume rise is assumed to be buoyancy dominated, otherwise it is momentum dominated.

2.1.3.4 Unstable or Neutral – Buoyancy Rise

When the plume rise is determined to be buoyancy dominated, as described above, then the distance to final rise, x_f (m), is determined as follows:

For F_b < 55:

$$x_f = 49 F_b^{5/8}$$

And for F_b $ 55:

$$x_f = 119 F_b^{2/5}$$

The final effective plume height is then given by:

For F_b < 55:

$$h_e = h_s' + 21.425 \frac{F_b^{3/4}}{u_s}$$

And for F_b $ 55:

$$h_e = h_s' + 38.71 \frac{F_b^{3/5}}{u_s}$$

2.1.3.5 Unstable or Neutral – Momentum Rise

When the stack gas temperature is less than or equal to the ambient air temperature, or if ΔT is less than the crossover temperature, $(\Delta T)_c$, then the plume rise is assumed to be dominated by momentum. The effective plume height is then given by:

$$h_e = h_s' + 3 d_s \frac{v_s}{u_s}$$

2.1.3.6 Stability Parameter

For stable atmospheric conditions, the stability parameter, s (s^{-2}), is required for plume rise calculations. In ASPEN, as in the ISCLT2 model, the stability parameter is calculated from the following equation given by Briggs (1975):

$$s = g \frac{\partial\theta / \partial z}{T_s}$$

As a default approximation, Mθ'Mz is taken as 0.020 K/m for stability class E, and for class F, Mθ'Mz is taken as 0.035 K/m.

2.1.3.7 Stable – Crossover between Momentum and Buoyancy

As in the case of unstable conditions, a crossover temperature difference is used to determine whether the plume rise is buoyancy or momentum dominated for stable atmospheric conditions. In this case the crossover temperature difference, $(\Delta T)_c$, is given by:

$$(\Delta T)_c = 0.019582\, T_s v_s \sqrt{s}$$

If the difference between stack gas temperature and ambient air temperature exceeds or equals $(\Delta T)_c$, the plume rise is assumed to be buoyancy dominated; otherwise it is momentum dominated.

2.1.3.8 Stable – Buoyancy Rise

For buoyancy dominated plume rise, ΔT exceeds $(\Delta T)_c$ as determined above. The distance to final plume rise, x_f, is calculated as

$$x_f = 2.0715 \frac{u_s}{\sqrt{s}}$$

And the effective plume height, h_e, is given by the following equation:

$$h_e = h_s' + 2.6\left(\frac{F_b}{u_s s}\right)^{1/3}$$

2.1.3.9 Stable – Momentum Rise

In stable conditions, if the stack gas temperature is less than or equal to ambient air temperature, or if ΔT is less than the crossover temperature difference $(\Delta T)_c$, it is assumed that the plume rise is momentum dominated. The effective plume height is then given as:

$$h_e = h_s^{'} + 1.5\left(\frac{F_m}{u_s\sqrt{s}}\right)^{1/3}$$

For this case, the unstable-neutral momentum rise is also evaluated. The smaller of these results is then used as the resulting plume height.

2.1.3.10 All Conditions – Distance Less Than Distance to Final Plume Rise

When gradual rise is to be estimated and the downwind distance from source to receptor, x, is less than the distance to final rise, then the effective plume height is given as:

$$h_e = h_s^{'} + 1.60\left(\frac{F_b^{1/3}x^{2/3}}{x_s}\right)$$

This relation is used only for buoyancy dominated plumes. In addition, if this relation results in a plume height which exceeds the final plume rise for the appropriate condition, then the final plume rise is used instead.

For momentum dominated plumes, stable and unstable conditions are treated separately as follows:

a) Unstable Conditions

$$h_e = h'_s + \left(\frac{3F_m x}{\beta_j^2 u_s^2}\right)^{1/3}$$

Where x is the downwind distance in meters, with a maximum value, x_{max}, defined by:

$$x_{\max} = \frac{4d_s\left(v_s + 3u_s\right)^2}{v_{su_s}} \qquad for \qquad F_b = 0$$

$$= 49F_b^{5/8} \qquad for \qquad 0 < F_b \le 55 \quad m^4/s^3$$

$$= 119F_b^{5/8} \qquad for \qquad F_b \ge 55 \qquad m^4/s^3$$

b) Stable Conditions

$$h_e = h_s^{'} + \left[3F_m \frac{\sin\left(x\sqrt{s}/u_s\right)}{\beta_j^2 u_s \sqrt{s}} \right]^{1/3}$$

Here the maximum downwind distance is defined by:

$$x_{\max} = 0.5\frac{\pi u_s}{\sqrt{s}}$$

The jet entrainment coefficient, β_j, is given as,

$$\beta_j = \frac{1}{3} + \frac{u_s}{v_s}$$

As in the case of buoyant gradual rise, the minimum of the distance-dependent momentum rise, as calculated above, and the final rise for the appropriate condition is used for the effective plume rise.

2.1.4 Dispersion Parameters

The standard deviation of the vertical concentration distribution, σ_z , for point sources is calculated using a procedure similar to that used in the ISCLT2 model. For a rural point source, the dispersion parameter, σ_z , is calculated using equations which approximately fit the Pasquill-Gifford curves (Turner, 1970) and are of the form,

$$\sigma_z = ax^b$$

where x, the downwind distance, is in kilometers and σ_z is in meters. The coefficients a and b are given as in Table 1-2 of the ISC2 Users' Guide (EPA, 1992) and are a function of both the downwind distance as well as stability class.

For urban point sources, the vertical dispersion parameter is computed using the Briggs' formulas to approximate vertical diffusion data of McElroy and Pooler (1968). Table 1-4 of EPA (1992) gives the appropriate relations for σ_z as a function of stability class and downwind distance from the source. As noted in EPA (1992), although these relations are assumed valid for downwind distances less than 100m, concentrations calculated at receptor locations within 100m of a source should be treated as suspect.

As in the ISCLT2 model, the ASPEN modeling system assumes a uniform lateral distribution across sector widths and therefore does not make use of the standard deviation of the lateral dispersion, σ_y .

The preceding approximations for dispersion parameters are applicable for ideal point sources. In general, a variety of processes can affect the initial growth and evolution point source plume. The ISC models use various treatments for consideration of many of these processes including the initial plume dimensions, building wake and downwash effects, and buoyancy-induced dispersion. Of these, ASPEN treats only the enhancements to the vertical dispersion parameter due to buoyancy-induced dispersion. (Treatment of building wake and downwash effects in ASPEN differs from ISCLT2, and is discussed in Section 2.1.7)

The current treatment of buoyancy-induced dispersion in the ASPEN modeling system follows that of Pasquill (1976) as implemented in the ISC2 model. Buoyancy-induced dispersion enhances the vertical dispersion due to ambient turbulence by taking into account the initial plume dispersion caused by turbulent motion and turbulent entrainment of ambient air. Then effective vertical dispersion, σ_{ze}, is given by the following relation:

$$\sigma_{ze} = \left[\sigma_z^2 + \left(\frac{\Delta h}{3.5}\right)^2\right]^{1/2}$$

where σ_z is the vertical dispersion due to ambient turbulence, and Δh is the plume rise due to momentum and/or buoyancy. Note that Δh is the distance-dependent plume rise when the receptor location is between the source and the distance to final plume rise, and is the final plume rise when the receptor location is beyond the distance to final rise.

2.1.5 The Vertical Term

In general, the vertical term which appears in the Gaussian sector average equation includes the effects of source elevation, receptor elevation, plume rise, limited mixing in the vertical and the gravitational settling and dry deposition of larger particles. In the ASPEN dispersion module, receptor elevation, as well as gravitational settling of large particles, is neglected. In addition, dry deposition of particles is treated separately, as discussed below. The vertical term is then given as in the ISC2 model for gases and small particles as follows:

$$V = \exp\left[-0.5\left(\frac{z_r - h_e}{\sigma_z}\right)^2\right] + \exp\left[-0.5\left(\frac{z_r + h_e}{\sigma_z}\right)^2\right]$$

$$+ \sum_{i=1}^{\infty}\left\{\exp\left[-0.5\left(\frac{H_1}{\sigma_z}\right)^2\right] + \exp\left[-0.5\left(\frac{H_2}{\sigma_z}\right)^2\right]\exp\left[-0.5\left(\frac{H_3}{\sigma_z}\right)^2\right]\exp\left[-0.5\left(\frac{H_4}{\sigma_z}\right)^2\right]\right\}$$

where:

$$h_e = h_s + \Delta h$$

$$H_1 = z_r - (2iz_i - h_e)$$

$$H_2 = z_r + (2iz_i - h_e)$$

$$H_3 = z_r - (2iz_i + h_e)$$

$$H_4 = z_r + (2iz_i + h_e)$$

z_r = receptor height above ground (m)

z_i = mixing height (m)

In the above equation, the infinite series accounts for the effects of restriction on vertical plume growth at the top of the mixed layer. It should be noted that if the effective stack height, h_e, exceeds the mixing height, z_i, then the plume is assumed to fully penetrate the elevated inversion and the ground-level concentrations are set to zero. At long downwind distances, the vertical term, as defined above, changes the form of the vertical concentration distribution from Gaussian to rectangular. Thus, the equation for the vertical term for downwind distances where the ratio of σ_z/z_i is greater than or equal to 1.6 is changed to the following form:

$$V = \frac{\sqrt{2\pi}\sigma_z}{z_i}$$

A more detailed discussion of the Vertical Term, including special treatments for mixing heights in rural and urban modes under various stability conditions may be found in the ISC2 Users' Guide (EPA, 1992).

2.1.6 The Decay Term

The decay term is used as a simple means of accounting for the pollutant removal by physical and/or chemical processes. The decay term takes the following form:

$$D = \exp\left(-\psi \frac{x}{u_s}\right) \qquad for \qquad \psi > 0$$

or

$$D = 1 \qquad for \qquad \psi = 0$$

where:

D	=	decay term (unitless)
ψ	=	decay coefficient (s^{-1})
x	=	downwind distance (m)
u_s	=	wind speed at stack height (m/s)

2.1.7 Building Wake Effects

The procedures used by the ASPENA model to account for the effects of building wakes and downwash effects are considerably different than those employed in the ISC2 model. Within the ISC2 model, the effects of building wakes on the plume dispersion coefficients are treated in a manner following those of Huber and Snyder. Following their suggestions, the vertical dispersion parameters are adjusted using a vertical virtual distance which is dependent on various factors including the relative dimensions of nearby buildings, stability class, and urban or rural classification of the emission source.

ASPENA uses a simpler treatment which also involves adjusting the plume dispersion parameters for a vertical virtual distance. Within ASPENA, the virtual distances are determined using an empirical formulation involving the building cross-sectional area and stability class, but are treated in the same way for both the rural and urban option. The formula used for calculating the vertical virtual distance, x_z, is given by,

$$x_z = bA^c \exp\left(A^d\right)$$

where A is the building cross-sectional area and the coefficients b, c, and d are dependent on the stability class and are given in the following table. This virtual distance is then added to the physical downwind distance and used through for all plume rise and dispersion parameter calculations.

Stability Category	b	c	d
A	1.95	0.504	0.754e-08
B	2.72	0.504	0.15799e-07
C	4.05	0.511	0.156395e-06
D	4.95	0.54	0.1039e-05
E	4.95	0.54	0.1039e-05
F	4.95	0.54	0.1039e-05

2.2 AREA SOURCE EMISSIONS

The ASPEN modeling system treats area sources (including motor vehicles) as a pseudo-point source located within each census tract. Pseudo-point sources are assumed to be vented point sources with an effective stack height of 5 meters and for which no plume rise calculations are made. The annual average concentration for area sources are processed within the mapping

module (ASPENB) in one of two ways depending upon the relative area of the census tract with respect to the location of the receptor grid locations. For large census tracts, five dispersion grids resulting from the pseudo-point treatment are distributed symmetrically throughout the tract in order to estimate ambient concentrations due to area source emissions. For small census tracts, only a single dispersion grid is used, located at the census tract centroid. A more detailed description of the treatment of area sources may be found in the discussion of the ASPENB module.

2.3 DRY DEPOSITION

Deposition of pollutants onto surfaces has the effect of reducing the average ambient concentrations and may be significant for particles. The dry deposition of gaseous HAPs is slow, so for most of these species, the deposition is less important than chemical reaction as a removal mechanism. Therefore, neglecting dry deposition for gas phase pollutants has little effect on the modeled concentrations. The ASPEN model therefore accounts for the deposition of particulate phase HAPs but does not include deposition of gas phase pollutants.

For particles, dry deposition rates are primarily a function of the particle size, and are thus much larger for coarse particles than for fine particles. In addition, the deposition of coarse particles is also highly dependent on gravitational settling. The dry deposition rates are also a function of the land-use type and vary for urban and rural environments. Deposition velocities, V_d (m/s), for the fine and coarse particles were obtained for different land-use types using the dry deposition algorithms of the Variable-grid Urban Airshed Model (UAM-V) photochemical model (SAI, 1992). These values are further parameterized as functions of stability class and wind speed. ASPEN's predicted atmospheric concentrations for particulate matter take into account different rates of particle deposition on urban and rural lands. The deposition velocities used in ASPENA are shown in Table 2.1.

TABLE 2.1 Deposition velocities for particulate matter

	Deposition Velocities (m/s) for coarse particles -- Rural*					
Stability	Wind speed (m/s)					
	1.5	2.5	4.5	7.0	9.5	12.5
A	1.33E-02	1.98E-02	3.32E-02	5.02E-02	6.73E-02	8.78E-02
B	1.28E-02	1.95E-02	3.30E-02	5.01E-02	6.72E-02	8.78E-02
C	1.25E-02	1.93E-02	3.29E-02	5.01E-02	6.72E-02	8.78E-02
D	1.24E-02	1.92E-02	3.29E-02	5.00E-02	6.72E-02	8.77E-02
E	1.13E-02	1.86E-02	3.25E-02	4.98E-02	6.70E-02	8.76E-02
F	1.04E-02	1.79E-02	3.22E-02	4.96E-02	6.68E-02	8.75E-02

	Deposition velocities (m/s) for coarse particles -- Urban*					
	Wind speed (m/s)					
Stability	1.5	2.5	4.5	7.0	9.5	12.5
A	3.10E-02	4.78E-02	8.27E-02	1.27E-01	1.71E-01	2.24E-01
B	2.99E-02	4.71E-02	8.24E-02	1.27E-01	1.71E-01	2.24E-01
C	2.92E-02	4.68E-02	8.22E-02	1.27E-01	1.71E-01	2.24E-01
D	2.89E-02	4.66E-02	8.22E-02	1.27E-01	1.71E-01	2.24E-01
E	2.64E-02	4.51E-02	8.13E-02	1.26E-01	1.71E-01	2.24E-01
F	2.42E-02	4.37E-02	8.05E-02	1.25E-01	1.70E-01	2.24E-01

	Deposition velocities (m/s) for fine particles -- Rural*					
	Wind speed (m/s)					
Stability	1.5	2.5	4.5	7.0	9.2	12.5
A	5.55E-05	8.48E-05	1.45E-04	2.21E-04	2.98E-04	3.89E-04
B	5.39E-05	8.38E-05	1.45E-04	2.21E-04	2.97E-04	3.89E-04
C	5.29E-05	8.32E-05	1.44E-04	2.21E-04	2.97E-04	3.89E-04
D	5.22E-05	8.29E-05	1.44E-04	2.21E-04	2.97E-04	3.89E-04
E	4.86E-05	8.06E-05	1.43E-04	2.20E-04	2.97E-04	3.89E-04
F	4.53E-05	7.85E-05	1.42E-04	2.19E-04	2.96E-04	3.88E-04

	Deposition velocities (m/s) for fine particles -- Urban*					
	Wind speed (m/s)					
Stability	1.5	2.5	4.5	7.0	9.5	12.9
A	1.15E-04	1.79E-04	3.13E-04	4.81E-04	6.50E-04	8.53E-04
B	1.11E-04	1.77E-04	3.12E-04	4.81E-04	6.50E-04	8.53E-04
C	1.09E-04	1.76E-04	3.11E-04	4.80E-04	6.49E-04	8.52E-04
D	1.08E-04	1.75E-04	3.11E-04	4.80E-04	6.49E-04	8.52E-04
E	9.98E-05	1.71E-04	3.08E-04	4.78E-04	6.48E-04	8.51E-04
F	9.25E-05	1.66E-04	3.05E-04	4.77E-04	6.47E-04	8.50E-04

*ASPEN computes particulate matter deposition rates for urban and rural lands, and also incorporates the resulting particle removal rates into predicted air concentrations.

Within the ASPEN dispersion module the deposition of particulate phase pollutants is treated using an equation similar to the Gaussian sector average equation. To account for dry deposition, an additional decay term is included in the calculation of ambient concentrations while the deposition rate, R_d, is given as,

$$R_d = V_d \chi$$

where:

R_d = dry deposition rate ($\mu g/m^2$-s)
V_d = deposition velocity (m/s)
χ = ground-level concentration ($\mu g/m^3$)

The decay rate Ψ for dry deposition is determined as a function of the deposition velocity, the downwind distance from the source and the relative dimensions of the plume with respect to the

mixing height. Both the plume dimensions and the mixing height are assumed to be dependent on the atmospheric stability as well as time of day. The decay term associated with the dry deposition is given as follows:

$$D_{dep} = \exp\left(\frac{-\psi_{dep} r^*}{u_s}\right)$$

where:

Ψ_{dep} = decay rate for deposition
r^* = 0 if $2\sigma_z < h'_s$
= $(r_i - r_{i-1})/2$ where r_i is the distance at which $2\sigma_z > h'_s$

The deposition decay rate, ψ_{dep}, is calculated from the deposition velocity and the dimensions of the plume with respect to the mixing height as follows,

$$\psi_{dep} = \frac{V_{dep}}{\left[\min\left(h'_e, 2\sigma_z\right) + \min\left(\left(z_i - h'_e\right), 2\sigma_z\right)\right]}$$

As examination of the above relations reveals, dry deposition, and hence reductions in ambient concentration, is not considered until the plume dimensions are such that the plume impacts the surface of the ground.

Separate decay terms are calculated in order to account for plumes which may impact urban or rural areas, in addition to accounting for whether the pollutant source is classified as urban or rural.

2.4 WET DEPOSITION

The ASPEN dispersion module uses the wet deposition algorithm from the revised version of the CAP88-PC model to estimate the wet deposition of particles. The algorithm is based on the approximate method described by Rodhe (1980, Model3) and uses the fraction of time during which precipitation is occurring in conjunction with the total annual precipitation to calculate both the decay rate for the modeled ambient concentrations as well as the deposition fluxes.

As with the dry deposition calculations, an additional decay term is used to account for the effects of wet deposition. In this case, the decay rate is a function of the scavenging coefficient, λ' (sec^{-1}), where the scavenging coefficient is proportional to the precipitation rate:

$$\lambda' = 10^{-7} p'$$

where p' is the average annual precipitation rate, (cm/yr). Defining f_p as the fraction of time that precipitation actually occurs, then the actual average precipitation rate during periods of precipitation becomes,

$$p = \frac{p'}{f_p}$$

and the scavenging coefficient is,

$$\lambda = 10^{-7}\,\frac{p'}{f_p}$$

The decay term associated with wet deposition is then given as,

$$D_{wet} = \exp\left(\frac{-\lambda r}{u_s}\right)$$

While the wet deposition rate is given as,

$$R_{wet} = \frac{\lambda Q}{2\pi r u_s} D_{wet}$$

where:

R_{wet}	=	wet deposition rate ($\mu g/m^2$-s)
λ	=	scavenging coefficient (sec^{-1})
Q	=	emission rate ($\mu g/s$)
r	=	downwind distance from source (m)
u_s	=	windspeed (m/s)
D_{wet}	=	decay rate due to precipitation scavenging

2.5 SECONDARY SPECIES FORMATION

Many of the toxic species treated within the ASPEN modeling system are formed through atmospheric reactions with nontoxic precursor species. The formation of these secondary species is treated using a post-processing procedure to estimate the annual average concentration increments. These precursor-product pairs are modeled within the dispersion module using the appropriate precursor reactive decay rates. ASPEN calculate the secondary product concentration as the difference between the precursor concentration in an inert model run and the concentration in the presence of reactive decay. The resulting concentration differences are adjusted for molar yield and molecular weight to provide an estimate for the concentration of the secondary species.

As an example, consider the treatment of secondary acrolein production. Since butadiene is the precursor species, two separate ASPENA runs would be performed, one with the appropriate decay rate for butadiene (reactive run), and one with a decay rate of zero (inert run). The concentrations of secondary acrolein are then calculated as:

$$\chi_{acrolein} = 1.04\left(\chi_{butadiene_{inert}} - \chi_{butadiene_{reactive}}\right)$$

where:

$\chi_{acrolein}$	=	ambient concentration of secondary acrolein ($\mu g/m^3$)
$\chi_{butadiene\ inert}$	=	ambient concentration of butadiene for inert run ($\mu g/m^3$)
$\chi_{butadiene\ reactive}$	=	ambient concentration of butadiene for reactive run ($\mu g/m^3$)

Other secondary species concentrations are calculated similarly.

