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Workbook for Comparison of Air Quality Models - Appendices

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Workbook for Comparison of Air Quality Models - Appendices

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Monitoring and Data Analysis Division
Research Triangle Park, North Carolina 27711

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OAQPS GUIDELINE SERIES

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Appendix A: TECHNICAL SUPPORT MATERIAL

Sections A.1-A.8 of this Appendix contain technical discussions of the application elements and describe methods of treating them in models. Brief discussions of the rationale for the importance ratings are given in Section A.9.

A.1 EMISSION CHARACTERISTICS

A.1.1 General

To predict the concentration of a pollutant, a model must treat the emissions of that pollutant and its precursors, if any, as well as the emissions of those substances which react with the pollutant or its precursors. The emissions and their distribution can be characterized by specifying the:

- Source-receptor relationships,
- Emission rates, and
- Composition of the emissions.

These three application elements are discussed together here but the user should make separate comparisons of their treatments.

The source-receptor relationship includes:

- Source location,
- Height at which emissions are released into the atmosphere,
- Receptor location,
- Receptor height,
- For line and area sources, the orientation of the source to a fixed direction, and
- Downwind and crosswind distances between source-receptor pairs.

Thus defined, source-receptor relationship comprises the positional factors which determine the extent to which dispersive, chemical, and removal processes affect pollutant concentrations. Once released at a particular location and height, pollutants travel downwind and are dispersed, ultimately to

be detected at the receptors of interest. It is during this time of travel that dispersion, secondary generation, and removal processes are active in altering the concentrations of the pollutant of interest.

Emission rates are clearly important because they determine the total quantities of materials emitted into the atmosphere during the time of interest. A source's emission rate generally varies with time. For example, emission rates from a stack generally vary over time scales ranging from minutes to years. For line and area sources, spatial variation within a single source may also be important. The treatment of these temporal and spatial variations must be considered when two models are compared and are discussed in Appendix A.1.3 dealing with the treatment of emission rates.

Finally, the composition of emissions must be considered in some applications. Chemical composition is important for secondary or reactive pollutants and in some situations where several species of particulate matter are of interest. The size distribution of particulate emissions is also important when fallout, deposition, or precipitation scavenging must be considered. It should be noted that the identification of possible sinks and secondary production mechanisms can depend upon knowing the composition of emissions other than those with which the user is mainly concerned.

The following three subsections describe the treatments of these application elements.

A.1.2 Treatment of Source-Receptor Relationship

In this discussion, location means a specification of the source's horizontal position. The release height specifies the vertical position of the release of emissions to the atmosphere, and does not include a specific discussion of treatments of plume rise, which are discussed as a separate element, plume behavior, in Appendix A.2.

For point sources, there are basically two levels of detail with which horizontal location can be treated. The first allows each source to be accurately located at its true position with respect to some horizontal grid system, thus allowing a maximum degree of spatial resolution. The second and less detailed approach locates each point source only to the extent of identifying a grid cell containing the source, thus sacrificing some degree of spatial resolution. This latter treatment is used by numerical models that treat all point sources lying within a given basic grid cell without regard to their

precise location but that do distinguish between sources located in different cells. The loss of resolution between the first and second levels is essentially the same as that incurred in developing an emissions inventory when small point sources are aggregated to area sources. For the purpose of this workbook, however, the inventory is assumed to be given and the less detailed treatment then involves the assignment of the point sources to grid cells despite the availability of more precise information. If the aggregation to area sources is part of the inventory, it should not be considered when comparing models. The comparison should be based on the treatments of the point, area, and line sources given in the inventory.

The location of point sources by grid cell can, of course, be treated at various levels of detail. The most detailed treatments preserve significant spatial resolution on a relatively fine grid. The least detailed sacrifice all spatial resolution and do not distinguish between sources regardless of their location within the region of interest. Models using the least detailed treatment cannot adequately treat situations involving alterations in the spatial distribution of emissions. Detailed treatments also frequently permit a finer grid to be used in areas where the user desires a high degree of spatial resolution. This treatment is somewhat more detailed than one using a fixed grid size, if the block size is smaller while allowing the user the added flexibility of matching the degree of resolution to the needs of the specific application.

Occasionally, a model may aggregate sources on a basis not directly related to location. This occurs when sources are aggregated, for example, by industrial category. Unless this type of treatment is used in conjunction with one of the locational treatments described above, it provides no information on the location of sources and is equivalent to the least detailed treatment of horizontal location.

The release height of point sources is treated in its most detailed form when both the physical stack height (without plume rise) and the elevation of the base of the stack above some reference elevation can be specified for each source. A less detailed treatment assumes flat terrain and considers only the physical stack height or release height above grade. These treatments can be used even when the horizontal locations of the sources are "gridded" by the model onto subareas of the region of interest. Less detailed treatments are

frequently used when the model grids the point sources. These involve specifying one or several representative release heights, which may include an elevation correction, for each subarea of the grid. Less detail is available when the same release heights are applied to all the subareas. (When representative release heights must be assigned, the user frequently calculates a representative plume rise and adds it to the physical release height, since models using such treatments generally make no provision for the internal calculation of a typical plume rise.) At the least detailed level release height is not treated explicitly; all emissions are treated as if they are released at the same height. This non-explicit treatment is used in numerical models in which all emissions are treated as part of the boundary condition at ground level.

Before proceeding, it is convenient to discuss receptor location because receptors are usually taken as points. As is the case with point sources, the horizontal locations of receptors can be specified as precise points or as locations in some grid block. When the receptors are located precisely two methods or a combination of the two are generally used. The first allows the user to locate the receptors arbitrarily. The second places the receptors at the intersections of a grid network, the spacing or scale of which may be fixed or under the user's control. Both methods may provide equivalent levels of detail and the user must decide which is better suited to the particular application. It may also be, of course, that specifying receptor locations by subarea only is sufficient to the user's purpose, but here such treatments will be rated as less detailed than treatments that locate receptors precisely in the horizontal. The level of detail of receptor locations also depends upon whether the elevation of the receptor can be specified. Given comparable specification of horizontal receptor locations, a treatment which allows the user to specify arbitrary receptor heights is more detailed than one which assumes that all receptors are at the same height (usually ground level).

In the context of source and receptor locations, it must be stressed that the user should not always rate one treatment against another solely on the level of detail. Consideration should also be given to whether the level of detail provided is necessary in the particular application. For instance, if the application involves the impact of a single source at a

specific location, the ability to locate numerous sources and receptors precisely is irrelevant as long as the pair to be studied can be located as desired. Thus, the comparisons made by use of the tables in the workbook should be modified to reflect the specific requirements of the application of interest. The table assumes that it is desired to locate a number of sources and receptors at arbitrary locations. Since all required cases could not be foreseen, the user must modify this general list to reflect the application of interest.

For area sources, the treatments of source location and release height follow the same general progression as for point sources, that is, a full specification in three dimensions (both horizontal location and release height) at the most detailed level and a complete lack of explicit recognition of different source locations and heights at the least detailed level. Two additional considerations must be given to area sources, however, because of their two dimensional nature. First, a model which accepts area sources at arbitrary locations provides more detail than one which places all area sources on a fixed grid even if the size of the grid can be changed by the user. In the latter case, the user's area sources must be mapped onto the model's gridded areas and hence the differences between areas tend to be averaged out. Such a loss of detail may be unimportant when the difference in emission rates in adjacent areas is small. The user must decide this based on his knowledge of the situation of interest. Second, models which treat arbitrarily sized area sources generally allow greater flexibility than those which limit area sources to one or several set sizes. This can be particularly important when dealing with "true" area sources such as open pit mines or dusty fields. Again the user must decide when comparing models whether this consideration is important in the particular application of interest.

Another difference between point and area sources arises because an area can have an arbitrary orientation with respect to the wind direction. Most models treat area sources on some type of grid system that is fixed in space and hence the orientation of an area cannot be adjusted even when the real physical source is tilted with respect to the model grid. For computational purposes, some models assume a specific orientation which may be unrelated to the actual orientation of the source. This assumption is

frequently reasonable when the area sources are aggregates of many small point or line sources. A somewhat more detailed treatment permits the area sources to assume an arbitrary orientation; such treatments may be useful when dealing with true area sources where the orientation of the actual sources can be arbitrary.

The most detailed treatment of line sources specifies the precise location and orientation of the line by, for example, using its endpoints and provides for some width and height for the line (thus really treating it as an elongated volume source). For infinite lines, only the orientation of the line is specified. Curved lines are usually approximated as series of straight line segments and for highways some width can be provided by allowing the number of lanes, medial strip width, and roadway width to be specified. Less detailed treatments specify only the horizontal location and fail to allow for width; a release height may be specified. Care must be taken with line source models to ascertain whether they allow the line to assume an arbitrary orientation with respect to the receptor. Some models, for example, require that the receptor be located near the perpendicular bisector of the line and will not properly treat a receptor lying near the axis of the line source. As with point and area sources, increasing degrees of aggregation within the model produce less detailed treatments.

In applications involving a combination of source types, the degree of detail of the treatment can be different for different source types. However, an overall evaluation can still be made by comparing the reference model treatment with the study model treatment for each source category and making some assessment of the importance of each category to the particular application.

Some modeling parameters determined by the source-receptor relationship may depend explicitly on the downwind or crosswind distances between source-receptor pairs. For instance, in Gaussian plume models the dispersion parameters are normally functions of the downwind distance. When this is the case, these distances must be calculated. It should be noted, however, that a model may not ever need to calculate the downwind or crosswind distance explicitly. For example, a numerical dynamic model may move an air parcel along a trajectory but never use the distance along the trajectory. In such cases, the downwind/crosswind distances are not calculated and their treatment

can be ignored. When required by the model these distances are usually assumed to be determined by the horizontal separation between pairs and hence do not depend upon release height or receptor height. When point sources are involved and both the sources and receptors are located as points, the capability exists to calculate a unique downwind and crosswind distance for each source-receptor pair either along a curved trajectory or assuming a steady-state wind in a single direction. When a model grids either sources or receptors, less detail is available, since only average or representative separations can be determined. This is also the case for area and line sources. Finally, no downwind or crosswind distances can be determined if no distinctions between sources and receptors are made on the basis of location. This is the case, for instance, when a box model includes an entire region in a single box.

These treatments of source-receptor relationship are listed by their level of detail in Table 5.1. Treatments by suggested reference models are given in Table B.2.

A.1.3 Treatment of Emission Rate

Once the positional relationships between sources and receptors have been determined, the emission rate of each source must be specified. Two aspects of the element emission rate are important:

- Spatial distribution of emissions and
- Temporal variation of emissions.

The treatment of the spatial distribution of emissions is closely related to the treatment of horizontal location discussed in Appendix A.1.2, since the degree of spatial resolution available depends upon how close to their real positions the model locates sources. For point sources, no additional information is required to describe the spatial distribution beyond what is already given in the treatment of source-receptor relationship. In the case of line or area sources, however, the manner in which the distributed nature of the source is taken into account requires consideration and is discussed in this section. Two points of view exist regarding the treatment of distributed sources. In determining the treatment of distributed sources by a model it is useful to identify which point of view is adopted simply in order to clarify the treatment. In many cases, there is no intrinsic difference in the level of detail associated with the two possibilities.

From the first point of view, the total contribution of the entire emission distribution is estimated by adding up estimates of the contributions from many individual parts, each consisting of a uniformly emitting area or line segment. For example, sulfur dioxide emissions from residential space heating in an urban area are most commonly represented as a rectangular array of square area sources, each characterized by a given emission rate per unit area. Another example is the representation of automotive emissions as a set of finite line sources, each of which is characterized by a given emission rate per unit length. Each part is considered to be a separate source, and the contribution from each of these parts to the pollutant concentration is estimated. The total contribution from the entire distribution is then estimated by summing all these individual contributions.

From the other point of view, the overall distribution is regarded as a single entity in which, however, the local emission rate may vary from point to point. A single estimate of the total contribution from the given emission distribution is made without explicitly estimating the contribution from each of the individual parts comprising the source inventory, even though the source inventory may have exactly the same form as before. This point of view may be adopted for an array of square area sources as in the first example above, as well as in cases in which only one line or area source is of interest. In the latter situation, the emission rate per unit length or per unit area may be allowed to vary within the source itself.

There is no intrinsic difference in the levels of detail associated with these two points of view if only the total contribution to the estimated pollutant concentration is of interest. If the individual contributions are desired, a treatment which adopts the first point of view is likely to be superior to one which adopts the second. However, much depends upon the level of detail of the methods used to make the individual estimates in the two treatments. In order to estimate individual contributions within a model adopting the second approach, an algorithm for allocating the total calculated contribution among the individual parts must be incorporated. In the first approach the individual contributions are independently estimated.

Whatever point of view is adopted, some technique must be used to estimate the contribution of either the overall distribution or of each of its component parts. The rest of the discussion addresses methods of making these

estimates. The various possible methods fall into two general categories:

- Analytic or numerical integration, and
- Source substitution - the replacement of a line or area source with a small number of point sources.

In principle, the most detailed treatment of the spatial distribution of emissions involves the integration over the given distribution of the contribution from an infinitesimal area or line segment, assumed to contribute as a point source. If the spatial distribution and the infinitesimal contribution have a sufficiently simple form, the integral may be evaluated analytically. Thus, for example, the pollutant concentration downwind of a uniform horizontal line source of specified length oriented perpendicular to the wind may be estimated by means of a formula obtained by integrating the Gaussian plume expression for the contribution from each infinitesimal segment of the line. In general, however, the spatial distribution and the point source concentration estimates are sufficiently complicated that such an analytic expression cannot be derived. In such cases, alternative methods must be used.

One alternative is to evaluate the integral by some appropriate numerical procedure. If the numerical procedure is sufficiently detailed that the spatial variation present in both the emissions and the point source formula is taken into account, the result may be equivalent to that which would be obtained by an analytic integration. The level of detail of the treatment is directly related to the distance between sampling points at which the emission rate and point source estimate are evaluated; the smaller the distance, the higher the level of detail. Since for a given receptor the nearby emissions are expected to contribute more heavily than those futher away, treatments which incorporate high resolution near the receptor and progressively lower resolution at greater distances involve a relatively high level of detail.

Another alternative is to simplify the integration by introducing additional approximations so that either an analytic expression may be derived or the numerical integration is made significantly easier. For example, a common approximation used in dealing with an array of area sources is to assume that emissions are uniformly distributed in the crosswind direction. In most urban areas, this may be a reasonable assumption; in general, the level of the treatment depends upon the appropriateness of the assumptions in the user's

specific application. The example just given corresponds to what is often called the narrow plume approximation. In this approximation, only the emissions from those area sources which are directly upwind of the receptor, or in general those which are intersected by a trajectory which subsequently passes through the receptor location, have an effect on the estimated pollutant concentration. Further discussion may be found in Appendix A.4.2.

The least detailed treatments involve the replacement of a line or area source by a small number of point sources having a combined emission rate equal to that of the source they are replacing. The smaller the number of effective point sources is, the less detailed is the treatment; a treatment involving the use of a large number of points amounts to the use of a numerical integration procedure. The position of the effective points may be chosen to approximate the spread of emissions within the source being replaced, and the strength of each may depend upon their position.

There are two components to the treatment of temporal variation of emission rates:

- The degree of temporal resolution which the model allows and
- The suitability of the technique for treating the variations to the particular application.

The degree of temporal resolution is determined by the interval at which emission rates can be changed in the model. Even the most detailed treatments can usually handle properly at most hourly variations in emission rates. The overall temporal resolution of a model is often limited by the temporal resolution of the meteorological data. The emission data should reflect a similar resolution at the most detailed level. If a large number of time intervals must be treated, say all 8760 hours in a year, some models take a sample of all the hours and thus treat only a subset of all available time intervals. This approach provides somewhat less detail than accounting for all time intervals but may give results which are equivalent to those obtained from a fully detailed treatment particularly when the accuracy of the model is considered. Less detail is offered by treatments which allow no temporal variation, permitting only constant emission rates to be specified. Within these limits, the shorter the interval over which changes in emission rates can be specified, the more detailed the treatment.