3.0 MAPPING MODULE (ASPENB) DESCRIPTION

3.1 ASPENB OUTPUT FILE STRUCTURE AND UPDATE PROCEDURE

The ASPEN mapping module (ASPENB) produces a separate output file for each HAP/source category combination. Each of these files contains a record for each census tract with estimates of annual average concentrations for each of eight 3-hour time blocks. The procedure for producing these files by ASPENB is as follows:

- As ASPENB processes the an input file of the normalized source concentrations/depositions (ASPENA output file), each time a HAP is encountered ASPENB checks the local directory to determine if an output file for that HAP/source category combination already exists. If not, ASPENB creates the output file, and initializes it by creating a record for each census tract. An initial tract record contains a state/county FIPS and tract number, and eight concentration fields (each with a value of zero), and two deposition fields (each with a value of zero). If an output file already exists, it is opened.

- ASPENB then proceeds with the processing of the HAP. ASPENB interpolates the normalized concentrations/depositions of the grid receptors around the emission source to all the census tracts which fall within the source 50 kilometers impact zone. (See sections 3.2 and 3.3 for detailed discussions of the interpolation procedures and the determination of impacted census tracts, respectively.) It then applies the HAP emission rate to the normalized interpolated concentrations to obtain the population concentration/deposition estimates. For example, if the normalized concentration from the emission source for time block 1 at census tract A is 0.5 $\mu g/m^3$, and HAP emission rate is 2 g/sec, the HAP concentration is 1 $\mu g/m^3$ for time block 1 at census tract A.

- The HAP output file is then updated by incrementing the previous values with the current estimates, to obtain cumulative estimates for each census tract. After the output file is updated, it is closed.

3.2 INTERPOLATING TO CENSUS TRACT CENTROIDS

The normalized concentrations/depositions estimated by ASPEN's dispersion module (ASPENA) for grid receptors surrounding each emission source are interpolated to the census tract centroids within the 50 kilometers impact zone in the ASPENB. (See section 3.3 for a detailed discussion of the determination of impacted census tracts.)

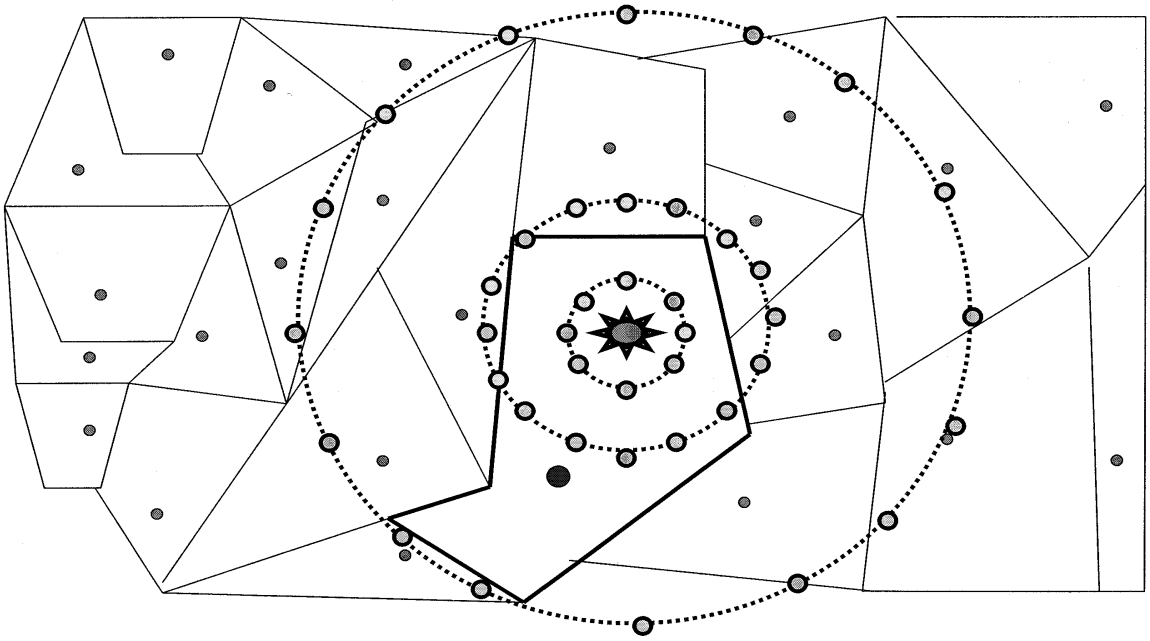

Figure 3-1. ASPENB receptor grid and census tract centroids

Figure 3-1 illustrates the relationship between the ASPEN model receptor grid and census tract centroids. The concentric rings represent the inner three rings of the ASPEN receptor array; and the irregular polygons represent the census tracts. A dark circle within each polygon represents the centroid of the tract.

The ASPENB designates the tract in which the source is located as the resident tract. Near sources, where ambient concentration gradients are likely to be steep, the position of a tract centroid relative to the source may result in a significant over- or underestimate of the population-weighted average exposure concentration in the tract. The coarser the spatial resolution of the population, the more significant the uncertainty in the average exposure concentration is likely to be. Therefore, for resident tracts, instead of estimating the ambient concentration increment at a single point in the tract (i.e., at the centroid), the average concentration increment over the entire area of the tract is estimated for the resident tract.

Detailed descriptions of the different interpolation procedures for the non-resident and resident census tract centroids are provided in the following sections.

3.2.1 Interpolating to Non-Resident Census Tract Centroids

The normalized concentrations/depositions for grid receptors are interpolated to the non-resident census tract (population) centroids with log-log interpolation in the radial direction and linear interpolation in the azimuthal direction (see Figure 3-2). The estimates are designed to represent average concentration for the tract. The interpolation to non-resident census tract centroids is implemented as follows:

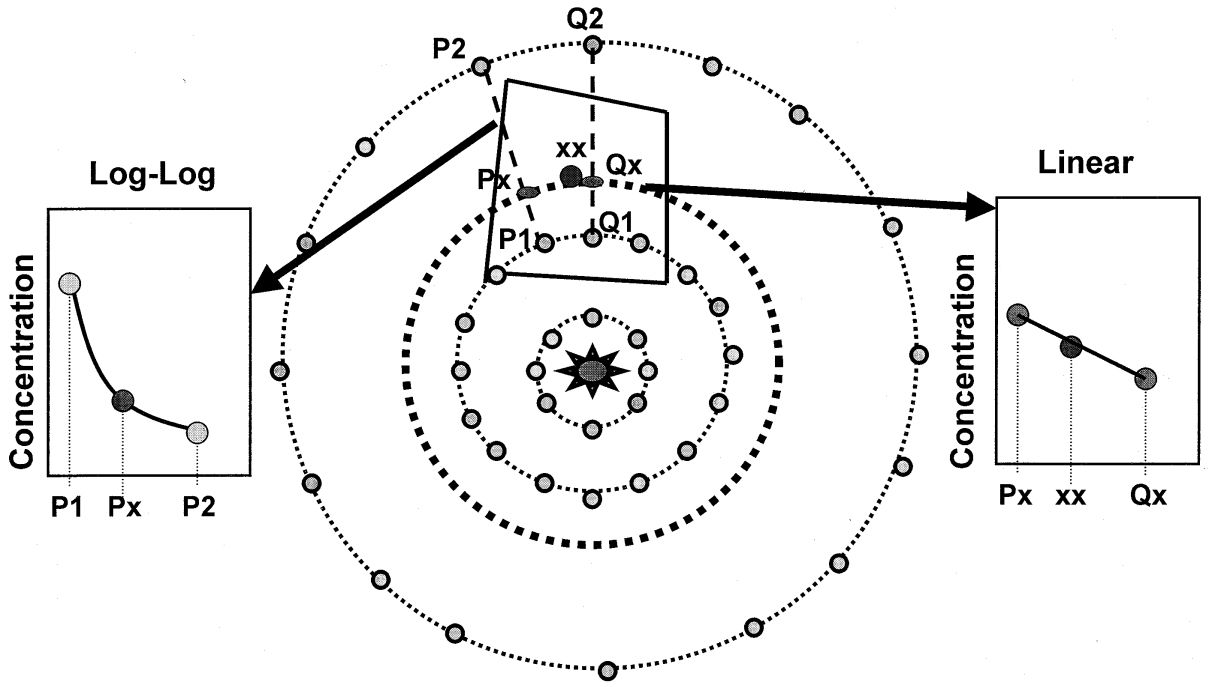

Figure 3-2. Interpolation to non-resident tract centroids

- For each census tract that falls within the 50 kilometer radius of the source impact zone, calculate the distance between the census tract centroid and the source, *d*, and its azimuth *az* (the clockwise angle measured from north).

- Locate the angular (*a1 and a2)* and radial indices (*r1 and r2)* in the receptor grid surrounding the non-resident census tract. The angular indices are the 2 closest azimuths of the polar receptor grid to the centroid azimuth. The radial indices are the 2 closet ring distances of the polar grid to the centroid. For example, the default polar grid has the following azimuths and ring distances with respect the emission source location:

Radial Index	Radial Distance (km)
1	0.1
2	0.5
3	1.0
4	2.0
5	5.0
6	10.0
7	15.0
8	20.0
9	25.0
10	30.0
11	40.0
12	50.0

Angular Index	Azimuth (Degree)
1	0.0
2	22.5
3	45.0
4	67.5
5	90.0
6	112.5
7	135.0
8	157.5
9	180.0
10	202.5
11	225.0
12	247.5
13	270.0
14	292.5
15	315.0
16	337.5

If a centroid is located at azimuth 110 degrees, and distance 0.65 km with respect to the emission source, the angular indices are 5 (90 degree) and 6 (112.5 degree), and the radial indices are 2 (0.5 km) and 3 (1.0 km) as shown below.

- Calculate the ratios for log-log interpolation in the radial direction (*rratio)*, and linear interpolation in the azimuthal direction (*aratio)*

$$rratio = \frac{\ln d - \ln radiir1}{\ln radiir2 - \ln radiir1}$$

where:

d	=	distance between the census tract centroid and the source
$radii_{r1}$	=	radial distance in the receptor grid for the radial index r1
$radii_{r2}$	=	radial distance in the receptor grid for the radial index r2
$rratio$	=	ratio for log-log interpolation in the radial direction

$$aratio = a - a1$$

where:

a	=	azimuth of the census tract in the receptor scaling
$a1$	=	azimuth for the angular index a1 in the receptor scaling
$aratio$	=	ratio for linear interpolation in the azimuthal direction

- Set the logarithm of the concentrations for each time block at the four corners of the receptor grid surrounding the census tract

$$c1 = \ln ca1, r1, h$$
$$c2 = \ln ca1, r2, h$$
$$c3 = \ln ca2, r1, h$$
$$c4 = \ln ca2, r2, h$$

where:

$c_{1,}\, c_{2,}\, c_{3,}\, c_{4}$	=	the logarithm of the concentrations at the four corners of the grid for time block h
$c_{a1,r1,h,}\, c_{a1,r2,h,}\, c_{a2,r1,h,}\, c_{a2,r2,h}$	=	the concentration for the receptor with indices (a1,r1), (a1,r2), (a2,r1), and (a2,r2) for time block h

- Log-log interpolation in the radial direction:

$$ca1 = c1 + (c2 - c1) \times rratio$$

$$ca2 = c3 + (c4 - c3) \times rratio$$

where:

ca_{1}, ca_{2}	=	the logarithm of the interpolated concentrations for time block h
$c_{1,}\, c_{2,}\, c_{3,}\, c_{4}$	=	the logarithm of the concentrations at the four "corners" of the grid for time block h

- Take the exponent of the logarithm of the interpolated concentrations in the radial direction:

$$cca1 = \exp(ca1)$$

$$cca2 = \exp(ca2)$$

where:

cca_1, cca_2	=	the interpolated concentration for time block h
ca_1, ca_2	=	the logarithm of the interpolated concentrations for time block h

- Finally, linearly interpolate in the azimuthal direction:

$$tc = cca_1 + (cca_2 - cca_1) \times aratio$$

where:

tc	=	concentration at the census tract centroid for time block h
cca_1, cca_2	=	interpolated concentrations at time block h
$aratio$	=	ratio for linear interpolation in the azimuthal direction

3.2.2 Concentration/Deposition Estimates for the Resident Census Tract

The procedures for estimating concentration and deposition for the resident census tracts are different for point sources and pseudo point sources.

3.2.2.1 Major Point Sources

For tracts with centroids close to a major point source, the ambient concentration is estimated in ASPEN by spatial averaging of the ambient concentrations of receptors estimated to fall within the bounds of the tracts, instead of by interpolation to the centroid. Figure 3-3 (a,b) illustrates the spatial averaging procedure. Since inclusion of detailed information on the boundaries of the census tracts was judged to be excessively resource-intensive, a circle of equal area to the census tract, centered at the centroid (Figure 3-3a), was used as an estimate of the tract boundary in the spatial averaging procedure.

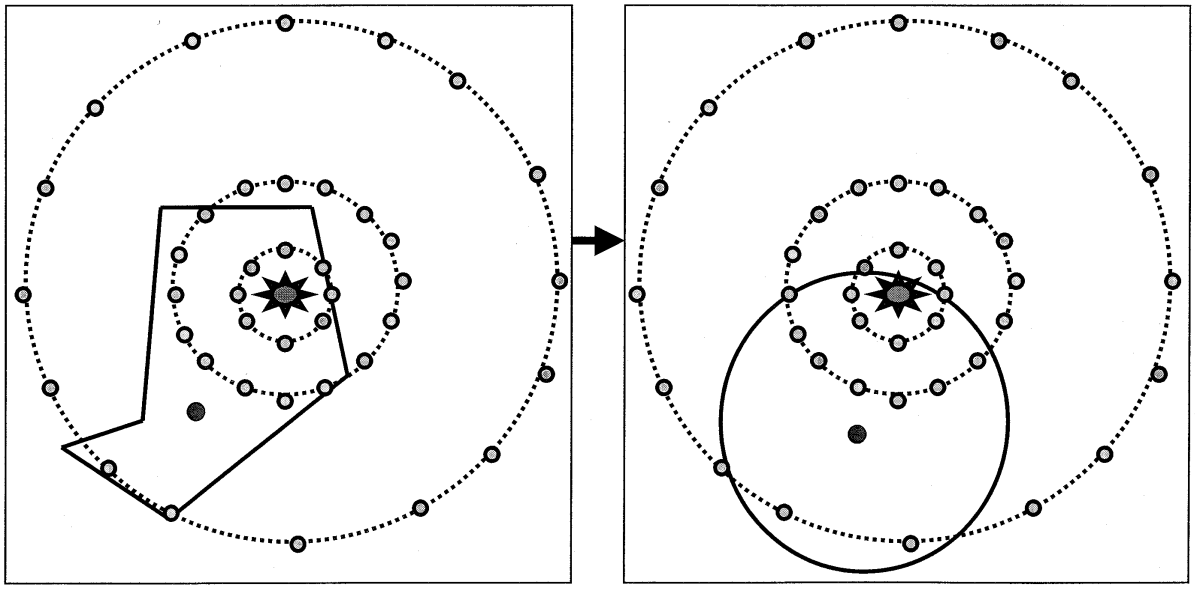

Figure 3-3 (a) Resident tract spatial averaging for point sources.

That procedure is implemented as follows:

- For each point source, the tract with the closest centroid is determined, i.e., the resident tract is defined.

- An effective or pseudo-radius is calculated for the resident tract based on the known tract area and the assumption that the shape of the tract is circular.
- Each modeling receptor for the source is evaluated to determine if it falls within the pseudo-radius of the tract.

- Based on the configuration and spacing of the modeling receptors, an area of representation is assigned to each receptor.

- The resident tract's average outdoor concentration is calculated as the area-weighted average of the modeling receptors that fall within its pseudo-radius (Figure 3-3b). The calculation is shown as follows:

$$conck = \frac{\Sigma sci, j, k \times ai, j}{totarea}$$

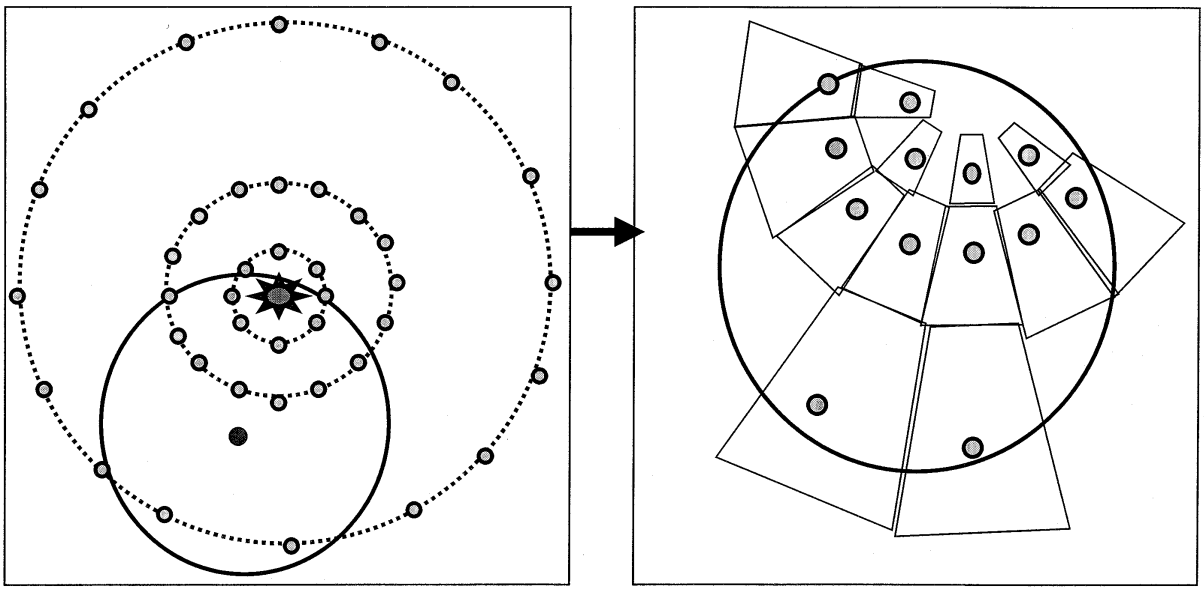

Figure 3-3 (b) Resident tract spatial averaging for point sources.

where:

$conc_k$	=	area-weighted average concentration for time block k at the resident tract
$sc_{i,j,k}$	=	normalized concentration for the receptor at the i^{th} direction, j^{th} distance within the bound of the resident tract for time block k
$a_{i,j}$	=	the area associated with the receptor at the i^{th} direction, and j^{th} distance
totarea	=	the accumulated area for the receptor grid fall within the bound of the resident tract

If no receptor fall within the pseudo-radius of the closest tract, then the tract concentration is estimated with the standard interpolation procedure described in Section 3.2.1.

3.2.2.2 Interpolation for Motor Vehicle and Area Sources

Each motor vehicle and area source is treated as a single pseudo-point source located at the centroid of each census tract in the ASPEN. Outside of the resident census tract of the pseudo-point source, resulting ambient concentration estimates are interpolated to tract centroids, as is done for major point sources.

However, the default interpolation approach cannot be implemented within the resident census tract, since the concentration cannot be estimated at the emission point (the tract centroid) with the long-term Gaussian formulation. For the resident tract, ASPEN represents motor vehicle and area sources as multiple pseudo-point sources geographically dispersed throughout the census tract (see Figure 3-4a).

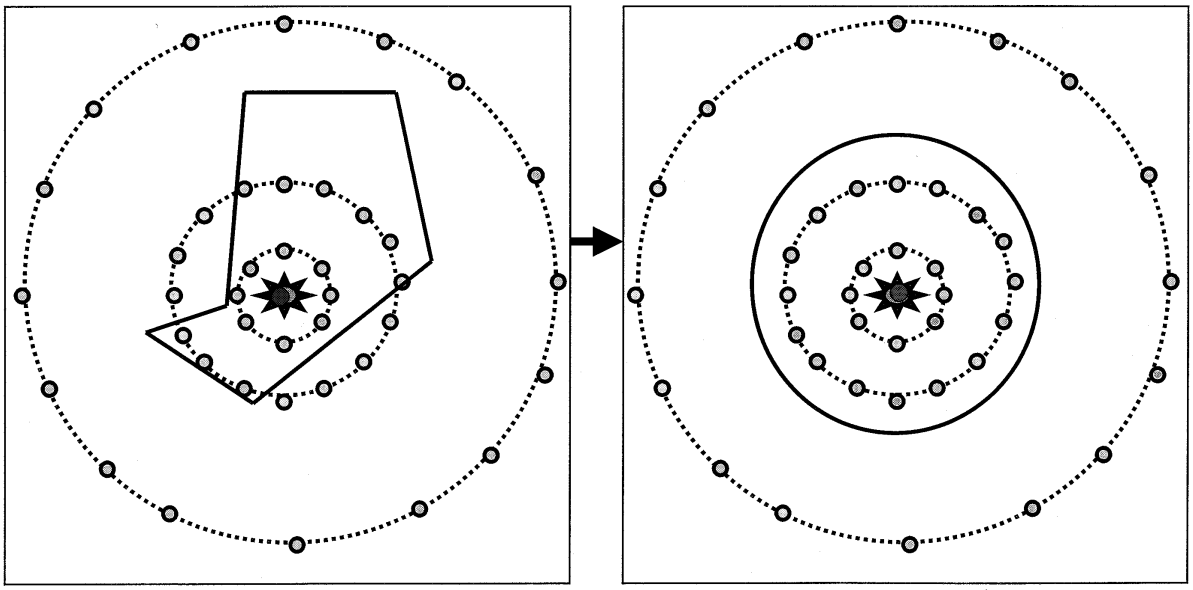

Figure 3-4 (a) Resident tract spatial averaging for area and mobile sources.