For those models which allow some temporal variation in emission rates, the suitability of the technique of handling the variations must also be considered. One technique is commonly used in dynamic models. The total time period of interest is divided into intervals. Each time interval is modeled in succession, the pollutant distribution at the end of one interval serving as the initial distribution for the next. This type of detailed approach is necessary when significant variations in emission rates occur over the averaging time of interest. In simpler situations, a second technique treating the situation as a set of steady states is applicable; the steady-state approach is generally simpler to implement. This approach looks at each time period separately. It can account for the time sequence, but it ignores the pollutant distribution remaining at the end of each interval when a new interval is considered. The steady state treatment is the more common. Some models allow the entire set of steady-state situations to be treated. Others simulate only a single situation at a time and must be applied repetitively when longer time periods are of interest.

The repititious application of a model allows temporal variations in emission rates to be treated using only constant rates. For example, if it is desired to use a climatological model designed to estimate annual averages from average emissions rates and the sources have significant monthly variations, the model could be run twelve times with emission rates appropriate for each month and the twelve individual results averaged. It would, of course, also be necessary to use meteorological data appropriate to each month in the individual runs.

As was the case with spatial variation, a model that aggregates sources is inherently less detailed than one which treats each source individually. In aggregating, each source's emission pattern is masked in an average value and some details of the situation are lost.

One further aspect of emission rate must be discussed: the treatment of the amount of emissions based on other input parameters such as vehicle miles traveled (VMT), vehicle mix, or population. When actual emission rates (or a sequence of rates) are supplied to the model, the degree of detail depends upon the degree of detail used in generating these numbers and is not limited by the model itself. When the model itself calculates the emission rates, a model requiring more detailed input generally provides a more detailed treatment. For example,

a model which estimates vehicular emissions based on VMT, average speed, and vehicle mix is less detailed than one which uses VMT, vehicle mix, and allows a different average speed to be assigned to each class of vehicles. Since the number of possibilities is large, no attempt to rank treatments will be made here. As a general guideline, the user should compare the levels of detail required in the inputs of the models being evaluated. It should also be noted that evaluating this aspect of emission rate may be impossible; for example, one model might require specific emission rates to be input, while a second model calculates emission rates from other information.

Table 5.2 gives the general treatments of emission rates in order of decreasing level of detail. Specific treatments used by suggested reference models are given in Table B.3.

A.1.4 Treatment of Composition of Emissions

Chemical Composition

In applications involving chemical reactions (secondary generation or reactive pollutants), the chemical composition of emissions is important. At the most detailed level, the emissions of all relevant individual compounds are treated. Somewhat less detail is obtained when several or many related compounds are "lumped" together into a single class and only the total emissions of all members of the class are treated. Two things must be considered when a model treats the emissions of at least some of the relevant compounds in terms of lumped classes. First, the criterion for determining in which class a particular compound belongs must be appropriate for the chemistry to be modeled. Second, the compound chosen to represent the class must also be chosen appropriately; in some cases, it may not be an actual compound but a hypothetical representative compound. For example, in the case of photochemical oxidants, it would be impractical to use full detail and treat the emission of every possible organic compound individually. Consequently, they may be lumped into classes depending upon their degree of photochemical reactivity. Thus, if five reactivity classes were used, each source could have associated with it up to five different emission rates for organic compounds, one emission rate for each reactivity class. This classification would also be appropriate to the oxidant problem whereas classification by, for instance, molecular weight may not be. In general, the greater

degree of classification into appropriate, distinct classes, the greater the level of detail of the treatment. Less detail is available when assumptions regarding the composition of emissions are built into the model, such as when a photochemical oxidant model assumes a certain percentage of the organic emissions to be reactive regardless of the actual nature of the sources involved. Still less detailed treatments describe the emissions of only one of several compounds known to interact.

Model treatments must also be checked to ascertain whether all relevant emissions have been treated. For example, models for photochemical oxidants that treat reactive organic compounds but not NO and NO_2 emissions are inherently less detailed than those which treat NO and/or NO_2, because NO can act as an ozone scavenger and the NO_x/organics ratio is important in determining the extent of ozone formation. Expert advice may be needed in making these determinations. With regard to this last point, care must be exercised to consider here only compounds which are actually "emitted" by the sources. These may only be a subset of the total number of compounds which are involved in the chemical kinetics and may not even include the pollutant of interest. For example, ozone "emissions" are negligible or zero but the emissions of the organic precursors must be treated in models for photochemical oxidant. The user would not deem a photochemical model inappropriate because ozone emissions are not treated.

Size Distribution of Particulate Matter

The most detailed treatment of the size distribution of emitted particulate matter would take into account a continuum of particle sizes by allowing the functional form of the particle size distribution to be specified. In somewhat less detail an appropriate distribution is assumed and the parameters necessary to describe that distribution are input. Less detail is available in treatments which treat all particles within a given range of sizes as if they had the same representative size. This treatment is analogous to the lumping of various chemical species described above. Similarly, a treatment using smaller size intervals offers more detail (generally, more size intervals) than a treatment that divides the total range of sizes into fewer, wider intervals. Even less detail is contained in treatments that assume that some fraction of the particulates are affected by the mechanism of interest. This is really a two-class treatment: a fraction of the particulates, for example

might be assumed large enough to fall out of a plume, while the remainder are assumed to behave like a gas. The least detail, of course, is offered by treatments which fail to treat the size distribution explicitly in situations in which it may be important. Such is the case when all particulate emissions are treated as a gas, including that fraction which is sufficiently large to be subject to significant gravitational settling.

It should be noted that a complete characterization of the composition of emissions may require a joint treatment of chemical composition and the size distribution. In such cases, the appropriate size distribution may not only vary from source to source but may also vary from chemical compound to chemical compound. Such detail is beyond the level at which models presently operate but the user should be aware of the complexity of a complete specification of the application.

Tables 5.3 and B.4 give the treatments of the composition of emission in general and by suggested reference models, respectively.

A.2 PLUME BEHAVIOR

A.2.1 General

Upon release, an effluent generally has some upward momentum and buoyancy. Mixing with the ambient air begins immediately and continues as the effluent travels downwind and disperses. In the initial phases of this travel, the plume centerline is determined simultaneously by the rise due to the initial momentum and buoyancy and the downwind advection. As mixing continues, the plume centerline is determined by the initial conditions to progressively lesser degrees until it is determined predominantly by the downwind advection. The height to which the initial momentum and buoyancy carry the effluent is called the "plume rise" and this height plus the physical release height is termed the "effective stack height."

As these definitions indicate, some models treat plume rise only for point sources. When area and line sources are aggregates of small point sources, the plume rise associated with each individual area or line source is an average or representative value. This discussion focuses on plume rise from point sources and certain other types of plume behavior. The user should be aware, however, that the same factors as discussed herein must be considered if a model explicitly treats plume rise from area or line sources.

Many interacting factors affect plume behavior. When the stack exit velocity is small compared to the wind speed, the plume may bend over immediately after release and downwash may occur behind the stack. This is one of several special situations to be considered when plume behavior is treated. If the stack exit velocity is large, mixing of the effluent and ambient air will be increased, rapidly dissipating the plume's buoyancy and momentum and causing a low plume rise. Plume rise also depends on stability, atmospheric temperature gradient, plume buoyancy and wind speed. The buoyancy of a hot plume is determined by the heat release rate; hotter plumes rise higher than colder plumes, other conditions being the same. The heat release rate depends on the stack exit velocity; the effluent's temperature, molecular weight, and specific heat; the stack diameter; and the atmospheric temperature and pressure. A formula relating these variables may be found in Moses and Kraimer (1972). In addition, the relative humidity and moisture content of the plume may be important. Many plumes contain some water and after release the condensation of gaseous water or vaporization of liquid water adds or removes heat from the plume and hence affects buoyancy. The condensation of water vapor can be large enough to cause a very low plume rise, as can be the case with cooling tower plumes.