For the resident tracts with radius larger than 0.3 kilometers (the average radius of two innermost modeling receptor rings), ambient concentrations in the resident census tract are estimated on the basis of five dispersed pseudo- point sources in ASPEN, with spatial averaging of the ambient concentrations of receptors estimated to fall within the bounds of the tract.

For purposes of the spatial averaging, the tract is assumed to be perfectly round (Figure 3-4a). One of the five pseudo-point sources is located at the center of the tract. The others are located halfway between the center and the hypothetical circumference in each of the four primary compass directions (Figure 3-4b).

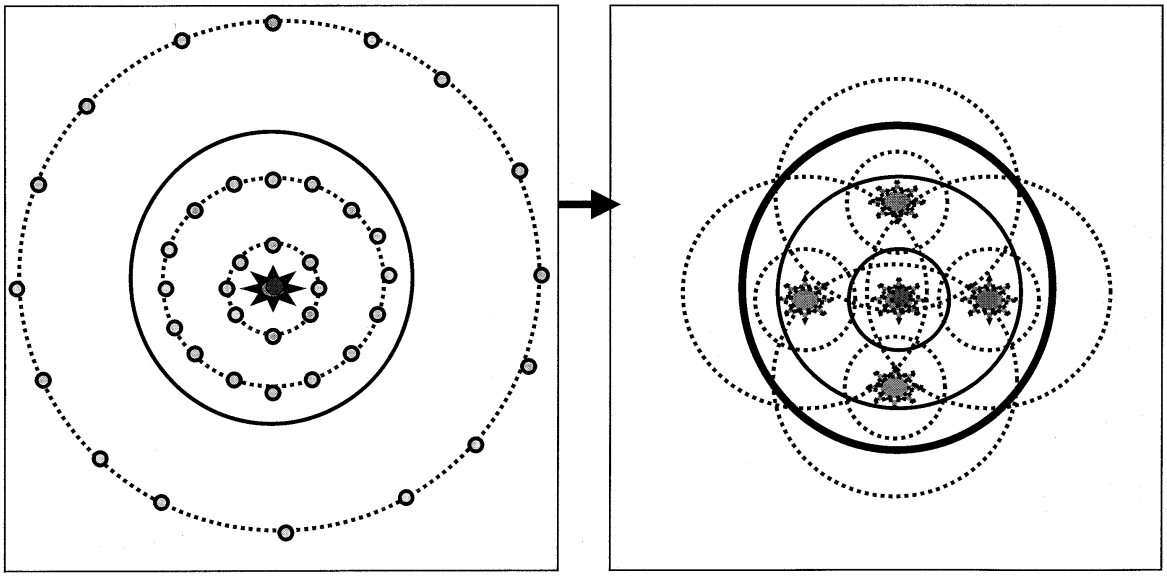

Figure 3-4 (b). Resident tract spatial averaging for area and mobile sources.

The area-weighted average concentration are estimated for the resident tract for the pseudo point sources as following:

$$ac_{k,m} = \sum sc_{i,j,k,m} \times a_{i,j,m}$$

where:

$ac_{k,m}$ = the cumulative area-weighted concentration associated with the pseudo point m for time block k at the resident tract

$sc_{i,j,k,m}$ = normalized concentration for the receptor surrounding pseudo point m at the i^{th} direction, j^{th} distance within the bound of the resident tract for time block k

$a_{i,j,m}$ = the area associated with the receptor surrounding pseudo point m at the i^{th} direction, and j^{th} distance

$$resc_k = \sum_{m=1}^{5} ac_{k,m} \times div_m$$

where:

$resc_k$ = spatially-averaged ambient concentration for time block k

$ac_{k,m}$ = the cumulative area-weighted concentration contributed by pseudo point m for time block k at the resident tract

div_m = the relative size of the receptor grid surrounding pseudo point m to the total area for the all 5 receptor grids: 1/9 for m=1; 2/9 otherwise.

For the resident tracts smaller than 0.3 kilometers, the concentration/depositions are set to zeros.

3.3 DETERMINATION OF IMPACTED CENSUS TRACTS

The normalized concentrations/depositions estimated by ASPEN's dispersion module (ASPENA) for grid receptors surrounding each emission source are interpolated to the census tract centroids within the 50 kilometers impact zone in the ASPENB. The determination of which census tracts fall within this zone is facilitated by the structure of the census tract index and census tract data files.

The tract index file contains the state and county index data. First the state index data are listed with the following information for each state.

- State FIPS code
- Maximum and minimum longitude and latitude of the state
- Total number of counties in the state
- Pointer to the first county of the state, i.e., the record number of the first county of that state in the list of all counties (to follow in the tract index file)

Next, the county index data are listed in the tract index file with includes the following information for each county.

- County FIPS code
- Maximum and minimum longitude and latitude of the county
- Total number of tracts in the county
- Pointer of the first tract of the county, i.e., the record number of the first tract of that county in the list of all tracts (in the tract data file)

For each census tract, the census tract data file contains the following:

- State/County FIPS code and tract FIPS code
- Location of census tract centroid in longitude and latitude
- Urban/rural designation
- Hypothetical tract radius

ASPENB finds tract data for the tracts with centroids within the 50 kilometer impact zone of each emission source as follows:

- Check the locational parameters of each state to determine if there is a potential overlap between that state and the 50 km radius circle of grid receptors around the emission source.

- If there is a potential state overlap, go to the records of the counties in that state and check each for a potential overlap between the county and the 50 km radius circle of grid receptors around the emission source.

- If there is a potential county overlap, go to the tract records of the county and for each tract determine if the centroid falls within the 50 km radius circle of grid receptors around the emission source.

4.0 DISPERSION MODULE (ASPENA) USER'S INSTRUCTION

ASPENA's required data inputs include HAP emission rates, modeling options, and meteorological data. Groups of HAPs that are of the same species type (gaseous, fine particulate, coarse particulate), use the same reactive decay rates, and use the same dry/wet deposition options may be simulated together in a single run. ASPENA estimates the normalized source concentration/deposition for the receptor grid surrounding each source. The normalized concentration/deposition estimates and HAP emission rates are then input to ASPENB, the mapping module of the modeling system, along with the census tract data. (The HAP emission rates are carried over from the ASPENA emission/control file to the ASPENA normalized source concentration/deposition output file.) The final outputs from the ASPEN modeling system are estimates of annual average concentrations (in $\mu g/m^3$) at each census tract for each of eight 3-hour time blocks for each HAP/source category combination.

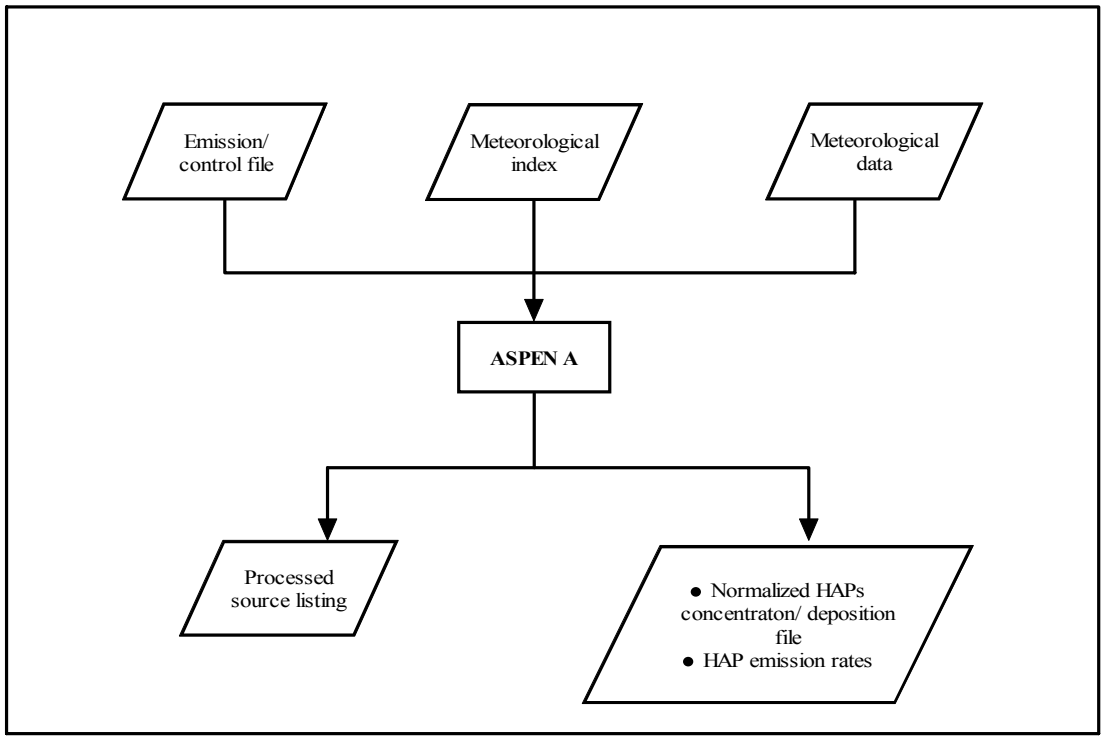

Figure 4-1 Flow diagram of the ASPENA dispersion module

A description of the input and output files of the ASPENA module are provided in Table 4-1.

Table 4-1 ASPENA file descriptions

File Name	File Type	Description	Data Contents
Emission/control	ASCII	ASPENA input file	Modeling options; reactive decay rates ; emission rates for a group of HAPs with the same species type, reactivity class, and selections for dry/wet deposition; Emission rates by stack for point sources and by census tract for pseudo point sources (area or mobile sources) for each of eight 3-hour time blocks; stack parameters for point sources
Meteorological Index	Binary	ASPENA input file	NWS station ID and location; annual average temperatures (max, min, and mean) and precipitation (avg. and frequency); annual average mixing heights for eight 3-hour blocks
STAR meteorological data	Direct access binary	ASPENA input file	Joint frequencies of 6 wind speeds, 16 wind directions and 6 stability categories at each NWS station for each of eight 3-hour time blocks
SYS file	ASCII	ASPENA run stream	List of ASPENA input and output filenames
Normalized source concentration and deposition file	Binary	ASPENA output file (ASPENB input file)	Normalized concentration/deposition estimates for the polar grid receptors surrounding each emission source for each of eight 3-hour blocks; emission rates of the associated HAPs from each source for each of eight 3-hour time blocks
Source listing	ASCII	ASPENA output file	List of processed sources used by ASPENA (used for QA purposes)

4.1 MODELING OPTIONS

ASPEN provides the user with a range of options to meet the needs of a variety of modeling applications. This section gives an overview of the dispersion, source, receptor and meteorological options that are available in the ASPENA dispersion module. Section 4.2 discusses the input files in which these modeling parameters are set.

4.1.1 Dispersion Options

The dispersion parameters in ASPENA are consistent with those in ISCLT2 (EPA, 1992), the EPA-recommended model(when ASPEN was developed) for estimating long-term average concentrations resulting from both rural and urban emission sources. ISCLT2 algorithms for stack-tip downwash, buoyancy-induced dispersion, and final plume rise, and default values for wind profile exponents and for vertical potential temperature gradients are used for ASPENA simulations and cannot be overridden by the user.

The user can select either rural or urban dispersion parameters, depending on the characteristics of the source location. The user also has the option of calculating dry and/or wet deposition flux values for a simulation of particulate HAPs. Finally, the user may select to invoke ASPENA's building downwash algorithms for point sources. However, it should be noted that these algorithms differ from those in (see Section 2.1.7).

Note that ASPENA does not treat the effect of terrain elevation on ground-level ambient concentration estimates, but implicitly assumes flat terrain throughout the modeling domain.

4.1.2 Source Options

ASPENA is capable of modeling three pollutant species types, two types of emission sources, and up to ten source categories. Each of these source options are listed here.

Species types: (1) gaseous HAPs, (2) fine particulate HAPs, (3) and coarse particulate HAPs

Source types: (1) point/stacked sources and (2) pseudo point/non-stacked sources (area and mobile sources are treated as pseudo point source in ASPEN). Detailed description of source types, release parameters, emission rates and multiple sources is given in section 4.2.

Source categories: The emission rates of the emission sources can be aggregated into up to ten different categories. For example, for the Cumulative Exposure Project, the following emission source categories were used:

- Metal manufacturing point sources (CAT09)
- Non-metal manufacturing point sources (CAT00)
- Petroleum refineries (CAT02)
- Municipal waste combustors (CAT07)
- Hazardous waste incinerators (CAT08)
- Other point sources (CAT01)
- Manufacturing area sources (CAT05)
- Non-manufacturing area sources (CAT06)
- Onroad mobile sources (CAT03)
- Nonroad mobile sources (CAT04)

The emission rates of the sources are specified for eight 3-hour time blocks in the model. The emissions of the sources can be constant or vary by time block.

The modeled HAPs must be assigned a set of reactive decay rates that vary by stability class and time block. A single ASPENA simulation can include emission rates for a group of HAPs with the same species type, reactivity class, and selection of dry/wet deposition.

4.1.3 Receptor Options

Surrounding each modeled source, ASPENA uses a default polar receptor grid of 12 concentric rings in 16 radial directions for a total of 192 receptors. The default ring distances from each modeled source are 0.1, 0.5, 1.0, 2.0, 5.0, 10.0, 15.0, 20.0, 25.0 30.0, 40.0, and 50.0 km. Following the caution of the ISC user's guide (EPA, 1992) that concentrations at receptors less than 100 meters from a source may be suspect, the closest receptor distance is 100 meters. Fifty km is the maximum distance recommended by the EPA for application of a Gaussian model (EPA, 1992).

ASPENA also allows the user to replace the default distances with user-specified values (between 100 meters and 50 km) for the 12 rings surrounding the modeled source.

4.1.4 Meteorological Options

ASPENA uses **ST**ability **Ar**ray (STAR) meteorological data which includes joint frequency distributions of 6 wind speeds, 16 wind directions, and 6 stability categories for each of eight 3-hour time blocks. The user can select the STAR data to be used for a particular modeled source by specifying the National Weather Service (NWS) station ID. If no selection is made, ASPENA will use the STAR data from the NWS station in the data base that is nearest the source.

ASPENA allows the user to customize the meteorological data inputs by excluding specified stability classes, wind speeds, and wind directions for a certain NWS station. If certain meteorological parameters are excluded ASPENA will re-normalize the joint frequency distributions for the station.

4.2 ASPENA INPUTS

The three types of input files needed to run the ASPENA dispersion model are: emission/control file, a STAR meteorological data file, and a meteorological index file.

4.2.1 Emission/Control File

The emission/control input file allows users of ASPENA to select the appropriate dispersion, source and receptor options in order to simulate the modeling conditions of interest. The modeling parameters include specifying species type, source type, source location, source release

parameters, emissions rates, and decay rates. The format of the emission/control file is provided in Table 4-2.

4.2.1.1 Run Information, Species Types and Deposition Options

The run information, species type and deposition selections is specified in the first record of the emissions/control input file. There are three species types in ASPEN: gaseous, fine particles, and coarse particles. Each emission input file should include only HAPs with the same species type, reactive decay rates, and dry/wet deposition selection. The syntax, type, and order for specifying the required information are summarized below.

Table 4-2 Description of the emission/control file

Record No.	Variables	Format	Description
1	IDRUN	A40	Run identification
	IDFILE	A20	Emission file identifier
	ISPTYP	I1	Species type (0 = gas; 1 = fine part.; 2 = coarse part.)
	IDDEP	I1	= 0, include dry deposition; = 1 no dry deposition
	IWDEP	I1	= 0, include wet deposition; = 1, no wet deposition
2	DK(IC,1)	6F10	Decay rates for 6 stability classes for time block 1
3	DK(IC,2)	6F10	Decay rates for 6 stability classes for time block 2
4	DK(IC,3)	6F10	Decay rates for 6 stability classes for time block 3
5	DK(IC,4)	6F10	Decay rates for 6 stability classes for time block 4
6	DK(IC,5)	6F10	Decay rates for 6 stability classes for time block 5
7	DK(IC,6)	6F10	Decay rates for 6 stability classes for time block 6
8	DK(IC,7)	6F10	Decay rates for 6 stability classes for time block 7
9	DK(IC,8)	6F10	Decay rates for 6 stability classes for time block 8
10	IFIPS	I5	State/County FIPS code
	IDSRC	A10	Plant ID for points; census tract no. for pseudo points
	UTMX	F10	Longitude (decimal degrees)
	UTMY	F10	Latitude (decimal degrees)
	ITYPE	I1	Source type (0 or blank for points; 3 = pseudo points)
	IURB	I1	Urban/Rural flag (1 = urban; 2 = rural)
11	INWS	I5	Star station (NWS) ID (blank or 0 = use nearest station)
	NOSC(6)	6I1	Excluded stability classes
	NOWS(6)	6I1	Excluded wind speeds
	NOWD(6)	6I1	Excluded wind direction
12	RAD (12)	12F5	Polar grid radial distances (km) (blank – use defaults)
13	IDSTK	A5	Stack ID for points; FIPS code for pseudo points
	RLON	F10	Longitude (decimal degrees)
	RLAT	F10	Latitude (decimal degrees)
	STAKH	F10	Stack height (m)
	STAKD	F10	Stack exit diameter (m)
	STAKV	F10	Stack exit velocity (m/sec)
	STAKT	F10	Stack exit temperature (Deg K)
	IVENT	I1	Vent/Stack flag (0 = stacked; 1 = non-stacked)
	IBLDG	I1	Build flag (0 = no building; 1 = building)
	BLDW	F10	Width of nearby building (m)
	BLDH	F10	Height of nearby building (m)
14	SAROAD	I5	5-digit Saroad code
	IDCAT	I1	1-digit source category code
	Q	8F10	Emissions (g/sec) for eight 3-hour time blocks Note that ASPEN treats the SAROAD code/source category code as a single combined code to refer to a unique chemical and is therefore technically not separable.

Notes: UTMX/UTMY and RLON/RLAT specify the locations of point sources, or the locations of the census tract centroid for pseudo point sources (i.e., area and mobile sources).

Record 14 is repeated for each HAP emitted from the stack or census tract; terminate with blank record.

Records 13 and 14 are repeated for each source/stack within facility; terminate with blank record. (Last stack and chemical for each facility will be followed by two blank lines to signal new facility.)

Records 10 through 14 are repeated for each facility or census tract, terminate with blank record. (Last facility, stack and chemical in file will be followed by three blank lines to signal no more facilities.)

Four blank records are required at the end of file to signal the end of the run.

Syntax:	IDRUN, IDFILE, ISPTYP, IDDEP, IWDEP
Type:	Mandatory
Order:	1st record of emission/control input file

IDRUN and IDFILE are the character variables in the header which allow the user to specify the title and the run information. ISPTYP is the species type: 0 for gaseous, 1 for fine particulate and 2 for coarse particulate. IDDEP and IWDEP are the selections for dry and wet deposition: 0 is the code to include deposition and 1 is the code to exclude deposition. Note that for the gaseous pollutant species type, ASPENA will not calculate deposition, regardless of how the deposition selection variables are set.

4.2.1.2 Reactive Decay Rate Inputs

The reactive decay rates are specified in the emission/control input file by stability class and time block. ASPENA requires that all the HAPs included in a single emission/control input file have the same decay rates. Therefore, a unique emission/control file is required for each set of HAPs with different decay rates. The decay rates are specified in the emission/control input file for each stability class and time block according to the following pattern: decay rates for time block 1 are entered in the second record, for time block 2 in the third record, and so on. The decay rate for the last time block, time block 8, is entered in the ninth record of the emission input. The syntax, type, and order for specifying reactive decay rates are summarized below. The reactivity classes and corresponding decay rates normally used are presented in Appendix C.

Syntax:	DK(IC,IH)
Type:	Mandatory
Order:	2nd - 9th record of emission/control input file

4.2.1.3 Source Types and Locations

ASPENA currently handles two source types, identified as point sources and pseudo point sources. Area and mobile sources are treated as pseudo point source. The location of a source is indicated by specifying the geodetic coordinates in latitude and longitude. The syntax, type, and order for identifying source types and locations are as follows.

Syntax:	IFIPS, IDSRCE, UTMX, UTMY, ITYPE, IURB
Type:	Mandatory, Repeatable
Order:	10th record of emission/control input file

IFIPS is the FIPS code. IDSRCE is the plant ID for a point source, and census tract FIPS code for pseudo point source. UTMX and UTMY are either the longitude and latitude of a point source, or the census tract centroid in the case of a pseudo point source. ITYPE is source type: 0 or blank for point source, and 3 for pseudo point source. IURB is urban/rural designation: 1 for urban and 2 for rural.

The source locations are also specified along with source parameters in record 13 of the emission input described in the next section.