The momentum of the plume depends upon the mass of the effluent and the stack exit velocity. The density of the plume is thus important and the product of velocity and stack diameter is a measure of the square root of the momentum release rate. For stacks with very high exit velocities, the momentum term may be much larger than the buoyancy term. This "momentum only" case is not encountered in most common applications, in which the principal interest is in buoyancy effects.

There are other factors which also affect plume rise:

- Terrain and nearby buildings,
- Number of nearby stacks and local heat sources,
- Shape of the stack opening,
- Wind direction in directionally inhomogenous situations,
- Wind shear, and
- Precipitation.

No single treatment of plume rise deals with all these factors and there is no generally accepted treatment; over twenty separate formulae are available and new ones continue to appear. Most analytical formulations make the plume rise directly proportional to the reciprocal of the wind speed at the top of the stack. Two terms, one proportional to the square root of momentum and the other to some power of the heat release rate, are also included but the momentum term is frequently omitted, its effect being negligible in many common situations. When plume rise is treated as a function of distance, data for power plant plumes indicates that the plume rise varies as the 2/3 power of the downwind distance. There may be separate formulae for different sized stacks and different stabilities but the treatment of special plume behavior is generally not included in the treatment of plume rise.

The special plume behaviors usually considered include:

- Downwash
- Plume trapping, and
- Inversion breakup fumigation.

The conditions leading to downwash were noted above. A rule-of-thumb says that downwash should be considered whenever the physical stack height is less than about 2 1/2 times the height of the building it is on or the height of nearby obstacles to airflow or whenever the stack exit velocity is less than about 1 1/2 times the windspeed at the top of the stack. This rule-of-thumb is only a rough guide and in many situations, for instance, with a cold plume having little buoyancy, downwash may need to be considered even for stacks whose heights exceed those indicated. Plume trapping occurs when a stable layer exists above a neutral or unstable layer. A plume emitted into the lower neutral or unstable layer will rise until it reaches the base of the stable layer where it becomes trapped between the stable layer and the ground. Very hot plumes may be able to "punch through" the stable layer and thus may not be trapped. Fumigation occurs when a stable surface-based inversion is broken up by heating from the ground. Pollutants that were emitted into the stable layer are then thermally mixed in the vertical and relatively high ground level concentrations can result, as discussed in Appendix A.4.

A.2.2 Treatment of Plume Behavior

As noted previously, there is no generally accepted method of treating plume rise. Several types of treatments of various degrees of detail exist. Within each type, the appropriateness of a given treatment depends upon whether the method has been verified in the field for the application of interest. In fact, the best comparison of two plume rise formulae is obtained by comparing their predictions with observed plume rise values under the conditions of interest.

The most detailed level of treatment would account for the simultaneous rising and dispersing of the plume. This problem is extremely complex and has been treated only in very specialized applications such as self-contamination of buildings where the behavior of the plume immediately after release is of primary concern.

Most models are unable to handle dispersion during the initial rising phase of plume travel and usually treat the situation by separating the rising plume from the dispersing plume and considering two distinct steps:

> First, the plume rise is determined based on stack and meteorological parameters. This plume rise may be a function of the downwind distance.
>
> Second, dispersion is treated by assuming a virtual source emitting at an effective stack height equal to the physical release height plus the plume rise.

This is the type of treatment found in most dispersion models for primary pollutants. However, many formulae are used to estimate the plume rise. As noted above, comparison to a reference model's treatment should be based upon which treatment gives better agreement with observed plume rises for the application under consideration. Such comparative results are scanty and another method must normally be used if a comparison is to be made.

Without prejudice to other treatments, models using the following plume rise formulae can be considered applicable in many situations, unless comparative field studies indicate otherwise for the case at hand:

- Briggs' 2/3 power law,
- Holland,
- CONCAWE or CONCAWE simplified, and
- ASME.

The Briggs' and Holland formulae have been "verified" for power plants. Only Holland has a separate momentum term and correction factors have been suggested to account for stability. Briggs uses separate formulae for different stability classes and is the only one that treats plume rise as a function of downwind distance. The CONCAWE formulations consist of single formulae and are the only ones in which plume rise is inversely proportional to a fractional power of the wind speed, except for the Briggs (stable) formula. It must be stressed that this list does not mean that other formulae should not be used. These four are widely used and do a fairly good job of prediction in many cases. Other formulae may be better in specific applications, but the only valid evidence of this is direct comparison with observations.

If the user has an unverified formula in a study model, the following general guidelines, valid for hot, buoyant plumes only, may be helpful:

- Plume rise should be proportional to the reciprocal of wind speed to some power between 1.0 and 0.70 for nonstable conditions. Calm conditions require the omission of wind speed from the formulae used.
- A buoyancy term must be included (heat release rate should be raised to a power between 1/3 and 1).
- Other things being equal, a formula with a momentum term would be preferred.
- Other things being equal, a formula giving plume rise as a function of downwind distance would be preferred. (This consideration is more important for low level sources than for elevated sources.)

It must again be stressed that verification in the field for the application of interest is the preferred decision parameter. Use of the above guidelines is recommended only as a last resort. For ease in comparison, the widely used formulae are compared in Table A.1.

Table A.1. Comparison of Widely Used Plume Rise Formulae[a]

Formula	Wind Speed Proportionality	Buoyancy Proportionality	Momentum Term Included?	Function of Stability?	Function of Downwind Distance?
Briggs	$(1/u)^{1/3}$ stable 1/u neutral, unstable	$Q^{1/4}$ stable[b] $Q^{1/3}$ neutral, unstable	no[b]	yes	yes
Holland	1/u	Q	yes	yes[c]	no
CONCAWE	$(1/u)^{0.70}$	$Q^{0.58}$	no	no	no
CONCAWE simplified	$(1/u)^{0.75}$	$Q^{1/2}$	no	no	no
ASME	$(1/u)^{1/3}$ stable 1/u neutral, unstable	$Q^{1/3}$ stable $Q^{1/3}$ neutral, unstable	no	yes	no

[a] u = wind speed at top of stack
Q = heat release rate

[b] A momentum term is included in the literature but is omitted in the most common formulations used in models.

[c] When recommended correction factors are used.

The next lower level in detail still uses the two-step procedure but does not attempt to estimate a specific plume rise based on stack parameters. Instead, the user specifies a value for the product of some power of the wind speed and plume rise. The model then calculates a plume rise for each wind speed. This method usually assumes that plume rise is inversely proportional to the wind speed but does not allow differences between sources or other meteorological parameters to affect the plume rise.

A still less detailed treatment allows plume rise to be considered but only permits a small number of specific values. This treatment is used frequently for aggregate sources and hence is common in the treatment of area sources in urban models. The values of plume rise chosen are average or representative values and are often included in the release height (see Appendix A.1.2).

The least detailed treatment does not deal with plume rise explicitly. This is the case, for example, in proportional models and models which treat vertical dispersion by assuming uniform mixing.

There are only a limited number of treatments of the special plume behavior. Downwash is typically not treated explicitly. Treatments of downwash are normally developed expressly for that problem alone. Halitsky (1965, 1968) and Turner (1969) discuss downwash in general and should be consulted if downwash is expected to be significant. More recent studies of downwash near buildings are found in Huber and Snyder (1976) and Robins and Castro (1977). Several techniques of accounting for building influences on plume dispersion are presented by Huber (1977). In general, many additional studies are necessary to thoroughly understand the complex effects of downwash on ground-level concentrations.

Plume trapping can be accommodated in two-step models by assuming that the plume is reflected from the base of the stable layer aloft and from the ground. Repeated reflections lead to uniform mixing. The plume is assumed to be unaffected by the inversion lid until its vertical spread reaches the stable layer and to be uniformly mixed after some suitable downwind distance thereafter. Between these two distances, interpolation of concentrations is used. (See the discussion of boundary conditions in Appendix A.7.) Carpenter et al.

(1971), Pooler (1965), Hales (1956) and Bierly and Hewson (1962) give treatments that can be used for trapping. The formula developed independently in the latter two papers, and included in Turner (1969), frequently is used in Gaussian plume models.