Line 11 can be left blank. In this case, the closest meteorological station will be used by latitude/longitude. Line 12 can be left blank. In this case default receptor grid will be used

4.2.1.4 Source Release Parameters

The input source parameters vary depending on the source type. For a point source, the stack height, stack exit diameter, stack gas exit temperature, and stack gas exit velocity are required. For a pseudo point source, no source parameters are required and ASPENA will use a default stack height. The syntax, type, and order for specifying source release parameters are summarized below.

Syntax: IDSTK, RLON, RLAT, STAKH, STAKD, STAKV, STAKT, IVENT, IBLDG, BLDW, BLDH
Type: Mandatory/Optional, Repeatable
Order: 13th record of emission/control input file

IDSTK is the stack ID for point source, and census tract FIPS code for pseudo point source. RLON and RLAT are either the longitude and latitude of a point source or the location of the census tract centroid, in the case of a pseudo point source. STAKH is the stack release height above ground (in meters). STAKD is the inside stack diameter (in meters). STAKV is stack gas exit velocity (in m/sec). STAKT is the stack gas exit temperature (in degrees K). IVENT is the vent/stack designation: 0 for stacked and 1 for non-stacked. IBLDG is the building flag: 1 to include consideration of building downwash, 0 otherwise. BLDW and BLDH are the width and height of nearby buildings (in meters).

4.2.1.5 Emission Rates

The emission rates are specified in ASPENA in eight 3-hour time blocks. The syntax, type and order for specifying emission rates are summarized below.

Syntax: SAROAD, IDCAT, Q
Type: Mandatory, Repeatable
Order: 14th record of emission/control input file

IDCHEM is the 5-digit HAP SAROAD code plus 1-digit source category code. Q is the source emission rates (in grams/second).

Multiple sources can be repeated as shown in the example in Section 8 (tutorial). In this case lines 13 and 14 are repeated for each source/stack within facility.

4.2.1.6 Secondary Compounds

ASPENA models atmospheric transformation processes as first-order reactive decay. Secondary formation is calculated as the difference between secondary precursor concentrations with and without reactive decay. This calculation is completed in the post-processing program SEC_DAT. For a detailed description of the treatment of secondary HAPs see Section 6.1.

4.2.1.7 Deposition Rates

For particles, dry deposition rates are primarily a function of the particle size and land-use type. The fine and coarse particle deposition velocities used in ASPENA were obtained for urban and rural land-use types using the dry deposition algorithms in the Variable-grid Urban Airshed Model (UAM-V) photochemical model (SAI, 1995). These values were further parameterized as function of stability class and wind speed.

The ASPENA dispersion module uses the wet deposition algorithm from the revised version of the CAP88-PC model to estimate the wet deposition of particles. The algorithms are based on the approximate method described by Rodhe (1980) and use the fraction of time during which precipitation is occurring in conjunction with the total annual precipitation to calculate both the decay rate for the modeled ambient concentrations as well as the deposition fluxes.

4.2.2 STAR Meteorological Data File

ASPENA utilizes a climatological modeling approach. As with other climatological models (e.g., the EPA's CDM and ISCLT), the dispersion module is supplied with **ST**ability **Ar**ray (STAR) meteorological data. STAR data include the joint frequencies of 6 wind speeds, 16 wind directions and 6 stability categories (Pasquill - Gifford: A through F).

For each ASPENA model run, the STAR data is prepared for eight 3-hour time blocks for each surface station. The station number and time block number are specified at beginning of each STAR data record. The STAR input file is in binary format. Each record contains the STAR data for one time block of one star station, and includes the variables shown in Table 4-3.

The STAR data is prepared as follows:

- Split the surface data into eight 3-hour time blocks
- Generate STAR data for each time block
- Combine the eight STAR data sets into one file

The format of the star data is provided in detail in Appendix C.

Table 4-3 Description of the STAR meteorological data file

Variables	Data Type	Description
IWB	Integer	Star (NWS) station ID
IHR	Integer	Time block number
FSTAR	Real	STAR data for the time block

4.2.3 Meteorological Index File

The STAR data file is paired with a binary meteorological index file. The number and ordering of stations included in both the index file and the STAR data file must be the same. There is one record for each STAR station containing the following information: station number, station longitude, station latitude, annual average daily maximum temperature, annual average daily minimum temperature, annual average temperature, annual average precipitation, annual frequency of precipitation, and annual average mixing heights for each of eight 3-hour blocks. A description of the meteorological index file parameters is provided in Table 4-4.

Table 4-4 Description of the meteorological index file

Variables	Data Type	Description
ISTA	Integer	Star (NWS) station ID
STAX	Real	Longitude of the station (decimal degree)
STAY	Real	Latitude of the station (decimal degree)
ATEMP (1)	Real	Annual average daily maximum temperature (Deg K)
ATEMP (2)	Real	Annual average daily minimum temperature (Deg K)
ATEMP (3)	Real	Annual average temperature (Deg K)
PS	Real	Annual average precipitation (cm)
FPS	Real	Fraction of time with precipitation
STAS	Real	Not used (eight zeros)
HTMI	Real	Annual average mixing heights for eight 3-hour time blocks

4.2.3.1 Temperatures

For each surface meteorological station included in the STAR data, the annual average daily minimum, maximum and average temperature (in degrees Kelvin) is specified in the meteorological index file.

4.2.3.2 Mixing Heights

For each surface meteorological station included in the STAR data, annual average mixing heights (in meters) are specified for each of eight 3-hour time blocks in the meteorological index file.

4.2.3.3 Precipitation

For each surface meteorological station included in the STAR data, annual average precipitation (cm/year) and fraction of time that precipitation occurs (based on hourly values) are specified in the meteorological index file.

4.2.4 Polar Receptor Grid Network

Surrounding each modeled source, ASPENA uses a default polar receptor grid of 12 concentric rings in 16 radial directions for a total of 192 receptors. The ring distances from each modeled source are 0.1, 0.5, 1.0, 2.0, 5.0, 10.0, 15.0, 20.0, 25.0 30.0, 40.0, and 50.0 km.

Instead using the default concentric distances, the user can specify the distances for the 12 rings between 100 meters and 50 km surrounding the modeled source.

4.3 ASPENA OUTPUTS

ASPENA creates two output files when it is executed. The first of these is the normalized source concentration/deposition data file. This binary file contains the source information and the normalized concentration/deposition for each of eight 3-hour time block at each receptor location around the source, and the emission rates for each HAP. This file is used as input to the ASPENB mapping module. The utility program INV2ASCI_CON can be used to convert the ASPENA output from binary to ASCII format. Converting the file to ASCII allows the user to review the modeling results of the ASPEN dispersion module. The utility does not convert the deposition portion of the output, however. Note that a single binary output file is created which will contain data for all sources and all HAPs specified in the emission/control input file.

The second file created by ASPENA is a listing of all emission sources (source FIPS, ID, location, type and urban/rural destination) that were processed in the run. This file ends with a line of zeros. The number of non-zero lines included in the file should equal the total number of sources included in the emission/control file. This processed source listing file is written to Fortran unit 88.

The user has the option of creating a third output file that echoes all the information included in the meteorological index file, the emission/control file and the concentration/deposition output file. This large file is typically used in the testing stage of the modeling study.

Once ASPENA has been run a log file with a ".como" extension is created. The log file includes useful information including the input/output filenames and error messages. Table 4-5 presents a summary of error messages in ASPENA.

Table 4-5 Error messages in the ASPENA log file

Error Message	Module	Subroutine	Program Aborts
Too many chemicals *Comment: Max number of species is 150*	ASPENA	SKIP STACK	Yes
Too many star stations *Comment: Max number of stations is 500*	ASPENA	STARIN	Yes
Bad number in star data *Comment: Errors in star index file*	ASPENA	STARIN	Yes
Can not find star data for station *Comment: Missing star data for stations specified in the emission/control file*	ASPENA	STAR	Yes
WARNING: iNWS, istar *Comment: The star station IDs specified in the star data and index file are not in sync*	ASPENA	STAR	Yes
Illegal urban/rural flag *Comment: urban/rural flag must be 1 or 2*	ASPENA	MAIN	Yes
Illegal source type *Comment: Source type must be 0 or 3*	ASPENA	MAIN	Yes
Error … idummy *Comment:*	ASPENA	SKIP	Yes

4.4 RUNNING ASPENA

ASPENA can be run interactively by simply typing:

aspena aspena.sys

where "aspena.sys" is the run stream filename.

Figures 4-2 and 4-3 show example run stream files used to run ASPENA. The first record in the file contains the name of the emission/control file, the third record contains the name of the meteorological index file, the fourth record contains the name of the STAR meteorological data file, and the fifth record contains the name of the normalized source concentration/deposition output file. The second record in the file is a placeholder for those that want to create the optional "echo" output file described above. The creation of the testing file is invoked by including a file name in record 2, as shown in Figure 4-2. To prevent the creation of the testing file, "/dev/null" is entered in record 2, as shown in Figure 4-3.

```
1  aspena.ar.inp
2  aspena.ar.test
3  wtpmix.ind
4  star.dat
5  aspena.ar.con
```

Figure 4-2. Example ASPENA run stream file (filename: aspena.sys) that creates a testing file.

```
1  aspena.ar.inp
2  /dev/null
3  wtpmix.ind
4  star.dat
5  aspena.ar.con
```

Figure 4-3 Example ASPENA run stream file (filename: aspena.sys) that does not create a testing file.

A job file can be created to run ASPENA multiple times, in sequence, as shown in the Figure 4-4. For this example, ASPENA is run 3 times, using 3 different run stream files. The two statements preceding each run line delete any previously created versions of the ASPENA output files that will be created by the simulation. The statement after each run line renames the processed source listing file, so that it will not be overwritten during the subsequent simulation.

```
rm aspena.tri.lst
rm aspena.tri.con
/bin/time aspena aspena.tri.sys
mv fort.88 aspena.tri.lst
#
rm aspena.ar.lst
rm aspena.ar.con
/bin/time aspena aspena.ar.sys
mv fort.88 aspena.ar.lst
#
rm aspena.mv.lst
rm aspena.mv.con
/bin/time aspena aspena.mv.sys
mv fort.88 aspena.mv.lst
```

Figure 4-4 Example ASPENA job file

In the above examples, the files with a "*.inp" extension contain the emission/control information specifying the particular emission source for processing. In general, all chemicals of the same species type (gas, fine, or coarse particles) with the same reactive decay rates and deposition options may be processed in a single run, regardless of the source type or location.

5.0 ASPENB USER'S INSTRUCTIONS

ASPENB is the mapping module of the ASPEN modeling system. ASPENB takes the diurnally-stratified annual average concentration estimates from ASPENA and interpolates the results from grid receptors to census tract centroids. Further, the contributions from all modeled sources are summed to give estimates of cumulative ambient concentration increments in each census tract. An overview of the inputs and outputs of the ASPENB module is shown in Figure 5-1.

Output from ASPENB is post-processed using a series of programs described in detail in Section 6. By accounting for all identified source categories (including background concentrations where available), the sum of the concentration increments should yield an estimate of the overall concentration of each HAP within each census tract. These estimates are designed to represent population-weighted concentration averages for each census tract.

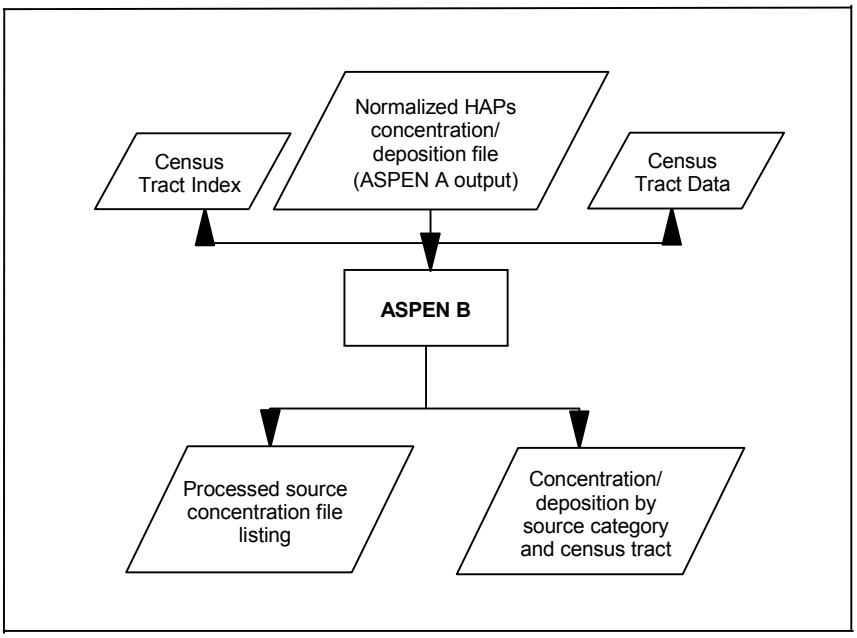

Figure 5-1 Flow diagram of the ASPENB mapping module

Several new features have been added to ASPENB (version 1.1). The detailed discussions of these new features, along with the comparisons to the previous version are as follows:

- ***Number of output files produced by the model***

Each output file produced from version 1.0 of the model contains the tract level concentration/deposition for a single source category for a particular HAP. If there are ten source categories for the HAP, there will be ten output files generated by the model. In version 1.1 of the model there is a single output file or each HAP which contains the tract level

concentration/deposition for all source categories. Therefore, the number of output files produced by the model is greatly reduced.

- ***Output file naming convention***

The naming convention for the output file generated by version 1.0 of ASPENB is 5-digit SAROAD code plus a 1-digit source category code, with a "*.exp" extension. The naming convention for the version 1.1 of ASPENB output file is simply the 5-digit SAROAD code with a "*.exp" extension, i.e., the extra digit to identify the source category has been eliminated.

- ***Number of source categories contained in the ASPENB output file***

Flexibility in the number of source categories, which can be included in a modeling simulation, has been added to the version 1.1 of the ASPENB. The user selects the desired number of source categories to be included in a particular modeling simulation. A maximum of ten source categories is allowed.

- ***Rerun for a single source category***

Each output file generated by version 1.0 of the model contains the tract level concentration/deposition for a single source category for a particular HAP. If there is a need for rerunning the simulation for that source category, the user can simply delete the output file generated by the previous simulation, then rerun the model.

The output file generated by version 1.1 of the model contains the tract level concentration/deposition estimates for all the source categories included in the modeling study. If revision is needed for a single source category, that source category alone can be rerun and the model will replace the previous estimates for that category in the output file. This feature avoids a requirement to rerun all source categories (i.e., start the output file from scratch) in order to revise a single source category.

5.1 ASPENB INPUTS

The ASPENB module requires three input files: the normalized concentration/deposition output file from ASPENA, a census tract data file and a census tract index file. The input data requirements are the same for both versions of ASPENB. A description of the input and output files of the ASPENB module are provided in Table 5-1.

Table 5-1 ASPENB input and output file descriptions

File Name	File Type	Description	Data Contents
Normalized source concentration and deposition file	Binary	ASPENB input file (ASPENA output file)	Normalized concentration/deposition estimates for the polar grid receptors surrounding each emission source for each of eight 3-hour blocks; emission rates of the associated HAPs from each source for each of eight 3-hour time blocks
Census tract data	Binary	ASPENB input file	Tract FIPS code, longitude and latitude of the centroid, urban/rural flag of the tract, and hypothetical tract radius
Census tract index	Binary	ASPENB input file	State/county FIPS codes; state/county max and min longitude/latitude; pointer to the first county in state and number of counties in state; pointer to the first tract in county and number of tracts in county
Population concentration and deposition file (naming convention {saroad}.EXP)	Direct access binary	ASPENB output file (AVGDAT input file)	Estimates of annual average concentrations (in $\mu g/m^3$) at each census tract for each of eight 3-hour time blocks, and annual average deposition fluxes over land and water (in $\mu g/m^2$-day) for each HAP/source category combination
File listing	ASCII	ASPENB output file	List of processed concentration filenames by ASPENB to prevent processing an input more than once

5.1.1 Source Concentration and Deposition File

The first input required by the ASPENB module is the normalized source concentration/ deposition data output file from ASPENA. This binary file contains the source information and the normalized concentration/deposition for each of eight 3-hour time block at each receptor location around the source, and the emission rates for each HAP. See Appendix C for further details.

5.1.2 Census Tract Data File

The second input required by ASPENB is the binary census tract data file. The format of this file is shown in Table 5-2. For each census tract, the tract data file contains the following:

- State/County FIPS code and tract FIPS code
- Location of census tract centroid in longitude and latitude
- Urban/rural designation
- Hypothetical tract radius

Table 5-2 Description of census tract data file

Variables	Data Type	Description
TRFIPS	Integer	State/County FIPS code, tract FIPS code
TRLON	Real	Longitude of the tract centroid (decimal degree)
TRLAT	Real	Latitude of the tract centroid (decimal degree)
UFLAG	Integer	Urban/Rural flag of the tract (1 = urban; 2 = rural)
TRRAD	Real	Hypothetical tract radius (m)

The data in the census file are derived from the 1990 US Census. The longitude and latitude represent an approximate population weighted census tract centroid. They are calculated as a population-weighted average of the US Census reported geographic centroids of the constituent block groups.

The urban/rural designation was specified based on residential population density: urban if greater than 750 people/km^2.

Finally, the hypothetical tract radius was derived from the tract area reported in the US Census, under the assumption of a perfectly round shape:

$$TRRAD = \sqrt{Area / \Pi}$$

5.1.3 Census Tract Index File

The final input required by ASPENB is the binary census tract index file, containing the state and county index data. The format of this file is shown in Table 5-3. The state index data are listed with the following information for each state:

- State FIPS code
- Maximum and minimum longitude and latitude of the state
- Total number of counties in the state

- Pointer to the first county of the state, i.e., the record number of the first county of that state in the list of all counties (to follow in the tract index file)

The county index data are listed in the tract index file with includes the following information for each county:

- County FIPS code
- Maximum and minimum longitude and latitude of the county
- Total number of tracts in the state
- Pointer to the first tract of the state, i.e., the record number of the first tract of that county in the list of all tracts (in the tract data file)

A utility program, MKTRACTS, generates the census index file utilizing ASCII formatted census data. Figure 5-2 presents an example MKTRACTS job file.

Table 5-3 Description of census tract index file

Record No.	Variables	Data Type	Description
1	NSTATES	Integer	Total number of states included in the data
	NCOUNTIES	Integer	Total number of counties included in the data
	NTRACTS	Integer	Total number of tracts included in the data
2	STFIP	Integer	State FIPS code
	STMNLN	Real	State minimum longitude (decimal degree)
	STMNLT	Real	State minimum latitude (decimal degree)
	STMXLN	Real	State maximum longitude (decimal degree)
	STMXLT	Real	State maximum latitude (decimal degree)
	COPTR	Integer	Pointer to the first county in the state
	NUMCO	Integer	Total number of counties in the state
3	COFIPS	Integer	County FIPS code
	COMNLN	Real	County minimum longitude (decimal degree)
	COMNLT	Real	County minimum latitude (decimal degree)
	COMXLN	Real	County maximum longitude (decimal degree)
	COMXLT	Real	County maximum latitude (decimal degree)
	TRPTR	Integer	Pointer to the first tract in the county
	NUMTR	Integer	Total number of tracts in the county

Record 2 is repeated for all states included in the census tract data file.
Record 3 is repeated for all counties included in the census tracts data file.

```
/bin/time src/mktracts << -eof-
DATA FILE          |smptracts
-eof-
```

Figure 5-2 Example MKTRACTS job file

In the above example, the user input the ASCII formatted census tract data SMPTRACTS.ASC, the utility MKTRACTS generates the corresponding binary formatted census tract data (SMPTRACTS.DAT) and index file (SMPTRACTS.IND) required by ASPENB.

Figure 5-3 presents an example of ASCII formatted census tract data. Each record contains the following variables: state FIPS, county FIPS, tract FIPS, longitude, latitude, tract hypothetical radius, and urban/rural flag.

```
 9  1 10101-73.679499 41.068223  3.26 2
 9  1 10102-73.633778 41.097472  3.31 2
 9  1 10201-73.623645 41.059098  1.91 2
 9  1 10202-73.588872 41.063468  1.75 2
 9  1 10300-73.637447 41.036887  1.75 2
.......
36119 15000-73.617674 41.334870  4.34 2
```

Figure 5-3 Example of ASCII formatted census tract data

5.2 ASPENB OUTPUTS

ASPENB creates two output files when it is executed. The first is the population concentration/deposition file. This is the binary output file which contains estimated outdoor concentrations ($\mu g/m^3$) and deposition fluxes ($\mu g/m^2$-day) for each HAP by census tract for each of eight 3-hour time blocks. The utility EXP2ASCI converts the ASPENB output from binary to ASCII format. This allows the user to easily view the modeling results of ASPENB. The format of the binary and ASCII output files are provided in Appendix C.

The second file created by ASPENB is the processed source concentration file. This file contains a list of all of the normalized source concentration/deposition input file names that have been processed. This is used to avoid running the same input file twice.

5.3 RUNNING ASPENB

Figure 5-4 shows an example run stream file for ASPENB. As discussed above, there are three required input files for the ASPENB: the normalized source concentration/deposition file (output from ASPENA), the census tract data file, and the census tract index file. ASPENB requires that the tract data and index files be located in the same directory where the job is run.

Note that the tract data and index files are specified in record 2 of the run stream file by their base name only (do not include any extensions). In the directory in which they reside, the two files should be distinguished by the following extensions: tract data file (*.dat) and index file (*.ind).

```
/bin/time aspenb << -ieof-
ONROAD MV FILE     |cat3.con
TRACT FILE BASENAME|tracts
FILE LIST FILENAME |filelist.ntl
NO. OF SRC CATEGORY|5
RERUN (Yes/No)     |No
-ieof-
```

Figure 5-4 Example ASPENB run stream file

The run stream file shown in Figure 5-4 is set up for a modeling simulation that includes total number of five source categories, and it is not a rerun. Important parameters for the run stream are as follows:

- Filename for input normalized source concentration/deposition file: cat3.con
- Base name of the census tract data file and index file: tracts
- Filename for output file listing: filelist.ntl
- Number of source categories included in the modeling: 5
- Status of the run, i.e., if it is a rerun: NO

A separate population concentration/deposition output file is created by ASPENB for each HAP. The naming convention for the output file is 5-digit SAROAD code with a "*.exp" extension. For example, the output file for toluene (with SAROAD code 45202) will be named as 45202.exp. Each time a HAP is encountered during the ASPENB simulation, the local directory is checked to determine whether an appropriate HAP output file already exists. If not, one is created. If so, the previous values for the current source category are incremented by the current estimates to obtain cumulative concentration and deposition estimates for each census tract for that source category.

In the example shown in Figure 5-4, if the emissions data for the CAT3 are revised, ASPENA can be rerun for that category to produce revised normalized source concentration/deposition data. A remodeling for the category can be completed using the rerun feature of ASPENB, without having to rerun the simulations for other source categories. Figure 5-5 presents the ASPENB run stream file using the rerun feature. Note that the only difference between the run stream shown in Figure 5-4 and 5-5 is the selection for the status of the run.

```
/bin/time aspenb << -ieof-
ONROAD MV FILE     |cat3.rev.con
TRACT FILE BASENAME|tracts
FILE LIST FILENAME |filelist.ntl
NO. OF SRC CATEGORY|5
RERUN (Yes/No)     |Yes
-ieof-
```

Figure 5-5 Example ASPENB run stream file using the rerun feature

To successfully execute a rerun for a particular source category, special attention should be paid to the following:

- Specify "Yes" for rerun status in the ASPENB run stream file
- Use the revised ASPENA output file (as shown in the example cat3.rev.con) as one of the input files
- Provide the ASPENB output files from the previous modeling runs. Those files contain results from the previous modeling for all source categories, and the rerun will modify the results for the single category specified in the input normalized concentration file
- If the normalized concentrations file name remains unchanged in the rerun from the previous modeling run (i.e., if cat3.con is the normalized concentrations file name used in both runs in the examples shown above), then the file name should be removed from filelist.ntl generated in the previous run, because the model will not allow running a file with a name included in filelist.ntl.

Once ASPENB has been run a log file with a ".como" extension is created. The log file includes useful information including the input/output filenames and errors. Table 5-4 presents a summary of error messages in ASPEN. At the end of a run, the log file displays the following message: "All done: X sources processed," where X is the total number of emission sources in the simulation. The number and type of sources processed by ASPENB should be the same as those processed in the corresponding ASPENA simulation.

Table 5-4 Error messages in the ASPENB log file

Error Message	Module	Subroutine	Program Aborts
Error reading source file *Comment: read error or unexpected of in normalized concentration/deposition file*	ASPENB	NEXTSOURCE	Yes

5.4 MODEL RE-START CAPABILITY

ASPENA has no direct re-start capability. However, it is possible to re-start ASPENB indirectly in some cases. For example, for large modeling domains ASPEN input files for the same HAP/source category combinations may be divided into several files (e.g., stratified by geographic region). When ASPENB processes the first ASPENA output file, it creates the appropriate ASPENB HAP output files. When subsequent ASPENA output files are processed by ASPENB, the previously created ASPENB HAP output files are incremented to accumulate the concentration increments from all sources for that HAP/source category combination.

To avoid losing output data in the event of ASPENB aborting while processing one of the multiple files, the user can make an intermediate copy of the ASPENB output files at the completion of the processing of each ASPENA output file. (See Figure 5-6 for an example job file.) Then if a run aborts, ASPENB can be re-started at the beginning of the aborted simulation, using the intermediate ASPENB output files as the starting point. Figure 5-7 presents an example job file for re-starting the job specified in the Figure 5-6 job file, if it were to abort during the second ASPENB simulation. First, the partially updated output files are deleted. Then the intermediate files are copied back into the local directory. Finally the ASPENB job is re-started at the beginning of the simulation that aborted. Note that this procedure requires knowledge of the HAPs that will be processed so that the names of the ASPENB output files are known.

```
/bin/time aspenb << -eof-
ON ROAD MV FILE    |cat3.epa1.con
TRACT FILE BASENAME|tracts
FILE LIST FILENAME |filelist.ntl
NO. SOURCE CATEGORY|5
RERUN(YES/NO)      |NO
-eof-
#
cp -p 45202.exp tmp/45202.exp
cp -p filelist.ntl tmp/filelist.ntl
#
/bin/time aspenb << -eof-
ON ROAD MV FILE    |cat3.epa2.con
TRACT FILE BASENAME|tracts
FILE LIST FILENAME |filelist.ntl
NO. SOURCE CATEGORY|5
RERUN (YES/NO)     |NO
-eof-
```

Figure 5-6 Example ASPENB job file that creates intermediate output files

```
rm 45202.exp
rm filelist.ntl
cp -p tmp/45202.exp 452023.exp
cp -p tmp/filelist.ntl filelist.ntl
/bin/time aspenb << -eof-
ON ROAD MV FILE    |cat3.epa2.con
TRACT FILE BASENAME|tracts
FILE LIST FILENAME |filelist.nt
NO. SOURCE CATEGOEY|5
RERUN (YES/NO)     |NO
-eof-
```

Figure 5-7 Example of an ASPENB re-start job file

6.0 POST-PROCESSING MODEL OUTPUTS

A series of software programs are used to post-process the ASPENB model output. A detailed descriptions of the post-processors are presented in this section.

There are three post-processors for ASPENB, they are:

- AVGDAT - calculates the annual average HAP concentration for each source category included in the ASPENB output, calculates the total annual average concentrations over all categories including the background value provided by the user
- EXTRDAT - converts the concentration data files from binary to ASCII format
- SECDAT - generates the secondary pollutant concentrations and combines the concentrations of the primary and secondary components

Note that the processing procedures, which were carried out by two post-processors in version 1.0 of the model (MRG_DAT and BACKGRND), have been incorporated into the post-processor AVGDAT. Therefore, those two processors are no longer needed for version 1.1 of the model. Figure 6-1 presents a flow chart of the relationships among the post-processors.

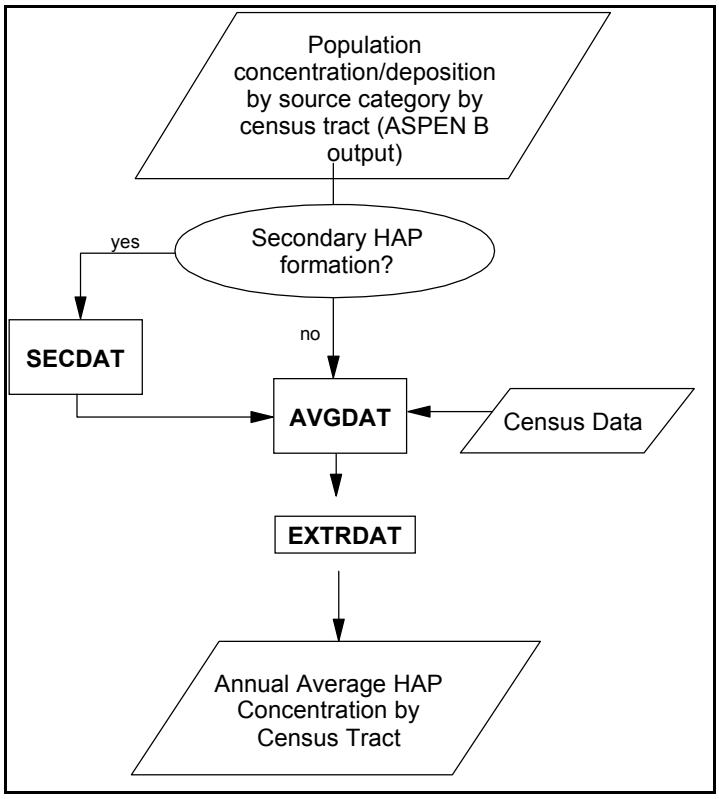

Figure 6-1 Flow chart of the ASPEN post-processors.

6.1 GENERATING CONCENTRATIONS FOR THE SECONDARY COMPOUNDS

ASPEN estimates the concentration of the secondary HAPs as the difference between the precursor concentration in an inert model run and its concentration in the presence of reactive decay. The resulting concentration differences are adjusted for molar yield and molecular weight to estimate the concentration of the secondary HAP.

The post-processor SECDAT is used for generating the concentration estimates of the secondary HAPs, and combining the concentrations of the primary and secondary HAPs. The SECDAT output file is in the same format as the population concentration/deposition file, so that it can be further processed by AVGDAT. Figure 6-2 present an example job file for generating secondary and total concentrations of acrolein.

The job file in Figure 6-2 is formatted as follows:

- Number of source categories included in the ASPENB output file: 5
- Filename of census tract list: ustracts.lst
- SAROAD code for secondary arolein: 80265
- Output filename: 80265.exp
- Scaling factor: -1.04
  Note: the negative sign indicates that concentration differences of the HAPs specified below should be calculated
- The inert concentration filename: 80302.exp (80302 is the SAROAD code for inert 1,3-butadiene)
- The reactive concentration filename: 43218.exp (43218 is the SAROAD code for 1,3-butadiene)

To generate the concentrations for the total acrolein, the job file is set up as follows:

- Number of source categories included in the ASPENB output file: 5
- Filename of census tract list: ustracts.lst
- SAROAD code of the total acrolein: 80266
- Output filename: 80266.exp
- Scaling factor: 1.0
  Note: the positive sign indicates to calculate the total concentration of the HAPs specified below
- The primary acrolein concentration filename: 435051.exp (43505 is the SAROAD code for acrolein)
- The secondary arolein concentration filename: 80265.exp

```
#
# Generate secondary species for all source categories
#
rm aspenb/output/80265.exp
/bin/time src/secdat << ieof
5
data/ustracts.lst
80265
aspenb/output/80265.exp
-1.04
aspenb/output/80302.exp
aspenb/output/43218.exp
ieof
#
# Generate total for all categories
#
rm aspenb/output/80266.exp
/bin/time src/secdat << ieof
5
data/ustracts.lst
80266
aspenb/output/80266.exp
1.0
aspenb/output/43505.exp
aspenb/output/80265.exp
ieof
```

Figure 6-2 Example job file for the SECDAT post-processor

The difference between the post-processor SECDAT and its predecessor SEC_DAT is that the new version greatly simplifies the processing procedure. In a single run SEC_DAT only treats the processing for one source category for a particular HAP; but SECDAT can complete the processing for all the source categories for the HAP included in the ASPENB output. The run stream set up for SECDAT is the same as the one for SEC_DAT, except that total number of source categories included in the ASPENB output file needed to be specified, and the file name will be in the format of 5-digit SAROAD code with ".EXP" extension (i.e., the source category code digit is no longer needed).

6.2 CALCULATING ANNUAL AVERAGE CONCENTRATION

The post-processor AVGDAT is used to convert the model results into annual average concentrations. The input concentration are estimated for eight 3-hour time blocks; the post-processor calculates the average for the time blocks. The post-processor reads in the concentrations in eight 3-hour time blocks for all the source categories included in the population concentration/deposition file. Then it calculates the annual average concentrations for each source category and total annual average concentration over all source categories, including the background value provided by the user.

Figure 6-3 presents an example job file for calculating the average concentration of benzene. Important parameters for this run stream are as follows:

- The number of source categories included in the ASPENB output file: 5
- Filename for census tract list: ustracts.lst
- Output filename: 45201.exp.avg
- HAP SAROAD code: 45201 (benzene)
- Path for input concentration file: aspen/
- Background value for the HAP in $\mu g/m^3$: 0.479

```
rm 45201.exp.avg
/bin/time avgdat << ieofa
5
ustracts.lst
45201.exp.avg
45202
aspen/
0.479
ieof
```

Figure 6-3 Example job file for the post-processor AVGDAT

Note that only the path is required for the input concentration files.

6.3 EXTRACT AND TABULATE ANNUAL AVERAGE CONCENTRATION

The output from AVGDAT is in binary format. The EXTRDAT post-processor converts this file from binary to ASCII format. The post-processor provides the following options to the user:

- Select the concentration units: $\mu g/m^3$, ppm, pphm, ppb or ppt, input as MGPCM, PPM, PPHM, PPB or PPT
- Select census tracts:
  To convert concentrations for all census tracts: input –1 (see Figure 6-4)
  To extract concentrations for the listed tracts only: input total number of tracts, and list the tracts of interest (see Figure 6-5)

Figure 6-4 presents an example job file for converting benzene concentrations from binary to ASCII for all tracts (in $\mu g/m^3$). Important parameters in the job file include:

- Number of source categories included in the ASPENB output: 5
- Name of input file: 45201.exp.avg
- Name of output file: 45201.exp.out
- HAP SAROAD code: 45201 (benzene)
- Filename for census tract list: ustracts.lst

- HAP name, desired measurement units, molecular weight: BENZENE, MGPCM, 78.11 (format: A10,A8,F10)
- Indicator of census tract selection: -1 (all census tracts)

```
rm 45201.avg.out
/bin/time extravg << ieofa
5
45201.exp.avg
45201.avg.out
45201
ustracts.lst
BENZ      MGPCM     78.11
-1
ieof
```

Figure 6-4 Example 1 job file for the EXTRDAT post-processor

Figure 6-5 presents an example run stream for converting benzene concentrations from binary to ASCII for only the 10 listed tracts (units in ppb).

```
rm 45201.avg.out
/bin/time extravg << ieof
5
45201.exp.avg
45201.avg.out
45201
ustracts.lst
BENZ      PPB     78.11
10
 9001 10101 -73.67950  41.06822
 9001 10102 -73.63378  41.09747
 9001 10201 -73.62364  41.05910
 9001 10202 -73.58887  41.06347
 9001 10300 -73.63744  41.03689
 9001 10400 -73.65913  41.02311
 9001 10500 -73.64153  41.01606
 9001 10600 -73.62646  41.02859
 9001 10700 -73.61841  41.02867
 9001 10800 -73.59914  41.04003
ieof
```

Figure 6-5 Example 2 job file for the post-processor EXTRDAT

7.0 COMPUTER NOTES

7.1 MINIMUM HARDWARE REQUIREMENTS

The computer resources required to run the ASPEN application are contingent upon the number of emission sources and HAPs to be processed. The disk storage requirements to run a simulation on a UNIX workstation (Sun Ultra Sparc 2 / Solaris 2.5.1), using the emissions from one source category (on-road mobile), one reactivity class (reactivity class 2 including emissions from 11 HAPs) in a single EPA region (EPA region 9) is approximately 1.3 Mbytes for ASPENA, and 2.7 Mbytes for ASPENB. It takes 6 CPU hours for both ASPENA and ASPENB for this simulation. Table 7-1 presents the disk storage requirements.

Table 7-1 ASPEN disk storage requirements for example simulation.

File	Disk Storage (Mbytes)
Inputs	
Meteorological (214 stations)	4.0
Census tract (48 states, 60,803 tracts)	1.8
Emissions	8.4
Outputs	
Normalized source concentration/deposition (binary)	4.2
Population concentration/deposition (binary)	31.9 (2.9 Mbytes / HAP × 11 HAPs)
Annual average concentration (ASCII)	106.7 (9.7 Mbytes / HAP × 11 HAPs)
Total	157

7.2 COMPILING AND RUNNING ASPEN ON A UNIX WORKSTATION

The commands for compiling ASPEN on a UNIX workstation are presented in Figure 7-1 and Figure 7-2.

```
FLGS = -O2

TARGT = aspena

OBJCTS = \
gauss.o \
gaussz.o \
header.o \
list.o \
notice.o \
opnfil.o \
point.o \
prise.o \
save.o \
aspena.o \
sigmaz.o \
stack.o \
star.o \
starin.o \
szcoef.o \
ddmpr.o \
vert.o \
depos.o \
biddisp.o \
vgausz.o \
blkmet.o \
blkdep.o \
skip.o

$(TARGT): $(OBJCTS)
      f77 -o $(TARGT) $(FLGS) $(OBJCTS)

.f.o    :
      f77 -c $(FLGS) $<
```

Figure 7-1 The commands for compiling ASPENA on a UNIX workstation

```
FLGS = -O2
TARGT = aspenb

OBJCTS = \
addSource.o \
areaAvg1.o \
areaAvg2.o \
aspenb.o \
findResTr.o \
findcloTr.o \
impacted.o \
initSearch.o \
initTarget.o \
inside.o \
interpolate.o \
loadTracts.o \
nextCo.o \
nextSource.o \
nextSt.o \
nextTarget.o \
nextTr.o \
openSource.o \
ptAverage.o \
receploc.o \
setPts.o \
tolog.o \
update.o

$(TARGT): $(OBJCTS)
      f77 -o $(TARGT) $(FLGS) $(OBJCTS)
.f.o  :
      f77 -c $(FLGS) $<
```

Figure 7-2 The commands for compiling the ASPENB on a UNIX workstation.

7.2.1 Modifying the Array Limits

In the current version of ASPEN, the array limits are configured as follows:

- Maximum number of meteorological station: 500
- Maximum number of pollutants: 150
- Maximum number of radial distances of the grid: 12 (in ASPENA)
- Maximum number of azimuth direction of the grid: 16
- Maximum number of time blocks: 8
- Maximum number of HAPs emits from a source: 100
- Maximum number of census tracts: 60,803
- Maximum number of the states included in the tracts data: 49

- Maximum number of counties included in the tracts data: 3,111
- Maximum number of the tracts included in a county: 2,000
- Maximum number of the fields included in the population concentration/population file: 12. The 12 fields are: State/County FIPS code, tract FIPS code, concentrations in eight 3-hour time blocks, deposition over the land and water

Most of the array limits are specified in PARAMETER statements. Exceptions, which are hard coded, include the number of receptor grid radial distances (12), the number of receptor grid azimuthal directions (16), and the number of time blocks (8) in the ASPENA module. Depending on the amount of memory available on the particular computer system being used, and the needs for a particular modeling application, the other array limits can be easily changed, and the model can be recompiled.

If the user changes the number of time blocks in the ASPEN model, the ASPENA emission/control input file, and the number of the fields included in the ASPEN output files would also need to be changed.

7.3 PORTING THE MODEL TO THE OTHER HARDWARE ENVIRONMENTS

7.3.1 PC

The ASPEN models are designed and coded to allow them to run on most operating environments, including UNIX and DOS. The current version of the model is written to run on UNIX. Although the users do not need to make major changes, they may experience some minor differences between UNIX to PC environments, including the following:

- The suffix .f of all source files should be changed to .for
- The subroutine OPNFIL of ASPENA uses GETARG to read input run stream filename, which is compiler dependent. GETARG may be available under a different name for another compiler.

8.0 ASPEN MODEL TUTORIAL

This section presents examples of the setup and use of ASPEN. Several example applications are provided to demonstrate how to set up a basic modeling scenario and post-process the model output. A more detailed discussion of each module is provided in Sections 5, 6, 7 and Appendix C. Two main example scenarios are presented in this section: a gaseous HAPs and a particulate HAPs scenario. There are three examples provided for calculating annual average concentrations for a single gaseous HAP. The final example is for calculating concentrations and depositions for two particulate HAPs.

8.1 EXAMPLE 1 – GASEOUS HAPS

This example problem is to simulate gaseous toluene concentrations by census tract in one county (Fairfield, CT). For this example, multiple emission sources (point, area, and on-road mobile) are modeled. Users must prepare an emission/control input file for each source category. A description of the input file parameters required for the emission/control input file for each source category is provided. The reactivity for toluene for this example is assigned to category 4.