Inversion breakup is generally not treated by models. Carpenter et al. (1971), Turner (1969), and Pooler (1965) give formulas which can be used to estimate ground level concentrations during inversion breakup if the user must consider this condition. (See the discussion in Appendix A.4.)

One further treatment of plume behavior used to treat the deposition of particulate matter for which gravitational settling is important should be noted. This is called the "tilted plume" approximation and is discussed in Appendix A.6.2.

The various general treatments of plume rise are given in Table 5.4. Treatments of special plume behavior are not rated. The user should note how the study model compares to the reference model in the number of special cases of plume behavior each treats. These treatments should be compared to those given in the references cited above. Treatments by suggested reference models are described in Table B.5.

A.3 HORIZONTAL AND VERTICAL WIND FIELDS

A.3.1 General

The primary mechanism for the transport of pollution in the atmosphere is advection, the horizontal motion of air which carries pollutants along from one place to another. This transport of pollution by the wind must be accounted for by any deterministic model which attempts to predict the spatial distribution of some material being emitted from a set of known sources. In certain circumstance, there may also be a significant vertical component to the mean atmospheric motion and in these cases pollutants may be transported in the vertical direction as well. This appendix describes the general features of and methods for treatment of the horizontal and vertical transport of pollution by the wind.

Horizontal Wind Field

This term refers to the magnitude and direction of the horizontal component of the wind velocity as functions of horizontal position, height above ground, and time. Hereafter, when the terms wind speed and direction are used they will refer to the horizontal component, in accord with common usage.

The general properties of the wind speed and direction most relevant for pollutant transport are:

- A systematic increase in speed and shift in direction with height above ground which
  - Is very pronounced within an inversion,
  - Becomes less and less pronounced as the atmosphere ranges from stable through neutral to unstable conditions, and
  - Is significantly affected by variations in surface properties upwind and possibly downwind of the location in question;
- A sensitivity to the presence of topographic features such as
  - Hills or mountains
  - River valleys, and
  - Large bodies of water;
- A significant diurnal variation, reflecting the diurnal variation of atmospheric stability; and
- Significant seasonal variations, reflecting seasonal changes in the weather.

The variation with altitude is due to the frictional interaction between wind and the surface of the earth. Its effects are most pronounced near the surface and becomes less evident at higher elevations until at some altitude the surface effects become negligible. The effects of variations in atmospheric stability on the rate at which wind speed and direction change with altitude simply reflect variations in the extent to which the momentum of air at different levels is being mixed by turbulence. Enhanced vertical mixing such as exists under unstable conditions tends to smooth out and decrease the

dependence of wind speed and direction on height. In stable conditions, vertical mixing and with it the influence of one layer of air on another is decreased. As a result, both wind speed and direction can have a significant dependence on height in stable, and especially inversion, conditions.

The gross effect of hills, mountains, or river valleys on wind speed and direction is to channel the airflow and to promote the formation of local, organized circulation patterns. More subtle effects can occur as well, such as mountain and valley breezes and drainage flows, and the possibilities are numerous and varied. A useful summary and discussion is given by Slade (1968). The principal effect of large bodies of water is similar to some topographic effects. A surface-based breeze, called a lake or sea breeze depending on the body of water involved, tends to blow from the water toward the land during the day as a result of differences in air temperature above adjoining land and water surfaces. This breeze may blow in a direction opposite to the prevailing wind and may extend a considerable distance inland. In situations in which the lake or sea breeze acts against the prevailing wind, a convergence zone in which there are significant upward vertical motions is formed. Pollutants may be transported inland near the surface, rise in the convergence zone, and be transported back out over the water at heights of several hundred meters. Situations in which the lake or sea breeze acts in the same direction as the prevailing wind are less complex and "circulation cells" such as were just described do not form. Any movement of cool maritime air onto an adjacent, warm land surface results in an elevated temperature inversion extending some distance inland. Continuous fumigation of elevated plumes can occur during this condition, because the base of the inversion is eroded as the air moves onshore.

It should also be pointed out that urban areas themselves have a significant effect on the wind field, ranging from modification of the flow when regional wind speeds are high to the establishment of local circulation patterns due to the urban heat island effect when regional winds are weak. Systematic changes in wind direction and speed occur over urban areas. Even in strong regional flows there is a systematic tendency of the air to rise over cities, accompanied by a net inflow at low levels.

Both seasonal and diurnal variations in the mean wind speed and direction occur. We will not discuss seasonal variations except to point out that they depend on the location of the region of interest and can be significant.

Dramatic variations may also occur during frontal passages or other weather changes. Diurnal variations are related to the diurnal variation of stability and the effect of stability on the variations of the wind field with altitude. Diurnal variations are most important during periods of cloudless weather, in which there are strong diurnal variations in stability and correspondingly large variations in the extent of atmospheric mixing. In stable conditions at night, the wind speed near the ground may be very low while at the same time at heights of a few tens of meters it is often quite high. In unstable conditions the wind speed, although usually rather low, is not strongly dependent on altitude. Both high and low wind speeds may occur under neutral conditions, although high wind speeds tend to produce neutral conditions even on clear days and nights, as discussed in Appendix A.4.

The horizontal wind speed and direction are in fact randomly fluctuating quantities with fluctuations occurring over time scales from much less than a second up to years and beyond. Qualitatively, short-term fluctuations are perceived as turbulence while long-term fluctuations are perceived as part of the day-to-day changes in the weather. For the purposes of describing the transport of pollution, the interest is normally in the mean wind speed and direction over some specific time interval, or over each of a sequence of time intervals. The transport of pollutants by the mean wind is the operational definition of advection, and the transport of pollutants by the fluctuations about this mean is the operational definition of dispersion. In any given situation, the averaging time for which mean wind measurements are available determines the distinction between advection and dispersion. Typical averaging times in practice range from about 10 minutes up to about 3 hours.

Vertical Wind Field

The vertical component of the wind velocity is in many cases much less important than the horizontal components, for the simple reason that in many cases it is zero over the averaging time of interest. In some situations, however, primarily those in which there are significant topographic features in the region of interest, significant vertical wind components may be present. When they are, they provide an effective mechanism for vertical transport of pollution and should be taken into account.

A.3.2 Treatment of Horizontal and Vertical Wind Fields

The treatment of the wind field by an air quality model depends on the type of model according to the classification scheme introduced in Appendix A.4. For example, dynamic models treat the time dependence of the wind field in addition to its spatial dependence, numerical models can generally handle more complex spatial variations than semiempirical models, and so on. Thus, treatments of wind field may be classified by the way both spatial and temporal variations are handled.

Spatial variation in either horizontal or vertical directions is usually handled in numerical models by specifying the wind velocity components at discrete points defined by a suitable grid, the grid spacing being chosen to reflect the actual spatial resolution available in the data from which the model wind field is calculated. This grid spacing then determines the spatial resolution of the model as a whole. The grid may be one, two or three-dimensional depending on the model. Similarly, in dynamic models the temporal variation in wind speed and direction at a given point is usually handled by specifying a sequence of mean values representing averages over some basic time step, typically one hour.

An alternative to the use of measured wind speeds and direction in combination with an interpolation procedure is to model the wind flow within the region of interest in a separate calculation using fluid flow modeling techniques and to thereby determine the wind field in a manner suitable for use in the air quality simulation model. This approach is often used with dispersion models for complex terrain, and in principle allows great flexibility in the spatial and temporal variations in the wind field that can be described by the model. The user should be aware, however, that not only are simplifying assumptions generally introduced in practice, but also that the manner in which the basic equations are implemented in a computer code must be carefully considered in order to minimize numerical errors. Expert advice may be necessary to properly take these considerations into account.

Treatments at lower levels of detail involve progressively larger numbers of simplifying assumptions regarding both spatial and temporal variations. Most semiempirical models incorporate such assumption in their formulation and, if sufficient information is available, the user should consider whether they are appropriate or acceptable for the specific application of interest. Expert

advice may be necessary in these considerations. Often the utility of a semiempirical model designed for use in a limited set of circumstances is extended by making additional assumptions. An example illustrating this practice will be given below.