8.1.1 Setting up the Emission/Control Input File for Point Sources

For this example, the input file is prepared to simulate toluene concentrations from two point sources. The point source emissions data used in this example are from the U.S. EPA's Toxic Release Inventory (TRI) database. The emission/control input file for ASPENA is presented in Figure 8-1.

```
1   TRI Point Sources                          Reactive Catagory 4 011
2    9.870e-07 9.870e-07 9.870e-07 9.870e-07 9.870e-07 9.870e-07
3    9.870e-07 9.870e-07 9.870e-07 9.870e-07 9.870e-07 9.870e-07
4    1.180e-05 7.890e-06 3.950e-06 1.970e-06 9.870e-07 9.870e-07
5    7.890e-05 5.920e-05 3.950e-05 1.970e-05 9.870e-07 9.870e-07
6    6.710e-05 5.130e-05 3.550e-05 1.970e-05 9.870e-07 9.870e-07
7    2.370e-05 1.780e-05 1.180e-05 7.890e-06 9.870e-07 9.870e-07
8    1.970e-06 1.970e-06 1.970e-06 9.870e-07 9.870e-07 9.870e-07
9    9.870e-07 9.870e-07 9.870e-07 9.870e-07 9.870e-07 9.870e-07
10   09001     16269  -73.2694   41.141702
11
12
13   1  -73.2694   41.1417      8.90      0.67     12.00    323.0000      0.00      0.00
14  452020  1.25e-01  1.25e-01  1.25e-01  1.25e-01  1.25e-01  1.25e-01  1.25e-01  1.25e-01
15
16
17   09001     16291  -73.4167   41.366102
18
19
20   1  -73.4167   41.3661     24.00      0.49     20.53    332.0000      0.00      0.00
21  452020  2.62e-03  2.62e-03  2.62e-03  2.62e-03  2.62e-03  2.62e-03  2.62e-03  2.62e-03
23
24
25
26
```

Figure 8-1 Example emission/control input file for point sources (filename: "aspena.tri.inp")

A record by-record description of the input file data requirements is as follows:

- Line 1 (header): The run identifier (title), pollutant species type, and deposition parameters are specified here. For this example, the parameters are set to: gaseous species type (= 0); no dry deposition (=1), and no wet deposition (=1).
- Lines 2-9: The decay rates of reactivity category 4 are specified for each of the six stability classes (A-F) and eight 3-hour time blocks.
- Lines 10-14: For each point source modeled, the source location, emissions, and various stack parameters must be specified. Detailed information for the two TRI sources included in this example is provided in Table 8-1. For a description of the input file format for each of these variables, see Table C-1 in Appendix C.
- Lines 15-16: These lines are left blank to indicate the end of information for the emission source.
- Lines 17-21: This section contains data for a second point source, analogous to lines 10-14.
- Lines 22-26: These lines are left blank to indicate the end of the file.

Table 8-1 Point source data parameters entered into the emission/control input file

Variable	Source No. 1	Source No. 2	Remarks
FIPS code	09001	09001	Fairfield, CT
Plant ID	16269	16291	
Longitude	-73.2694	-73.4167	
Latitude	41.1417	41.3661	
Source type	0	0	Point source
Urban/Rural flag	2	2	Rural
NWS station ID	Blank	Blank	Use nearest station
Stack ID	1	1	
Longitude	-73.2694	-73.4167	
Latitude	41.1417	41.3661	
Stack height (m)	8.9	24.0	
Stack diameter (m)	0.67	0.49	
Stack exit velocity (m/sec)	12.0	20.53	
Stack exit temperature (Deg K)	323.0	332.0	
Vent/Stack flag	0	0	Stacked
Building flag	0	0	No building
Width of nearby building (m)	0.0	0.0	
Height of nearby building (m)	0.0	0.0	
HAP Saroad code	45202	45202	Toluene
Source category	0	0	TRI-Nonmetal
Emissions of each time block (g/sec)	0.125	2.62×10^{-3}	Flat temporal profile

8.1.2 Setting up the Emission/Control Input File for Mobile Sources

The example emission/control input file for mobile sources is presented in Figure 8-2.

```
1    On-Road MV Sources                      Reactive Category 4 011
2     9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07
3     9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07
4     1.18E-05  7.89E-06  3.95E-06  1.97E-06  9.87E-07  9.87E-07
5     7.89E-05  5.92E-05  3.95E-05  1.97E-05  9.87E-07  9.87E-07
6     6.71E-05  5.13E-05  3.55E-05  1.97E-05  9.87E-07  9.87E-07
7     2.37E-05  1.78E-05  1.18E-05  7.89E-06  9.87E-07  9.87E-07
8     1.97E-06  1.97E-06  1.97E-06  9.87E-07  9.87E-07  9.87E-07
9     9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07
10  09001     30400 -73.4919   41.0644 31
11  4781
12
13  09001 -73.4919   41.0644                                          1
14  4520230.1482E+000.1482E+000.1113E+010.9006E+000.9317E+000.1289E+010.5786E+000.1613E+00
15
16
17  09001     30500 -73.5024   41.0780 31
18  4781
19
20  09001 -73.5024   41.0780                                          1
21  4520230.1168E+000.1168E+000.8744E+000.6927E+000.7138E+000.1005E+010.4522E+000.1257E+00
22
23
24
25
26
```

Figure 8-2 Example emission/control input file for on-road mobile sources (filename: "aspena.mv.inp")

Mobile source emissions are specified at the census tract level as pseudo point sources. This example includes toluene emissions from on-road mobile sources for two census tracts (tracts 30400 and 30500).

- Lines 1-9: These records are identical to the point source emission/control input file shows in Figure 8-2 (except for the run identifier) because both include emissions for toluene.

- Lines 10-14: The format of these lines is the same as for the point source example discussed above. However, some of the variables represent somewhat different parameters for this case.

  Line 10: The census tract FIPS code (30400) is used instead of the plant ID, and the coordinates (longitude and latitude) of the census tract centroid is specified instead of the plant location. On-road mobile sources are considered "pseudo points", with a source category code of 3.

Line 11: For this example the NWS station ID for the desired meteorological station is specified. If left blank, as it was in the point source example, the closest station in the data base would be assigned. However, for "pseudo points" the meteorological stations are generally pre-determined so that sources can be grouped according to meteorological station and urban/rural designation to save computing time. This is discussed in Appendix C.

Line 13: The source type for mobile sources (and area sources) is designated as non-stacked (vent/stack flag = 1), and pseudo point source (source type = 3).

Line 14: In contrast to the point source example, for this case the emission rate varies among the eight time blocks.

- Lines 15-16: These lines are left blank to indicate the end of information for the emission source.

- Lines 17-21: This section contains data for a second pseudo point source, analogous to lines 10-14.

- Lines 22-26: These lines are left blank to indicate the end of the file.

8.1.3 Setting up the Emission/Control Input File for Area Sources

Like mobile sources, area sources are specified at the census tract level as pseudo point sources. Figure 8-3 shows an emission/control input file for simulating toluene emissions from two area sources in two census tracts (tract #s 35100 and 42700). The input file for area source emissions is very similar to the mobile source file discussed in Section 8.1.2. The only difference is that there are two emissions records in the area source file, corresponding to the two area source categories: manufacturing emissions (source category code = 5), and non-manufacturing emissions (source category code = 6). This can be seen in Figure 8-3, where the manufacturing and non-manufacturing emissions in census tract 35100 are represented by records 14 and 15, respectively.

8.1.4 Running ASPENA

The two types of input required to run ASPENA are the emission/control file, and the meteorological files. Procedures for preparing the emission/control file are discussed in Sections 8.1.1 – 8.1.3. The meteorological data input requirements include STAR meteorological data and a meteorological index file. Versions of the latter two files, containing national 1990 data, are provided as part of the ASPENA modeling system.

```
1   Area Sources                          Reactive Category 4 011
2     9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07
3     9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07
4     1.18E-05  7.89E-06  3.95E-06  1.97E-06  9.87E-07  9.87E-07
5     7.89E-05  5.92E-05  3.95E-05  1.97E-05  9.87E-07  9.87E-07
6     6.71E-05  5.13E-05  3.55E-05  1.97E-05  9.87E-07  9.87E-07
7     2.37E-05  1.78E-05  1.18E-05  7.89E-06  9.87E-07  9.87E-07
8     1.97E-06  1.97E-06  1.97E-06  9.87E-07  9.87E-07  9.87E-07
9     9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07  9.87E-07
10  09001     35100 -73.4919   41.1433 31
11   4781
12
13  09001 -73.4919   41.1433                                          1
14  4520250.0000E+000.0000E+000.1785E-010.5356E-010.5356E-010.5356E-010.5356E+010.5356E-01
15  4520260.1249E-010.5239E-010.1336E+000.1529E+000.1208E+000.9346E-010.4291E-010.2793E-01
16
17
18  09001     42700 -73.4209   41.1425 31
19   4781
20
21  09001 -73.4209   41.1425                                          1
22  4520250.0000E+000.0000E+000.8033E010.2410E+000.2410E+000.2410E+000.2410E+000.2410E+00
23  4520260.2810E+010.5116E010.1549E+000.2566E+000.2381E+000.2223E+000.1437E+000.9328E-01
24
25
26
27
28
```

Figure 8-3 Example emission/control input file for area source (filename: "aspena.ar.inp")

Once the input files have been prepared and formatted according to the specifications provided in Appendix C, run stream files need to be created that include the input and output filenames for the simulation.

Example run stream files for area, point and mobile and gaseous HAPs simulations are shown in Figures 8-4, 8-5, and 8-6. The filenames shown in the figures correspond to the following:

- aspena.xx.inp - emission/control input file (format: ASCII)
- wtpmix.ind - meteorological index input file (format: binary)
- star.dat - STAR meteorological data file (format: direct access binary)
- aspena.xx.con - ASPENA normalized source concentration/deposition output file (format: binary)

  where, "XX" refers to one of the following source category codes:
  ar – area source
  tri – point source
  mv – mobile source

```
aspena.ar.inp
/dev/null
wtpmix.ind
star.dat
aspena.ar.con
```

Figure 8-4 Run stream file for the gaseous HAPs ASPENA run (filename: "aspena.ar.sys")

```
aspena.tri.inp
/dev/null
wtpmix.ind
star.dat
aspena.tri.con
```

Figure 8-5 Run stream file for ASPENA point run (filename: "aspena.tri.sys")

```
aspena.mv.inp
/dev/null
wtpmix.ind
star.dat
aspena.mv.con
```

Figure 8-6 Run stream file for ASPENA mobile run (filename: "aspena.mv.sys")

In addition to the pollutant concentration output file, ASPENA also creates an output file with listing all the emission sources processed in Fortran unit 88. It is convenient to rename this file at the conclusion of each simulation, so that it will no be overwritten by the next simulation in the job. Figure 8-7 presents an example of a job file for ASPENA simulations made with the example files discussed above. In the example, the 3 processed source listing files produced for the three simulations are renamed from "fort.88" to "aspena.tri.lst", "aspena.ar.lst", and "aspena.mv.lst".

```
rm aspena.tri.lst
rm aspena.tri.con
/bin/time aspena aspena.tri.sys
mv fort.88 aspena.tri.lst
#
rm aspena.ar.lst
rm aspena.ar.con
/bin/time aspena aspena.ar.sys
mv fort.88 aspena.ar.lst
#
rm aspena.mv.lst
rm aspena.mv.con
/bin/time aspena aspena.mv.sys
mv fort.88 aspena.mv.lst
```

Figure 8-7 Example of ASPENA job file

```
plant FIPS number:    9001
plant ID:             35100 stack type:     3 Long/Lat coordinates :     -73.492    41.143 urban/rural  1=urban; 2=rural : 1
Species type                  : 0

 ambient temperatures (k):   289.000  279.000  284.000
 meteorological station:    4781
    utm coordinates (km):     -73.100    40.783
    excluded stabilities:        000000
          wind speeds:           000000
          wind directions:       0000000000000000
 Average Precip and freq :  110.2106    0.2067

 Stack ID    :            09001
 Long/Lat coordinates :       -73.492    41.143
 stack height (m):             0.00
       diameter (m):           0.00
       exit velocity (m/s):    0.00
       exit temperature (k):   0.00
 vent/stack class:               vent

 Calculated concentrations for hour  1 from--
 chemicals emitted:        452025  452026
 emission rate (g/s):    0.00E+00   0.12E-01
 receptor grid concentrations (micrograms/cubic meter) resulting from total emissions

 bearing                       distance (km)
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00

   0.0    5.0E+01  2.8E+00  8.4E-01  2.6E-01  6.0E-02  2.2E-02  1.2E-02  8.3E-03  6.1E-03  4.7E-03  3.2E-03  2.4E-03
  22.5    3.8E+01  2.1E+00  6.3E-01  1.9E-01  4.5E-02  1.6E-02  9.4E-03  6.3E-03  4.7E-03  3.7E-03  2.5E-03  1.9E-03
  ................
 Calculated concentrations for hour  8 from--
 chemicals emitted:        452025  452026
 emission rate (g/s):    0.54E-01   0.28E-01
 receptor grid concentrations (micrograms/cubic meter) resulting from total emissions

 bearing                       distance (km)
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00

   0.0    6.0E+01  3.5E+00  1.0E+00  3.2E-01  7.4E-02  2.7E-02  1.5E-02  9.8E-03  7.1E-03  5.5E-03  3.7E-03  2.7E-03
  22.5    4.7E+01  2.7E+00  7.9E-01  2.4E-01  5.7E-02  2.1E-02  1.2E-02  7.8E-03  5.7E-03  4.5E-03  3.0E-03  2.3E-03

 No Deposition Calculations Specified on Input ..
 ..........
Total Plants Processed :           2
```

Figure 8-8 ASPENA diagnostic file created by example area source run

```
plant FIPS number:    9001
 plant ID:              30400
 stack type:         3
 Long/Lat coordinates :       -73.492    41.064
 urban/rural  1=urban; 2=rural : 1
 Species type                  : 0

 ambient temperatures (k):   289.000  279.000  284.000
 meteorological station:    4781
    utm coordinates (km):     -73.100    40.783
    excluded stabilities:        000000
          wind speeds:           000000
          wind directions:       0000000000000000
 Average Precip and freq :  110.2106    0.2067

 Stack ID    :            09001
 Long/Lat coordinates :       -73.492    41.064
 stack height (m):             0.00
       diameter (m):           0.00
       exit velocity (m/s):    0.00
       exit temperature (k):   0.00
 vent/stack class:               vent

 Calculated concentrations for hour  1 from--
 chemicals emitted:        452023
 emission rate (g/s):    0.15E+00

 receptor grid concentrations (micrograms/cubic meter) resulting from total emissions

 bearing                      distance (km)
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00

   0.0    5.0E+01  2.8E+00  8.4E-01  2.6E-01  6.0E-02  2.2E-02  1.2E-02  8.3E-03  6.1E-03  4.7E-03  3.2E-03  2.4E-03
  22.5    3.8E+01  2.1E+00  6.3E-01  1.9E-01  4.5E-02  1.6E-02  9.4E-03  6.3E-03  4.7E-03  3.7E-03  2.5E-03  1.9E-03
    ...........
 Calculated concentrations for hour  8 from--
 chemicals emitted:        452023
 emission rate (g/s):    0.16E+00

 receptor grid concentrations (micrograms/cubic meter) resulting from total emissions

 bearing                      distance (km)
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00

   0.0    6.0E+01  3.5E+00  1.0E+00  3.2E-01  7.4E-02  2.7E-02  1.5E-02  9.8E-03  7.1E-03  5.5E-03  3.7E-03  2.7E-03
  22.5    4.7E+01  2.7E+00  7.9E-01  2.4E-01  5.7E-02  2.1E-02  1.2E-02  7.8E-03  5.7E-03  4.5E-03  3.0E-03  2.3E-03

No Deposition Calculations Specified on Input ..
```

Figure 8-9 ASPENA diagnostic file created by example mobile source run

```
plant FIPS number:   9001
 plant ID:           16269
 stack type:         0
 Long/Lat coordinates :       -73.269    41.142
 urban/rural  1=urban; 2=rural : 2
 Species type                  : 0

 ambient temperatures (k):   289.000  279.000  284.000
 meteorological station:    4781
    utm coordinates (km):     -73.100    40.783
    excluded stabilities:        000000
          wind speeds:           000000
          wind directions:       0000000000000000
 Average Precip and freq :  110.2106    0.2067

 Stack ID    :                1
 Long/Lat coordinates :       -73.269    41.142
 stack height (m):             8.90
       diameter (m):           0.67
       exit velocity (m/s):   12.00
       exit temperature (k): 323.00
 vent/stack class:               stack

 Calculated concentrations for hour  1 from--
 chemicals emitted:        452020
 emission rate (g/s):    0.12E+00

 receptor grid concentrations (micrograms/cubic meter) resulting from total emissions

 bearing                      distance (km)
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00

   0.0    1.1E-01  1.1E+00  6.9E-01  4.2E-01  1.6E-01  6.7E-02  3.9E-02  2.7E-02  2.0E-02  1.6E-02  1.1E-02  8.3E-03
  22.5    3.0E-01  1.2E+00  6.5E-01  3.5E-01  1.2E-01  5.0E-02  2.9E-02  2.0E-02  1.5E-02  1.2E-02  8.0E-03  6.0E-03
.............
 Calculated concentrations for hour  8 from--
 chemicals emitted:        452020
 emission rate (g/s):    0.12E+00

 receptor grid concentrations (micrograms/cubic meter) resulting from total emissions

 bearing                      distance (km)
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00

   0.0    9.5E-02  9.2E-01  7.3E-01  4.8E-01  1.9E-01  8.0E-02  4.7E-02  3.3E-02  2.4E-02  1.9E-02  1.3E-02  1.0E-02
  22.5    2.0E-01  1.2E+00  7.3E-01  4.2E-01  1.5E-01  6.2E-02  3.6E-02  2.5E-02  1.8E-02  1.4E-02  1.0E-02  7.5E-03
..............
No Deposition Calculations Specified on Input ..

 plant FIPS number:    9001
 plant ID:              16291
```

Figure 8-10 ASPENA diagnostic file created by example TRI source run

8.1.5 Running ASPENB

Two types of input files are required to run ASPENB. The first is the normalized source concentration/deposition output file from the ASPENA run. The second contains census tract information, including tract data (format: binary) and a tract index file (format: binary). For the purposes of this example, the tract data filenames are: “smptracts.dat” and “smptracts.ind”. Note that ASPENB requires that the tract data be located in the same directory as where the job is run. Also, the tract data files are specified in the job file by their base name only. So, for the example run, the census tract data file name is entered as smptract, with no suffix at the end. For a detailed description of how to run ASPENB, see Section 3. The ASPENB job file for the gaseous HAPs simulations is shown in Figure 8-11.

```
/bin/time aspenb << -eof-
POINT SOURCE FILE  |aspena.tri.con
TRACT FILE BASENAME|smptracts
FILE LIST FILENAME |runfile.lst
NO. SOURCE CATEGORY|7
RERUN (YES/NO)     |NO
-eof-
#
/bin/time aspenb << -eof-
ON ROAD MV FILE    |aspena.mv.con
TRACT FILE BASENAME|smptracts
FILE LIST FILENAME |runfile.lst
NO. SOURCE CATEGORY|7
RERUN (YES/NO)     |NO
-eof-
#
/bin/time aspenb << -eof-
AREA SOURCE FILE   |aspena.ar.con
TRACT FILE BASENAME|smptracts
FILE LIST FILENAME |runfile.lst
NO. SOURCE CATEGORY|7
RERUN (YES/NO)     |NO
-eof-
```

Figure 8-11 ASPENB example job file

ASEPENB creates a separate population concentration/deposition output file (format: binary) for each HAP encountered in the ASPENA output file. The naming convention for the output file is the 5-digit pollutant SAROAD code with an *.exp extension. For example, the ASPENB output filename for toluene (SAROAD code = 45202) is 45202.exp.

The ASPENB module also provides an output file containing a list of all the names of processed input ASPENA files. In the Figure 8-11 example, the name for the listing file is "runfile.lst"

which contains the input normalized source concentration filenames ("aspena.tri.con", "aspena.mv.con" and "aspena.ar.con" for the example).

Utility "exp2asci" converts the binary formatted ASPENB population concentration/deposition file into ASCII format. Figure 8-12 presents an example of the binary to ASCII conversion using "exp2asci". In the example, 45202.exp is the binary formatted ASPENB output, "smptracts" is the census tract data file, and 7 is the number of source categories included in "45202.exp". The utility generates the ASCII formatted output file named as "45202.txt".

```
rm 45202.txt/bin/time
exp2asci << -eof-
7
*.EXP FILENAME      |45202.exp
TRACTS DATA FILE    |smptracts
-eof-
```

Figure 8-12 Example EXP2ASCI job file

The ASCII formatted ASPENB output population concentration/deposition file generated by the utility "exp2asci" for the example is presented in Figure 8-13.

8.1.6 Post-Processing Model Output

The ASPENB output files are in binary format and contain pollutant concentration estimates for each of eight 3-hour time blocks for each source category. A series of software programs are available to post-process the model output. Detailed descriptions of these programs are provided in Section 4. (Deposition estimates are also contained in the ASPENB output files, but are not treated by the post-processors.) For this example the following two post-processors are used:

- AVGDAT - calculates the annual average HAP concentration for each source category, and calculates the total annual average concentration over all categories
- EXTRDAT - converts the concentration data files from binary to ASCII format

Figure 8-14 presents an example job file for post-processing the example model output.

The ASPEN ASCII output for the example simulations is shown in Figure 8-15. It contains the concentrations of toluene (in $\mu g/m^3$) by source category and census tract. The first two columns are the state and county FIPS codes and tract FIPS code. The output displays annual average concentrations for TRI, on-road mobile, manufacturing and non-manufacturing area sources, under the CAT00, CAT03, CAT05 and CAT06 columns, respectively.

```
9001   10101  0.632475E-03  0.602951E-03  0.385393E-03  0.154866E-03  0.142112E-03  0.224468E-03  0.419884E-03  0.694393E-03  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.964551E-03  0.123733E-02  0.632815E-02  0.236211E-02  0.143745E-02
0.331155E-02  0.298845E-02  0.196255E-02  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.308918E-03  0.297286E-03  0.244506E-03  0.311125E-03  0.648992E-03  0.953998E-03  0.176608E-03
0.422919E-03  0.102578E-02  0.456361E-03  0.317639E-03  0.346642E-03  0.415487E-03  0.396137E-03  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
9001   10102  0.653247E-03  0.731114E-03  0.435314E-03  0.185383E-03  0.165064E-03  0.268752E-03  0.468903E-03  0.896791E-03  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.631174E-03  0.153372E-02  0.709802E-02  0.232719E-02  0.175388E-02
0.361774E-02  0.521225E-02  0.149818E-02  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.369893E-03  0.388875E-03  0.317510E-03  0.415000E-03  0.892116E-03  0.141493E-02  0.231649E-03
0.545520E-03  0.126443E-02  0.596893E-03  0.431510E-03  0.475560E-03  0.582221E-03  0.591870E-03  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
9001   10201  0.844332E-03  0.706242E-03  0.493527E-03  0.200628E-03  0.188866E-03  0.277834E-03  0.530698E-03  0.765232E-03  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.184324E-02  0.203914E-02  0.104112E-01  0.385490E-02  0.274736E-02
0.579354E-02  0.496717E-02  0.297403E-02  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.441517E-03  0.455559E-03  0.322872E-03  0.383767E-03  0.658951E-03  0.983919E-03  0.214462E-03
0.670122E-03  0.151366E-02  0.722135E-03  0.421889E-03  0.428519E-03  0.415162E-03  0.405331E-03  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
9001   10202  0.988371E-03  0.806748E-03  0.578435E-03  0.239344E-03  0.226871E-03  0.325602E-03  0.615040E-03  0.862008E-03  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.272014E-02  0.315319E-02  0.154034E-01  0.614889E-02  0.447321E-02
0.952190E-02  0.766703E-02  0.463139E-02  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.566090E-03  0.604773E-03  0.404266E-03  0.467594E-03  0.699876E-03  0.110158E-02  0.261179E-03
0.929373E-03  0.199587E-02  0.971293E-03  0.533134E-03  0.526697E-03  0.438111E-03  0.454870E-03  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00
.....
36119   15000  0.164685E-03  0.494377E-03  0.249541E-03  0.138755E-03  0.129794E-03  0.256117E-03  0.936136E-03  0.485032E-03
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.759098E-03  0.277467E-03  0.146514E-02  0.103151E-02
0.112701E-02  0.303295E-02  0.317063E-02  0.582770E-03  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.845961E-04  0.227843E-03  0.196333E-03  0.389976E-03  0.112622E-02  0.702282E-03
0.924682E-04  0.128902E-03  0.229063E-03  0.316118E-03  0.242534E-03  0.420564E-03  0.713992E-03  0.288280E-03  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
0.000000E+00  0.000000E+00
       0      0 45202
```

Figure 8-13 ASPENB output population concentration/deposition file (in ASCII format) for the example run

```
rm 45202.exp.avg
/bin/time avgdat << ieof
7
smptracts.lst
45202.exp.avg
45202
samples/
0.0
ieof
#
rm 45202.avg.out
/bin/time extravg << ieof
7
45202.exp.avg
45202.avg.out
45202
smptracts.lst
TOLUENE   MGPCM   92.14
-1
ieof
```

Figure 8-14. Example post-processing job file

Average Concentrations

SAROAD Code 45202; Species TOLUENE MGPCM

FIPS Code		Cat00	Cat01	Cat02	Cat03	Cat04	Cat05	Cat06	Bkgrd	Total
9001	10101	0.4071E-03	0.0000E+00	0.0000E+00	0.2574E-02	0.0000E+00	0.3456E-03	0.4447E-03	0.0000E+00	0.3771E-02
9001	10102	0.4756E-03	0.0000E+00	0.0000E+00	0.2959E-02	0.0000E+00	0.4748E-03	0.5900E-03	0.0000E+00	0.4499E-02
9001	10201	0.5009E-03	0.0000E+00	0.0000E+00	0.4329E-02	0.0000E+00	0.4058E-03	0.5989E-03	0.0000E+00	0.5834E-02
9001	10202	0.5803E-03	0.0000E+00	0.0000E+00	0.6715E-02	0.0000E+00	0.4805E-03	0.7638E-03	0.0000E+00	0.8540E-02
9001	10300	0.4722E-03	0.0000E+00	0.0000E+00	0.4025E-02	0.0000E+00	0.3379E-03	0.5220E-03	0.0000E+00	0.5357E-02
9001	10400	0.4340E-03	0.0000E+00	0.0000E+00	0.3371E-02	0.0000E+00	0.2958E-03	0.4549E-03	0.0000E+00	0.4555E-02
9001	10500	0.4515E-03	0.0000E+00	0.0000E+00	0.3839E-02	0.0000E+00	0.3007E-03	0.4812E-03	0.0000E+00	0.5072E-02
9001	10600	0.4881E-03	0.0000E+00	0.0000E+00	0.4443E-02	0.0000E+00	0.3357E-03	0.5370E-03	0.0000E+00	0.5804E-02
9001	10700	0.5008E-03	0.0000E+00	0.0000E+00	0.4796E-02	0.0000E+00	0.3451E-03	0.5588E-03	0.0000E+00	0.6201E-02
9001	10800	0.5491E-03	0.0000E+00	0.0000E+00	0.6050E-02	0.0000E+00	0.3952E-03	0.6474E-03	0.0000E+00	0.7642E-02
9001	10900	0.6123E-03	0.0000E+00	0.0000E+00	0.8710E-02	0.0000E+00	0.4629E-03	0.7809E-03	0.0000E+00	0.1057E-01
9001	11000	0.5987E-03	0.0000E+00	0.0000E+00	0.8919E-02	0.0000E+00	0.4178E-03	0.7315E-03	0.0000E+00	0.1067E-01
9001	11100	0.5683E-03	0.0000E+00	0.0000E+00	0.7246E-02	0.0000E+00	0.3946E-03	0.6777E-03	0.0000E+00	0.8887E-02
9001	11200	0.4728E-03	0.0000E+00	0.0000E+00	0.4386E-02	0.0000E+00	0.3135E-03	0.5156E-03	0.0000E+00	0.5688E-02
9001	11300	0.4201E-03	0.0000E+00	0.0000E+00	0.3389E-02	0.0000E+00	0.2720E-03	0.4376E-03	0.0000E+00	0.4519E-02
9001	20100	0.7148E-03	0.0000E+00	0.0000E+00	0.1865E-01	0.0000E+00	0.5490E-03	0.1004E-02	0.0000E+00	0.2091E-01
9001	20200	0.5568E-03	0.0000E+00	0.0000E+00	0.5354E-02	0.0000E+00	0.7085E-03	0.8610E-03	0.0000E+00	0.7481E-02
9001	20300	0.5863E-03	0.0000E+00	0.0000E+00	0.5123E-02	0.0000E+00	0.8751E-03	0.1036E-02	0.0000E+00	0.7620E-02
9001	20400	0.6764E-03	0.0000E+00	0.0000E+00	0.9716E-02	0.0000E+00	0.1051E-02	0.1486E-02	0.0000E+00	0.1293E-01
9001	20500	0.6369E-03	0.0000E+00	0.0000E+00	0.7910E-02	0.0000E+00	0.6095E-03	0.9718E-03	0.0000E+00	0.1013E-01
9001	20600	0.6852E-03	0.0000E+00	0.0000E+00	0.9828E-02	0.0000E+00	0.7735E-03	0.1250E-02	0.0000E+00	0.1254E-01
9001	20700	0.7898E-03	0.0000E+00	0.0000E+00	0.1841E-01	0.0000E+00	0.1179E-02	0.2108E-02	0.0000E+00	0.2249E-01
9001	20800	0.7328E-03	0.0000E+00	0.0000E+00	0.1478E-01	0.0000E+00	0.8390E-03	0.1434E-02	0.0000E+00	0.1778E-01
9001	20900	0.8289E-03	0.0000E+00	0.0000E+00	0.3388E-01	0.0000E+00	0.1113E-02	0.2069E-02	0.0000E+00	0.3789E-01
9001	21000	0.8012E-03	0.0000E+00	0.0000E+00	0.3328E-01	0.0000E+00	0.8739E-03	0.1602E-02	0.0000E+00	0.3655E-01
9001	21100	0.8043E-03	0.0000E+00	0.0000E+00	0.4475E-01	0.0000E+00	0.7977E-03	0.1536E-02	0.0000E+00	0.4789E-01
9001	21200	0.7407E-03	0.0000E+00	0.0000E+00	0.1967E-01	0.0000E+00	0.7066E-03	0.1251E-02	0.0000E+00	0.2237E-01
9001	21300	0.6920E-03	0.0000E+00	0.0000E+00	0.1452E-01	0.0000E+00	0.5808E-03	0.1012E-02	0.0000E+00	0.1680E-01
9001	21400	0.6660E-03	0.0000E+00	0.0000E+00	0.1225E-01	0.0000E+00	0.5077E-03	0.8898E-03	0.0000E+00	0.1431E-01
9001	21500	0.6845E-03	0.0000E+00	0.0000E+00	0.1453E-01	0.0000E+00	0.5155E-03	0.9262E-03	0.0000E+00	0.1666E-01
9001	21600	0.7361E-03	0.0000E+00	0.0000E+00	0.2144E-01	0.0000E+00	0.6121E-03	0.1105E-02	0.0000E+00	0.2389E-01
9001	21700	0.7567E-03	0.0000E+00	0.0000E+00	0.2774E-01	0.0000E+00	0.6457E-03	0.1225E-02	0.0000E+00	0.3036E-01
9001	21800	0.8116E-03	0.0000E+00	0.0000E+00	0.4962E-01	0.0000E+00	0.7827E-03	0.1540E-02	0.0000E+00	0.5276E-01
9001	21900	0.8084E-03	0.0000E+00	0.0000E+00	0.6120E-01	0.0000E+00	0.8278E-03	0.1607E-02	0.0000E+00	0.6444E-01
.....										
.....										

Figure 8-15 ASPEN output in ASCII format for the example simulation

8.2 EXAMPLE 2 - PARTICULATE HAPS

Figure 8-16 presents an emission/control input file for an example simulation to calculate ambient concentrations of particulate HAPs from point source emissions. The input includes emissions of chromium (fine) and nickel (fine) from a TRI source. Differences between this file and the example for gaseous emissions from point sources are as follows:

7. Line 1: Both dry and wet depositions are selected in the example (= 0) for the fine particulate HAPs (species type=1)

8. Lines 2-9: Reactive decay rates for particulate HAPs are all set to 0.

```
1   TRI Point Sources                              Reactive Category 2 100
2   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00
3   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00
4   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00
5   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00
6   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00
7   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00
8   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00
9   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00   0.000e+00
10  9001      13777  -73.1483     41.185301
11
12
13      1   -73.1483    41.1853     6.10        0.15        5.00       308.0000   0.00       0.00
14  801410   7.19e-05   7.19e-05    7.19e-05    7.19e-05    7.19e-05   7.19e-05   7.19e-05 7.19e-05
15  802160   7.19e-05   7.19e-05    7.19e-05    7.19e-05    7.19e-05   7.19e-05   7.19e-05 7.19e-05
16
17
18
19
20
```

Figure 8-16 Example ASPENA input file for point source emits particulate HAPs

The other ASPEN model simulation and post-processing procedures for this example are the same as those described for gaseous HAPs starting in Section 8.1.1.

```
plant FIPS number:    9001 plant ID:              13777 stack type:         0 Long/Lat coordinates :       -73.148    41.185
urban/rural  1=urban; 2=rural : 1 Species type                  : 1

 ambient temperatures (k):   289.000  279.000  284.000
 meteorological station:    4781
    utm coodinates (km):     -73.100    40.783
    excluded stabilities:        000000
          wind speeds:           000000
          wind directions:       0000000000000000
 Average Precip and freq :  110.2106    0.2067

 Stack ID    :                1
 Long/Lat coordinates :       -73.148    41.185
 stack height (m):             6.10
       diameter (m):           0.15
       exit velocity (m/s):    5.00
       exit temperature (k): 308.00
 vent/stack class:               stack

 Calculated concentations for hour  1 from--

 chemicals emitted:        801410  802160
 emission rate (g/s):    0.72E-04   0.72E-04

 receptor grid concentrations (micrograms/cubic meter) resulting from total emissions

 bearing                      distance (km)
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00
   0.0    2.0E+01  2.1E+00  6.5E-01  2.0E-01  4.8E-02  1.7E-02  9.9E-03  6.6E-03  4.9E-03  3.8E-03  2.6E-03  1.9E-03
  22.5    1.8E+01  1.6E+00  4.9E-01  1.5E-01  3.5E-02  1.3E-02  7.5E-03  5.1E-03  3.7E-03  2.9E-03  2.0E-03  1.5E-03
  ...........

 Calculated concentations for hour  8 from--

 chemicals emitted:        801410  802160
 emission rate (g/s):    0.72E-04   0.72E-04

 receptor grid concentrations (micrograms/cubic meter) resulting from total emissions

 bearing                      distance (km)
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00
   0.0    2.3E+01  2.6E+00  7.9E-01  2.5E-01  5.9E-02  2.1E-02  1.2E-02  7.8E-03  5.7E-03  4.4E-03  3.0E-03  2.2E-03
  22.5    2.1E+01  2.0E+00  6.1E-01  1.9E-01  4.5E-02  1.6E-02  9.3E-03  6.2E-03  4.6E-03  3.6E-03  2.4E-03  1.8E-03

 Total Deposition 1 from--
  (deg)     0.10     0.50     1.00     2.00     5.00    10.00    15.00    20.00    25.00    30.00    40.00    50.00
   0.0    3.1E+03  2.0E+02  5.6E+01  1.6E+01  3.7E+00  1.4E+00  8.0E-01  5.6E-01  4.3E-01  3.4E-01  2.4E-01  1.9E-01
  22.5    3.5E+03  2.1E+02  5.9E+01  1.7E+01  3.9E+00  1.4E+00  8.5E-01  5.9E-01  4.5E-01  3.6E-01  2.6E-01  2.0E-01
```

Figure 8-17 ASPENA diagnostic file created by example point source run

```
9001   10101  0.887709E-07  0.774276E-07  0.779782E-07  0.336689E-07  0.245561E-07  0.273105E-07  0.490938E-07  0.847798E-07  0.954688E-06
0.954688E-06
 9001   10102  0.936549E-07  0.847418E-07  0.825023E-07  0.381454E-07  0.256891E-07  0.294738E-07  0.546769E-07  0.997266E-07  0.104341E-05
0.104341E-05
 9001   10201  0.106153E-06  0.891512E-07  0.903393E-07  0.360951E-07  0.286658E-07  0.312934E-07  0.561904E-07  0.903312E-07  0.108410E-05
0.108410E-05
 9001   10202  0.117312E-06  0.974810E-07  0.983083E-07  0.385422E-07  0.312283E-07  0.340161E-07  0.617253E-07  0.970862E-07  0.117850E-05
0.117850E-05
 9001   10300  0.106110E-06  0.868497E-07  0.897928E-07  0.338026E-07  0.287059E-07  0.307150E-07  0.539455E-07  0.823316E-07  0.105309E-05
0.105309E-05
 ..........
    0       080141
```

Figure 8-18 ASPENB output population concentration/deposition file (in ASCII format) for example point source run (for Saroad code 80141)

```
9001   10101  0.887709E-07  0.774276E-07  0.779782E-07  0.336689E-07  0.245561E-07  0.273105E-07  0.490938E-07  0.847798E-07  0.954688E-06
0.954688E-06
 9001   10102  0.936549E-07  0.847418E-07  0.825023E-07  0.381454E-07  0.256891E-07  0.294738E-07  0.546769E-07  0.997266E-07  0.104341E-05
0.104341E-05
 9001   10201  0.106153E-06  0.891512E-07  0.903393E-07  0.360951E-07  0.286658E-07  0.312934E-07  0.561904E-07  0.903312E-07  0.108410E-05
0.108410E-05
 9001   10202  0.117312E-06  0.974810E-07  0.983083E-07  0.385422E-07  0.312283E-07  0.340161E-07  0.617253E-07  0.970862E-07  0.117850E-05
0.117850E-05
 9001   10300  0.106110E-06  0.868497E-07  0.897928E-07  0.338026E-07  0.287059E-07  0.307150E-07  0.539455E-07  0.823316E-07  0.105309E-05
0.105309E-05
.........
    0       080216
```

Figure 8-19 ASPENB output population concentration/deposition file (in ASCII format) for example point source run (for Saroad code 80216)

9.0 REFERENCES

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APPENDIX A ASPENA SUBROUTINE DESCRIPTIONS

ASPENA

Main driving routine for ASPENA model.
Called by: None
Calls to: HEADER, OPNFIL, POINT, STARIN

BID_DISP

Adjusts dispersion parameters to account for buoyancy-induced dispersion.
Called by: GAUSS
Calls to: None

DDMPR

Calculates the distance dependent momentum plume rise.
Called by: PRISE
Calls to: None

DEPOS

Retrieves deposition velocities for specified wind speed and stability class
Called by: GAUSS
Calls to: None

GAUSS

Performs Gaussian plume computations for each point source.
Called by: STACK
Calls to: BID_DISP, DEPOS, PRISE, VERTF, VGAUSZ

GAUSSZ

Calculates vertical dispersion parameters at each radial distance for each stability class assuming no wake effects.
Called by: POINT
Calls to: SIGMAZ

HEADER

Writes header information to output files.
Called by: ASPENA
Calls to: None

LIST

Writes point source data to output files.
Called by: POINT, STACK
Calls to: None

OPNFIL

Opens and reads user input files.
Called by: ASPENA
Calls to: GETARG (System function)

POINT

Main routine to set up and process a single point source.
Called by: ASPENA
Calls to: GAUSSZ, LIST, SAVE, SKIP, STACK, STAR

PRISE

Calculates the plume rise for each type of plume (buoyant/momentum) and for each atmospheric stability class (unstable/neutral/stable).
Called by: GAUSS
Calls to: DDMPR

SAVE

Updates and saves concentration and deposition grids for each point source and time block
Called by: POINT, STACK
Calls to: None

SIGMAZ

Calculates the vertical dispersion parameter, σ_z, from dispersion curves as a function of downwind distance, stability class, and rural/urban classification.
Called by: GAUSSZ, VGAUSZ
Calls to: SZCOEF

SKIP

Routine to read point and stack parameters for "skipped" points. "Skipped" points are those for which the STAR data from previously processed point is used.
Called by: POINT
Calls to: None

STACK

Main routine to process individual point sources.
Called by: POINT
Calls to: GAUSS, LIST, SAVE

STAR

Sets up STAR data for current plant.
Called by: POINT
Calls to: None

STARIN

Reads STAR data file and creates index of STAR stations.
Called by: ASPENA
Calls to: None

SZCOEF

Determines coefficients and ranges for calculation of rural dispersion parameter.
Called by: SIGMAZ
Calls to: None

VERT

Computes the Vertical Term for use in Gaussian plume equation.
Called by: GAUSS
Calls to: None

VGAUSZ

Calculates vertical dispersion parameter with wake effects using virtual distances.
Called by: GAUSS
Calls to: SIGMAZ

APPENDIX B ASPENA COMMON BLOCKS

Parameters : MXSTA = 500 – maximum number of met stations
MXSPEC = 150 – maximum number of species in run

common/srcblk/	:	information concerning sources	
	ifips	INTEGER	plant FIPS code
	utmx,utmy	REAL	plant location
	itype	INTEGER	source type
	iurb	INTEGER	urban/rural flag
	isptyp	INTEGER	species type
	idsrce	CHAR	source ID
common/metblk/	:	information concerning STAR met data	
	istar	INTEGER	INWS index
	nosc(6)	INTEGER	array of excluded stability classes
	nows(6)	INTEGER	array of excluded wind speeds
	nowd(16)	INTEGER	array of excluded wind directions
	atemp(6)	REAL	array of temperatures
	fp	REAL	frequency of precipitation
	p	REAL	annual average precipitation
common/grdblk/	:	information concerning radial receptor grid locations	
	nr	INTEGER	number of radial grid locations
	rad(12)	REAL	radial distance to receptor locations
common/stkblk/	:	information concerning stacks	
	rlon,rlat	REAL	stack location
	stakh	REAL	stack height
	stakd	REAL	stack diameter
	stakv	REAL	stack exit gas velocity
	stakt	REAL	stack exit gas temperature
	ivent	INTEGER	stack/vent flag
	ibldg	INTEGER	building downwash flag
	bldw	REAL	building width
	bldh	REAL	building height
	idstk	CHAR	stack ID
common/chmblk/	:	information concerning chemical species	
	nchem	INTEGER	number of chemical species
	idchem	INTEGER	chemical ID
	q(mxspec,8)	REAL	emission rates
	dk(6,8)	REAL	reactive decay rates

common/oldblk/	:	information concerning building downwash	
	olda	REAL	area of nearby building at last stack
comon/sigblk/	:	information concerning vertical dispersion parameters	
	sigz(12,6)	REAL	vertical dispersion without wake effects
	vsigz(12,6)	REAL	vertical dispersion with wake effects
	delta(6)	REAL	contribution to vertical distance due to building
common/conblk/	:	information concerning ambient concentrations	
	c(16,12)	REAL	ambient concentrations
common/dep/	:	information concerning depositions	
	dep1(16,12)	REAL	dry deposition flux to land
	dep2(16,12)	REAL	dry deposition flux to agricultural land
	dep3(16,12)	REAL	dry deposition flux to water
	depw(16,12)	REAL	wet deposition flux
	iddep	INTEGER	dry deposition flag
	iwdep	INTEGER	wet deposition flag
common/runblc/	:	information concerning run ID	
	idrun	CHAR	run ID
	idfile	CHAR	run filename
common/runblk/	:		
	inps(10)	LOGICAL	
	invers	INTERGER	
common/stablk/	:	information concerning met data	
	nsta	INTEGER	number of met stations
	ista(mxsta)	INTEGER	met station ID
	stax,stay(mxsta)	REAL	met station location
	stas(8, mxsta)	REAL	average wind speeds
	htmi(8, mxsta)	REAL	mixing heights
	atmp(3, mxsta)	REAL	average temperatures
	fps(mxsta)	REAL	precipitation frequencies
	p(mxsta)	REAL	precipitation amounts
common/lmet/	:	information concerning various options	
	lpsuedo	LOGICAL	flag indicating pseudo-point
	lstrec	INTEGER	index of last record processed
	lskp	LOGICAL	flag indicating that station is skipped
	irec	INTEGER	index of current record
	iurblst	INTEGER	urban/rural flag of last processed source

common/maxcon/	:	information concerning concentrations	
	xc(16,12)	REAL	array of maximum concentrations
	xcavg(16,12)	REAL	array of average concentrations
common/totdep/	:	information concerning total depositions	
	deptot(16,12,3)	REAL	array of total depositions