The nature of the desired results may affect the amount of detail necessary in the treatment of the wind field, particularly in regard to the size of the region of interest and whether or not the entire spatial and temporal distribution of pollutant is desired. It is more important, for example, to be able to describe the spatial variations in the wind field over a large area than over a smaller one simply because the variations are expected to be more significant in the former case. Another example is the situation in which the maximum concentration for a given averaging time is to be estimated, rather than the expected mean concentration value. In this case, assumptions or information on wind persistence may be required.

Another major factor which determines the required level of detail in treating the wind field is the extent to which it is necessary to describe the vertical component. As mentioned above, it is often a reasonably good approximation to assume that the mean vertical component of the wind velocity is zero over the averaging time of interest. If this assumption is made, the practical treatment of the wind field is very much simplified; only the horizontal wind need be treated. The horizontal variation of the wind speed and direction is constrained by the physical requirement that air cannot accumulate anywhere, and normally the simplest possible approximation is made, i.e., that the wind speed and direction are independent of horizontal position over the region of interest and depend only on the height above ground. In practice, the dependence of wind direction on height is often ignored as well. The dependence of wind speed on height is usually given by an assumed functional form which may depend on the surface roughness and atmospheric stability. The most common form is a simple power law dependence with different exponents for different stabilities although a logarithmic form may be used near the ground under neutral conditions. Finally, the simplest treatment in the zero vertical component case is to assume that the wind speed and direction are uniform within the mixing layer over the region of interest. This treatment is often adopted in semiempirical models. The wind speed is normally chosen to be that which would be observed at a height equal to the emission height and this value is often estimated using a measured or assumed value at some lower reference height,

usually 10 meters, in combination with an assumed wind profile. This procedure results in a different effective wind speed for each different emission height and potentially each different source as well. Alternatively, a single effective wind speed can be used for all sources regardless of individual differences in emission height.

If the vertical component of the wind cannot be assumed to be zero, the treatment of the entire wind field is complicated again by the requirement that air cannot locally accumulate, except that now there is no constraint on the vertical component. In practice, this requirement provides a relationship between the horizontal and vertical components which is used to calculate the vertical wind speed, given measurements of the horizon components at several locations within the region of interest. Wind fields which satisfy this non-accumulation requirement are often called "mass-consistent" wind fields because the requirement is derived from the concept of the conservation of mass. Any wind field used in a dispersion model should be mass-consistent; otherwise, errors in the estimated concentration will result. Wind fields determined by fluid-flow models are generally designed to satisfy the mass-consistency requirement.

It is relatively easy to satisfy the mass consistency requirement if the vertical wind component may be assumed to be zero. In this case, for example, if the wind speed and direction do not depend on the horizontal position coordinates x and y, the mass consistency requirement is automatically satisfied regardless of the dependence of either speed or direction on height above ground.

An air quality model designed for use in complex situations may either require the wind field to be input and therefore place the burden of determining the proper wind field on the user or require the necessary measurements so that the wind field may be calculated internally. In the latter case, the wind field may be determined prior to or concurrently with the actual dispersion calculations. As indicated above, simplifying assumptions are often incorporated. For example, a model designed for use in flat terrain may be combined with assumptions regarding the flow of air over topographic features to produce a new model which may give results of sufficient validity for the user's purpose. Often such treatments of the vertical component are <u>implicit</u>, being incorporated, for example, in the form of assumptions about the height of the plume centerline above the terrain without an explicit determination of the vertical component

that would result in such behavior. For the purpose of this workbook, such assumptions represent an implicit treatment of the vertical wind speed and should be evaluated as such.

The situations in which treatment of the vertical component is desirable are those in which the region of interest contains significant geographic complexities such as mountains or hills, river valleys, large bodies of water, and so on. In the first two cases, the usual problem is to describe the channeling and vertical displacement effects of the terrain on the general wind flow. Models which are capable of doing this have been developed and are in current use. Near large bodies of water, the problem is to describe the effect of a temperature difference between adjacent surfaces. Although models of this situation have been developed, they are primarily of a research nature and have not been incorporated into a dispersion model.

In applications involving averaging times of a month or more, a climatological approach is often used. The entire range of possible wind directions is divided into several (usually 16 or 36) sectors, and the entire range of possible wind speeds is divided into several (typically six) discrete classes. At the same time, the possible range of atmospheric stabilities is also divided into some number (usually six) of discrete classes. The probability of observing simultaneously the wind direction in a given sector, the wind speed within a given class, and the stability within a given class is determined from local observations for each possible combination of wind direction, wind speed, and stability class. The resulting joint frequency distribution is called a stability wind rose. Each combination of the three elements defines a particular meteorological situation for which dispersion calculations are done, normally using a semiempirical model. The long-term average pollutant distribution is obtained by multiplying the results for each meteorological situation by the probability of observing that particular situation and summing over all possible cases. Thus, more information about the wind field than just the mean wind speed and direction over the averaging time of interest is used, although in each meteorological situation the assumption is commonly made that the wind is uniform and constant. The climatological approach is not necessarily restricted to semiempirical models; in principle, any type of model could be used to do the basic dispersion calculations as long as discrete wind field "classes" could be suitably defined and the probability of observing each determined.

The various treatments of the horizontal wind field are listed in Table 5.5 and the treatments of the vertical wind field are given in Table 5.6. Treatments used by suggested reference models can be found in Tables B.6 and B.7 for horizontal wind field and vertical wind field, respectively.

A.4 HORIZONTAL AND VERTICAL DISPERSION

A.4.1 General

One of the most important elements in assessing the impact of emissions on air quality is the estimation of the extent to which the effluent from sources is dispersed by the atmosphere. In comparing the treatments of dispersion by two different models, the user should keep the following three factors in mind:

- The operational definition of dispersion,
- The duration and size of the emission and the source-receptor distance or travel time, and
- The connection between the extent or rate of dispersion and the level of atmospheric turbulence.

These factors determine the applicability of the various treatments of dispersion and the physical features of the problem which need to be taken into account.

The term "diffusion" is used by some authors in exactly the same sense that the term "dispersion" is used throughout this workbook. The term dispersion is used here to avoid any confusion with the process of molecular diffusion, in which the spread of one substance in another is the result of entirely different phenomena than those responsible for atmospheric dispersion.

The operational definition of dispersion is interrelated with that of advection and depends upon the averaging time of interest. The wind speed and direction at a point are randomly fluctuating quantities; rapid fluctuations are perceived as turbulence and very slow fluctuations as part of the day-to-day variations in the weather. The operational definition of advection is the transport of pollutant by the mean wind as measured over some specified averaging time. The operational definition of dispersion is the transport of pollutant by fluctuations about this mean which occur over times less than the averaging time. In other words, advection is the overall downwind movement of the emission as a whole and dispersion is the spreading of the pollutant about this overall motion.

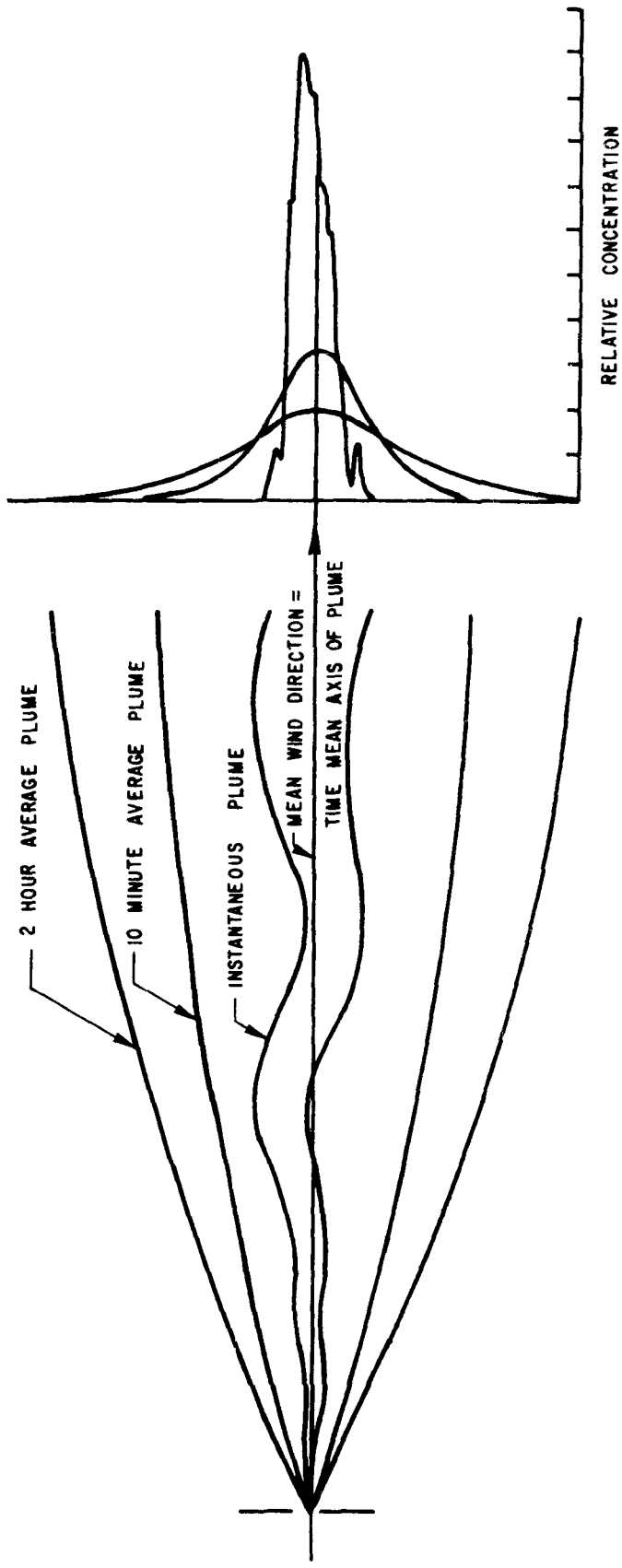


Figure A.1. Dependence of Crosswind Pollutant Distribution from a Continuous Point Source on Averaging Time.

To fix these ideas, consider two photographs of the same continuous plume taken from above: one is a snapshot and the other is a time exposure (Figure A.1). The plume in the snapshot is observed to follow a meandering path called the streakline. The width of the plume at any point is simply the actual physical spread of material about the instantaneous position of the plume centerline. In the time exposure, however, the plume appears to follow a much straighter path and is characterized by a much wider and more smoothly varying cross-section. The longer the exposure, the wider the cross-section appears. The time exposure shows only the mean wind direction over the exposure time, and the observed dispersion about the apparent plume centerline represents not only the physical spread but also the time-average effects of the meandering of the plume. Thus, meanders in the plume which take place over periods of time shorter than the exposure, or averaging, time are considered part of the dispersion. The snapshot clearly exhibits the effects of the short-term wind fluctuations responsible for meandering.

The practical consequence is that for the horizontal case the extent of the dispersion about the mean plume centerline depends on the averaging time. This effect does not occur for vertical dispersion for averaging times longer than about ten minutes due to absence of fluctuations in the vertical component of the wind over these time scales.

The example just given considered the case of a continuous release. A snapshot of the pollutant distribution following an instantaneous release during non-calm conditions shows a cloud of material centered at some point downwind of the source, whereas a time exposure shows a meandering path originating at the source. In both pictures, the observed extent of the dispersion represents the actual crosswind spread of material in the cloud, although dispersion in the downwind direction is not shown in the time exposure. Meandering in the path followed by the cloud should clearly not be treated as part of the dispersion of the cloud.

Based on this type of consideration, and assuming that only the mean wind speed and direction are known over the averaging time of interest, meandering should be considered part of the process of horizontal dispersion from a point source when both the following conditions are met:

- The duration of the release is greater than the averaging time, and
- The averaging time is greater than the source-receptor travel time.

If these conditions are not met, more information about the wind field is required so that a more realistic description of the actual trajectory followed by the pollutant emission may be obtained. In particular, variations in the wind which occur over times greater than the averaging time but less than the travel time should be explicitly taken into account either by assumption or by actual calculation of the trajectory. (See Appendix A.3 for a discussion of treatments of the wind field.)

The initial size of the emission determines the relative importance of any further dispersion in either the horizontal or vertical direction. The larger a plume or cloud of pollutant, the slower is the relative rate of growth due to the action of atmospheric turbulence because as the plume grows an increasingly large part of the turbulence acts over too small a scale to be effective. The effect on the horizontal dispersion estimates of changing the averaging time is also diminished for extended sources such as lines and areas for the same reason.

In order to quantitatively estimate the extent or rate of dispersion under specified conditions, the effect of those factors which determine the intensity of atmospheric turbulence must be suitably parameterized because dispersion is a direct result of the action of turbulence. The most important factors governing the production of turbulence are:

- The wind speed,
- The roughness of the ground surface, and
- The flux of heat being transferred between the ground surface and the air.

The first two factors govern the mechanical generation of turbulence by friction due to the variation of wind speed with height (wind shear), itself caused by the frictional interaction between the general flow of the wind and the roughness of the surface. The third governs the thermal generation of turbulence due to surface heating. The surface heat flux itself depends on:

- The solar angle (during the day),
- The extent of cloud cover (both day and night),

- Thermal properties of the ground surface, and
- The extent of anthropogenic heat generation (in urban areas).

In discussing atmospheric turbulence and dispersion, it is convenient to introduce the concept of atmospheric stability. At a given height, the atmosphere may be classified as unstable, neutral, or stable according to whether the rate of decrease of temperature with height (the lapse rate) is less than, equal to, or greater than a critical value called the dry adiabatic lapse rate (equal to approximately 1°C/100 meters), as shown in Table A.2. The significance of this classification is that near the ground, high levels of turbulence and high rates of dispersion are generally associated with unstable conditions and low levels of turbulence with stable conditions. The terms used in the classification are in fact descriptive of the effects of the different types of temperature gradient on vertical turbulent motions, vertical motion being enhanced under unstable conditions and suppressed under stable conditions. A temperature inversion is said to exist when the lapse rate is negative (temperature increasing with height). The atmosphere is extremely stable within an inversion and turbulence is strongly suppressed. As a consequence both the rate of vertical dispersion and the actual physical spread of a plume in the horizontal direction are strongly suppressed, although considerable meandering of the plume can occur.

Table A.2. General Atmospheric Stability Classification According to Temperature Lapse Rate[a]

Relation of Actual Lapse Rate to the Dry Adiabatic Lapse Rate	Atmospheric Stability Classification
Greater than	Unstable
Equal to	Neutral
Less than	Stable

[a]This classification is not the same as the widely used Pasquill stability classification scheme.

The temperature profile near the ground is itself determined by the same factors listed above as being significant determinants of atmospheric turbulence. At any given time, the difference between the actual lapse rate and the dry adiabatic lapse rate is determined by the balance between two

competing effects: 1) the addition to or removal from the air of heat energy due to solar heating or radiational cooling of the ground surface, tending to produce unstable or stable conditions respectively, and 2) the tendency of the turbulence itself, whether mechanically or thermally generated, to smooth out the temperature profile and produce neutral conditions.

In order for an atmospheric dispersion model to be useful in a variety of meteorological situations, some convenient measure of atmospheric stability or turbulence intensity is used to determine the appropriate values of those model parameters (such as σ_y and σ_z in Gaussian plume models) which determine the predicted extent or rate of dispersion. A number of different meteorological parameters or classification schemes have been used for this purpose and an increasing number of models make use of the more fundamental measures of turbulence intensity. Some of the more commonly used ones are given in Table A.3. The user should consult a standard reference (e.g., Slade, 1968) or an air pollution meteorologist for the definitions of the Richardson number or the Monin-Obukhov length if the model being evaluated makes use of one of these parameters. A discussion of the Pasquill-Gifford classification scheme is given by Turner (1969) and the Brookhaven scheme is discussed by Singer and Smith (1966). A review of various systems for characterizing turbulence is given by Gifford (1976).