APPENDIX C INPUT AND OUTPUT FILE FORMATS

C.1 DESCRIPTION OF ASPEN INPUT FILE CONTENT AND FORMAT

C.1.1 Description of Emission/Control File

Table C-1 Description of Emission/Control File

Record No.	Variables	Format	Description
1	IDRUN	A40	Run identification
	IDFILE	A20	Emission file identifier
	ISPTYP	I1	Species type (0 = gas; 1 = fine part.; 2 = coarse part.)
	IDDEP	I1	= 0, include dry deposition; = 1, no dry deposition
	IWDEP	I1	= 0, include wet deposition; = 1, no wet deposition
2	DK(IC,1)	6F10	Decay rates for 6 stability classes for time block 1
3	DK(IC,2)	6F10	Decay rates for 6 stability classes for time block 2
4	DK(IC,3)	6F10	Decay rates for 6 stability classes for time block 3
5	DK(IC,4)	6F10	Decay rates for 6 stability classes for time block 4
6	DK(IC,5)	6F10	Decay rates for 6 stability classes for time block 5
7	DK(IC,6)	6F10	Decay rates for 6 stability classes for time block 6
8	DK(IC,7)	6F10	Decay rates for 6 stability classes for time block 7
9	DK(IC,8)	6F10	Decay rates for 6 stability classes for time block 8
10	IFIPS	I5	State/County FIPS
	IDSRC	A10	Plant ID for points; census tract no. for pseudo points
	UTMX	F10	Longitude (decimal degrees)
	UTMY	F10	Latitude (decimal degrees)
	ITYPE	I1	Source type (0 or blank for points; 3 = pseudo points)
	IURB	I1	Urban/Rural flag (1 = urban; 2 = rural)
11	INWS	I5	Star station (NWS) ID (blank or 0 = use nearest station)
	NOSC(6)	6I1	Excluded stability classes
	NOWS(6)	6I1	Excluded wind speeds
	NOWD(6)	6I1	Excluded wind direction
12	RAD (12)	12F5	Polar grid radial distances (km) (blank – use defaults)
13	IDSTK	A5	Stack ID for points; FIPS code for pseudo points
	RLON	F10	Longitude (decimal degrees)
	RLAT	F10	Latitude (decimal degrees)
	STAKH	F10	Stack height (m)
	STAKD	F10	Stack exit diameter (m)
	STAKV	F10	Stack exit velocity (m/sec)
	STAKT	F10	Stack exit temperature (Deg K)
	IVENT	I1	Vent/Stack flag (0 = stacked; 1 = non-stacked)
	IBLDG	I1	Build flag (0 = no building; 1 = building)
	BLDW	F10	Width of nearby building (m)
	BLDH	F10	Height of nearby building (m)
14	IDCHEM	I6	5-digit Saroad code plus 1-digit source category code
	Q	8F10	Emissions (g/sec) for eight 3-hour time blocks

Note:

- UTMX/UTMY and RLON/RLAT specify the locations of point sources, or the locations of the census tract centroid for pseudo point sources (i.e., area and mobile sources).
- Record 14 is repeated for each HAP emitted from the stack or census tract.
- Records 10 through 14 are repeated for each facility or census tract, followed by two blank lines to indicate the end of the data record for the facility or census tract
- The emission record of the last facility or census tract will be followed by five blank lines to indicate the end of the file.
- For multiple pseudo point sources that use meteorological data from the same STAR station, and that have the same urban/rural designation, ASPEN will calculate the same normalized concentration/deposition receptor grid. To save computing time, the emission records for pseudo point sources should be entered so that all sources that will use the same meteorological station ID (NWS ID) and urban/rural designation are grouped together. ASPEN checks for this grouping, and omits redundant calculations. This is the preferred method for treating pseudo-point since the code will not need to re-search the STAR data for the appropriate station since the data will already be stored in memory.

C.1.2 Description of Meteorological Index File

The meteorological index file is in binary format. There is one record for each STAR station containing the following information.

Table C-2 Description of meteorological index file

Variables	Data Type	Description
ISTA	Integer	Star (NWS) station ID
STAX	Real	Longitude of the station (decimal degree)
STAY	Real	Latitude of the station (decimal degree)
ATEMP (1)	Real	Annual average daily maximum temperature (Deg K)
ATEMP (2)	Real	Annual average daily minimum temperature (Deg K)
ATEMP (3)	Real	Annual average temperature (Deg K)
PS	Real	Annual average precipitation (cm)
FPS	Real	Fraction of time with precipitation
STAS	Real	Not used (eight zeros)
HTMI	Real	Annual average mixing heights for eight 3-hour time blocks

C.1.3 Description of STAR Data

The STAR input file is in binary format Each record contains the STAR data for one time block of one star station, and includes the following variables.

Table C-3 Description of STAR Data

Variables	Data Type	Description
IWB	Integer	Star (NWS) station ID
IHR	Integer	Time block number
FSTAR (nd, ns, nc)	Real	STAR data for the time block nd = number of wind directions (16) ns: = number of stability classes (6) nc = number of wind speed categories (6)

C.1.4 Description of Census Tract Index File

The census tract index file is in binary format, and it contains the following variables.

Table C-4 Description of census tract index file

Record No.	Variables	Data Type	Description
1	NSTATES	Integer	Total number of states included in the data
	NCOUNTIES	Integer	Total number of counties included in the data
	NTRACTS	Integer	Total number of tracts included in the data
2	STFIP	Integer	State FIPS code
	STMNLN	Real	State minimum longitude (decimal degree)
	STMNLT	Real	State minimum latitude (decimal degree)
	STMXLN	Real	State maximum longitude (decimal degree)
	STMXLT	Real	State maximum latitude (decimal degree)
	COPTR	Integer	Pointer to the first county in the state
	NUMCO	Integer	Total number of counties in the state
3	COFIPS	Integer	County FIPS code
	COMNLN	Real	County minimum longitude (decimal degree)
	COMNLT	Real	County minimum latitude (decimal degree)
	COMXLN	Real	County maximum longitude (decimal degree)
	COMXLT	Real	County maximum latitude (decimal degree)
	TRPTR	Integer	Pointer to the first tract in the county
	NUMTR	Integer	Total number of tracts in the county

Note:
Record 2 is repeated for all states included in the census tract data file.
Record 3 is repeated for all counties included in the census tracts data file.

C.1.5 Description of Census Tract Data

The census tract data is in binary format. There is one record for each census tract containing the following variables.

Table C-5 Description of census tract data

Variables	Data Type	Description
TRFIPS	Integer	State/County FIPS code, tract FIPS code
TRLON	Real	Longitude of the tract centroid (decimal degree)
TRLAT	Real	Latitude of the tract centroid (decimal degree)
UFLAG	Integer	Urban/Rural flag of the tract (1 = urban; 2 = rural)
TRRAD	Real	Hypothetical tract radius (m)

C.2 DESCRIPTION OF ASPEN OUTPUT FILE CONTENT AND FORMAT

C.2.1 Description of Normalized Source Concentration/Deposition File

The normalized source concentration/deposition file is the output of the ASPEN dispersion module (ASPENA) and input to the ASPEN mapping module (ASPENB). It is in binary format.

Table C-6 Description of Normalized Source Concentration/Deposition File

Record No.	Variables	Data Type	Description
1	ID	Character	Emission file identifier
	VERSION	Integer	Version number
2	IDSRC	Character	Plant ID for points; census tract no. for pseudo points
	IDSTAK	Character	Stack ID for points; FIPS code for pseudo points
	ITYPE	Integer	Source type
	RLON	Real	Longitude (decimal degree)
	RLAT	Real	Latitude (decimal degree)
	IURB	Integer	Urban/Rural flag
	NCHEM	Integer	Number of HAPs with emissions
	ICHEM(I),(RATE (I,J),J=1,NUMGRD),I=1,NCHEM)	Integer Real	5-digit HAP SAROAD code plus 1-digit source category code, emission rates for eight 3-hour time blocks
	NC	Integer	Number of radial distances
	R(I),I=1,NC	Real	Polar grid radial distances (km)
	NL	Integer	Number of azimuth direction
	F	Real	Start bearing (0 degree)
4	(C(I,J,K),I=1,NL), J=1,NC	Real	Normalized concentration for the receptor grid
5	(DUL(I,J),I=1,NL) ,J=1,NC	Real	Normalized urban land deposition for the receptor grid
6	(DRL(I,J),I=1,NL) ,J=1,NC	Real	Normalized rural land deposition for the receptor grid
7	(DW(I,J),I=1,NL), J=1,NC	Real	Normalized wet deposition for the receptor grid

Note:
Record 4 is repeated for each of eight 3-hour time blocks.
Record 2 through record 7 is repeated for each facility or census tract.

C.2.2 Description of Population Concentration/Deposition File

The population concentration/deposition file is the output of the ASPEN mapping module (ASPENB). It is in binary format. There is one record for each census tract containing the following information.

Table C-7 Description of Population Concentration/Deposition File

Variables	Data Type	Description
STCO	Integer	State/County FIPS code
TRACT	Integer	Census tract FIPS code
CONC	Real	concentration in eight 3-hour time blocks ($\mu g/m^3$) for each source category
DLAND	Real	deposition flux on land ($\mu g/m^2$-day) for each source category
DWATER	Real	deposition flux on water ($\mu g/m^2$-day) for each source category

An empty record with zeros for the first two fields, followed by the 5-digit HAP SAROAD code and zeros for the rest of nine fields, indicates the end of the file.

C.2.3 Description of Source Listing File

The source listing file is the output of the ASPEN dispersion module (ASPENA) used for purpose of quality assurance. It is in ASCII format. There is one record for each emission source processed by ASPENA, containing the following variables.

Table C-8 Description of source listing file

Variables	Data Type	Description
IFIPS	Integer	State/County FIPS code
IDSRCE	Character	Plant ID for points; census tract no. for pseudo points
UTMX	Real	Longitude (decimal degrees)
UTMY	Real	Latitude (decimal degrees)
ITYPE	Integer	Source type (0 or blank for points; 3 = pseudo points)
IURB	Integer	Urban/Rural flag (1 = urban; 2 = rural)

The last record of the source listing contains zeros for the variables to indicate the end of the file.

C.2.4 Description of the Listing File

The listing file is an output file of the ASPEN mapping module (ASPENB). It lists the normalized source concentration/deposition input filenames processed by ASPENB. ASPENB checks this file each time a simulation is started to prevent processing a file twice.

C.3 DECAY RATES BY REACTIVITY CLASS

Reactivity Class 1 - non reactive

Stability Class	A	B	C	D	E	F
Time Block 1	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 2	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 3	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 4	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 5	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 6	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 7	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 8	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01

Reactivity Class 2 - particulate matter (five)

Stability Class	A	B	C	D	E	F
Time Block 1	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 2	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 3	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 4	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 5	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 6	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 7	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 8	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01

Reactivity Class 3 - particulate matter (coarse)

Stability Class	A	B	C	D	E	F
Time Block 1	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 2	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 3	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 4	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 5	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 6	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 7	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01
Time Block 8	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01	0.00E+01

Each pollutant is assigned a reactivity class (Rosenbaum, et al., 1998)

Reactivity Class 4 - medium low reactivity

Stability Class	A	B	C	D	E	F
Time Block 1	9.87E-07	9.87E-07	9.87E-07	9.87E-07	9.87E-07	9.87E-07
Time Block 2	9.87E-07	9.87E-07	9.87E-07	9.87E-07	9.87E-07	9.87E-07
Time Block 3	1.18E-05	7.89E-06	3.95E-06	1.97E-06	9.87E-07	9.87E-07
Time Block 4	7.89E-05	5.92E-05	3.95E-05	1.97E-05	9.87E-07	9.87E-07
Time Block 5	6.71E-05	5.13E-05	3.55E-05	1.97E-05	9.87E-07	9.87E-07
Time Block 6	2.37E-05	1.78E-05	1.18E-05	7.89E-06	9.87E-07	9.87E-07
Time Block 7	1.97E-06	1.97E-06	1.97E-06	9.87E-07	9.87E-07	9.87E-07
Time Block 8	9.87E-07	9.87E-07	9.87E-07	9.87E-07	9.87E-07	9.87E-07

Reactivity Class 5 - medium reactivity

Stability Class	A	B	C	D	E	F
Time Block 1	2.47E-06	2.47E-06	2.47E-06	2.47E-06	2.47E-06	2.47E-06
Time Block 2	2.47E-06	2.47E-06	2.47E-06	2.47E-06	2.47E-06	2.47E-06
Time Block 3	2.96E-05	1.97E-05	9.87E-06	4.93E-06	2.47E-06	2.47E-06
Time Block 4	1.97E-04	1.48E-04	9.87E-05	4.93E-05	2.47E-06	2.47E-06
Time Block 5	1.68E-04	1.28E-04	8.88E-05	4.93E-05	2.47E-06	2.47E-06
Time Block 6	5.92E-05	4.44E-05	2.96E-05	1.97E-05	2.47E-06	2.47E-06
Time Block 7	4.93E-06	4.93E-06	4.93E-06	2.47E-06	2.47E-06	2.47E-06
Time Block 8	2.47E-06	2.47E-06	2.47E-06	2.47E-06	2.47E-06	2.47E-06

Reactivity Class 6 - medium high reactivity

Stability Class	A	B	C	D	E	F
Time Block 1	4.93E-06	4.93E-06	4.93E-06	4.93E-06	4.93E-06	4.93E-06
Time Block 2	4.93E-06	4.93E-06	4.93E-06	4.93E-06	4.93E-06	4.93E-06
Time Block 3	5.92E-05	3.95E-05	1.97E-05	9.87E-06	4.93E-06	4.93E-06
Time Block 4	3.95E-04	2.96E-04	1.97E-04	9.87E-05	4.93E-06	4.93E-06
Time Block 5	3.35E-04	2.57E-04	1.78E-04	9.87E-05	4.93E-06	4.93E-06
Time Block 6	1.18E-04	8.88E-05	5.92E-05	3.95E-05	4.93E-06	4.93E-06
Time Block 7	9.87E-06	9.87E-06	9.87E-06	4.93E-06	4.93E-06	4.93E-06
Time Block 8	4.93E-06	4.93E-06	4.93E-06	4.93E-06	4.93E-06	4.93E-06

Reactivity Class 7 - very high reactivity

Stability Class	A	B	C	D	E	F
Time Block 1	5.01E-04	5.01E-04	5.01E-04	5.01E-04	5.01E-04	5.01E-04
Time Block 2	3.21E-05	3.21E-05	3.21E-05	3.21E-05	5.01E-04	5.01E-04
Time Block 3	9.00E-05	6.04E-05	3.08E-05	1.60E-05	5.01E-04	5.01E-04
Time Block 4	5.93E-04	4.45E-04	2.97E-04	1.49E-04	8.14E-06	8.14E-06
Time Block 5	5.04E-04	3.86E-04	2.67E-04	1.49E-04	8.14E-06	8.14E-06
Time Block 6	1.79E-04	1.34E-04	9.00E-05	5.99E-05	8.14E-06	8.14E-06
Time Block 7	3.95E-05	3.95E-05	3.95E-05	3.21E-05	5.01E-04	5.01E-04
Time Block 8	5.01E-04	5.01E-04	5.01E-04	5.01E-04	5.01E-04	5.01E-04

Reactivity Class 8 - high reactivity

Stability Class	A	B	C	D	E	F
Time Block 1	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05
Time Block 2	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05
Time Block 3	1.48E-04	9.87E-05	4.93E-05	2.47E-05	1.23E-05	1.23E-05
Time Block 4	9.87E-04	7.40E-04	4.93E-04	2.47E-04	1.23E-05	1.23E-05
Time Block 5	8.39E-04	6.41E-04	4.44E-04	2.47E-04	1.23E-05	1.23E-05
Time Block 6	2.96E-04	2.22E-04	1.48E-04	9.87E-05	1.23E-05	1.23E-05
Time Block 7	2.47E-05	2.47E-05	2.47E-05	1.23E-05	1.23E-05	1.23E-05
Time Block 8	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05

Reactivity Class 9 - low reactivity

Stability Class	A	B	C	D	E	F
Time Block 1	4.94E-07	4.94E-07	4.94E-07	4.94E-07	4.94E-07	4.94E-07
Time Block 2	4.94E-07	4.94E-07	4.94E-07	4.94E-07	4.94E-07	4.94E-07
Time Block 3	5.90E-06	3.95E-06	1.98E-06	9.85E-07	4.94E-07	4.94E-07
Time Block 4	3.94E-05	2.96E-05	1.97E-05	9.85E-06	4.94E-07	4.94E-07
Time Block 5	3.36E-05	2.57E-05	1.78E-05	9.85E-06	4.94E-07	4.94E-07
Time Block 6	1.19E-05	8.90E-06	5.90E-06	3.95E-06	4.94E-07	4.94E-07
Time Block 7	9.85E-07	9.85E-07	9.85E-07	4.94E-07	4.94E-07	4.94E-07
Time Block 8	4.94E-07	4.94E-07	4.94E-07	4.94E-07	4.94E-07	4.94E-07

APPENDIX D GLOSSARY

ASPEN -- Assessment System for Population Exposure Nationwide

ASCII -- American Standard Code for Information Interchange, a standard set of codes used by computers and communication devices. Sometimes used to refer to files containing only such standard codes, without any application-specific codes such as might be present in a document file from a word processor program.

Binary File -- A file written without the use of a FORTRAN FORMAT statement.

Directory -- A logical subdivision of a disk used to organize files stored on a disk.

Dispersion Model -- A group of related mathematical algorithms used to estimate (model) the dispersion of pollutants in the atmosphere due to transport by the mean (average) wind and small scale turbulence.

DOS -- Disk Operating System. Software that manages applications software and provides an interface between applications and the system hardware components, such as the disk drive, terminal, and keyboard.

EPA -- U. S. Environmental Protection Agency.

Error message -- A message written by the model to the error/message file whenever an error is encountered that will inhibit data processing.

ISCLT -- Industrial Source Complex - Long Term Dispersion Model.

Joint Frequency Distribution -- The joint frequency of wind direction sector, wind speed class and stability category (see also STAR).

Mixing Height -- The depth through which atmospheric pollutants are typically mixed by dispersive processes.

Pasquill Stability Categories -- A classification of the dispersive capacity of the atmosphere, originally defined using surface wind speed, solar insulation (daytime) and cloudiness (nighttime). They have since been reinterpreted using various other meteorological variables.

STAR -- STability ARray, a joint frequency distribution summary of stability category, wind speed and wind direction. The STAR data are used as input for the ISC Long Term dispersion model.

Station Identification -- An integer or character string used to uniquely identify a station or site as provided in the upper air (TD-5600 and TD-6201), mixing height (TD-9689), and surface weather (CD-144 and TD-3280) data formats available from NCDC.

Syntax -- The order, structure and arrangement of the inputs that make of the input runstream file, specifically, the rules governing the placement of the various input elements including pathway IDs, keywords, and parameters.

Wind Profile Exponent -- The value of the exponent used to specify the profile of wind speed with height according to the power law (see Section 1.1.3 of Volume II).

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(Please read Instructions on reverse before completing)

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16. ABSTRACT

This user's guide provides documentation for the Assessment System for Population Exposure Nationwide (ASPEN, Version 1.1), referred to hereafter as ASPEN. It includes a technical description of the ASPEN algorithms, user instructions for running the model and a tutorial for getting started. The ASPEN model consists of a dispersion and mapping module. The dispersion module is a Guassian formulation for estimating ambient annual average concentrations at a set of fixed receptors within the vicinity of the emission source. The mapping module produces a concentration at each census tract. Input data needed are emissions data, meteorological data and census tract data.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
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