The basic factors which determine atmospheric stability near the ground have already been mentioned. The dependence of these factors on the time of day, the nature of the topography, and the nature of the ground surface gives rise to certain characteristics of which the user should be aware.

Atmospheric stability near the ground undergoes very significant diurnal variations due to the rising and setting of the sun. On sunny days, the ground is warmed and heat is added to the air near the surface, causing the air temperature to rise and producing unstable conditions. On clear nights, the ground cools more rapidly than the air, heat is removed from the air near the ground, and a ground-based "radiation inversion" is produced. At any time, cloud cover tends to balance the exchange of heat and produce neutral conditions.

There are important differences between urban and rural areas. Urban areas are normally much rougher than the surrounding rural areas, and the heat produced by anthropogenic activity in the city is an important factor at night all year round as well as during the daytime in winter. The combination of these factors results in substantially higher levels of turbulence, and

Table A.3. Commonly Used Measures of Atmospheric Stability and Turbulence Intensity

Continuous Measures

1. **Temperature gradient or, equivalently, temperature difference between two reference heights.**
2. $S = \frac{g}{T} \frac{\partial \theta}{\partial z}$

   $\frac{\partial \theta}{\partial z}$ = (dry adiabatic lapse rate)-(ambient lapse rate)

   $= (1°C/100m + \partial T/\partial z)$

   g = acceleration due to gravity.

   T = ambient temperature.

   (S is negative in unstable conditions, zero in neutral conditions and positive in stable conditions.)
3. Standard deviation of the horizontal component of the wind direction (σ_θ) or of the vertical component (σ_ϕ).
4. Richardson number.
5. Monin-Obukhov length.

Discrete Classification Schemes

1. **Pasquill-Gifford stability classification.**
2. **Brookhaven gustiness classification.**

correspondingly higher rates of dispersion, over cities during both day and night. The frequency of surface inversions is much lower in cities than in rural areas; when a surface inversion exists in the surrounding countryside, the temperature profile within an urban area generally corresponds to neutral or weakly stable conditions.

Topography may significantly affect stability. The nocturnal inversion within a valley, for example, may be much deeper and longer lasting in the morning than that over flat terrain. This is caused by a combination of uneven heating of the ground surface due to the variable angle with which the sun's rays strike the ground and the tendency of cooler air to settle in low places in the terrain. The presence of fog also delays the heating of the ground and prolongs the existence of stable conditions. Forested areas and regions of complex terrain also have surface roughness comparable to those

of urban areas, and rates of dispersion are correspondingly higher than over gently rolling grassland, for example.

The stability of the atmosphere at higher elevations is also an important factor for atmospheric dispersion. At any given time the stability of the atmosphere at heights above a few hundred meters is determined mainly by the large scale features of the weather as well as by the general properties of the atmosphere as a whole. Below 10-15 km, the atmosphere is on the average slightly stable, so that turbulence generated at the surface can propagate upwards only so far before it is damped out. This results in an upper limit, called the mixing height, to the altitude to which pollutants will disperse over a short period of time. In the absence of an elevated inversion, this mixing height is determined by the same variables that determine the stability. An elevated inversion may exist, however, usually in association with a large high pressure area. Such inversions are called subsidence inversions and are very effective in limiting vertical dispersion. Subsidence inversions exist at altitudes of the order of 1000 m and the maximum mixing height on any given day is limited by the height of the base of these inversions. Since relatively low wind speeds are also associated with these large high pressure areas, they cause some of the worst pollution episodes.

An additional factor, relating primarily to vertical dispersion, is the fact that the earth's surface forms a barrier which limits not only the extent of mixing in the vertical direction but also the physical size of the turbulent fluctuations which cause the dispersion. The first effect is normally handled as a boundary condition, but the second implies that the higher the altitude above ground, the greater the size of fluctuation that can exist. In addition, the relative importance of mechanically generated turbulence compared to thermally generated turbulence decreases with altitude. Thus, the rate of vertical dispersion from elevated sources is somewhat different from that ground level sources, at least until the emission from the elevated source reaches the ground.

Since horizontal and vertical dispersion are considered to be separate elements in this workbook, and in order to tie the previous discussions together, it is useful to summarize here those factors which relate specifically to either horizontal or vertical dispersion, or both. These summaries are given in Tables A.4 and A.5.

Table A.4 Factors Affecting the Level of Atmospheric Turbulence and the Rates of Horizontal and Vertical Dispersion

- Wind shear, itself dependent on
  - Wind speed, and
  - Surface roughness
- Surface heat flux, itself dependent on
  - Solar angle,
  - Cloud cover,
  - Surface thermal properties, and
  - Anthropogenic heat production.
  - Orography (ground slope relative to solar angle)
- Atmospheric stability, itself dependent on
  - The factors listed above, and
  - Synoptic weather features (particularly above a few hundred meters altitude)

Table A.5. Factors Determining Meandering Contribution to Horizontal Dispersion

- Duration of pollutant release
- Source-receptor travel time
- Desired averaging time for pollutant concentrations
- Initial size of the emission
- Orographic barriers
- Street canyons

A.4.2 Treatment of Horizontal and Vertical Dispersion

In order to evaluate the treatments of horizontal and vertical dispersion in a specific model, the user should know:

- The technical benefits and limitations of the different types of treatments and
- The various ways of parameterizing the effects of the important meteorological variables in each type.

The remainder of this section addresses these points.

A.4.2.1 Treatment Classification

Treatments of dispersion may be usefully classified in the following two ways:

1) According to the general modeling approach adopted:

   - Numerical methods, which involve the numerical solution of equations describing the conservation of mass,
   - Semiempirical methods, which assume a particular functional form for the pollutant distribution, and
   - Methods which do not treat dispersion explicitly; and

2) According to the way the time dependence of the pollutant distribution is treated:

   - Dynamic treatments, which predict the pollutant concentration as a function of time as well as position,
   - Steady state treatments, which predict the average pollutant concentration as a function of position only for short averaging times, and
   - Climatological treatments, which predict the average pollutant concentration as a function of position only for long averaging times using a statistical distribution of meteorological conditions.

Methods which do not explicitly treat horizontal dispersion, vertical dispersion, or both may still in some cases be simulation models and examples will be discussed below. Empirical or statistical models, which also do not generally contain explicit treatments of dispersion, are discussed in Section 7.

Numerical Methods

The most advanced and sophisticated models of atmospheric dispersion fall into this category. The current state of the art is represented by "closure models" which consider both the concentration and the flux of pollutant as well as most of the meteorological variables as unknown functions of position and time to be determined by numerical solution of the relevant equations. The flux obtained in this approach is directly related to the rate of dispersion. This type of treatment is still in its formulative stage and has not yet been used in practical applications. For this reason, closure models will not be discussed further here.

The usual approach in numerical models is to describe the flux in terms of the concentration distribution, so that the flux is no longer an independent quantity. This is done by making the "gradient-transfer" approximation, which assumes that the pollutant flux is proportional to the concentration gradient. The proportionality factor is called the eddy diffusivity and is usually symbolized by the letter K, hence this approach is often referred to as "K-theory." The result of making this approximation is an equation, called the advection-diffusion equation, which predicts the pollutant concentration as a function of position and time. Treatments of the wind field are discussed in Section A.3. The advection-diffusion equation must usually be solved by any of a variety of numerical methods, including, for example, finite-difference or particle-in-cell techniques, but the user should not be too concerned with the details of the numerical method used by a model being evaluated. There are certainly advantages and disadvantages with the various approaches, but the focus here is more on the parameterization and treatment of meteorological and other factors.

The eddy diffusivities for dispersion in different directions are not necessarily equal, but this discussion will be restricted to what is by far the most common case, that in which only two eddy diffusivities are used, one for vertical dispersion and one for horizontal dispersion. The eddy diffusivity values reflect the level of atmospheric turbulence and their parameterization in terms of observable meteorological quantities should be considered by the user in evaluating a numerical model.

Semiempirical Methods

This category includes all treatments in which an explicit functional form is assumed for the concentration distribution. The assumed form may be based on observation, theoretical considerations, numerical simulation, or a combination of these. It may be a function determined elsewhere and assumed appropriate for the given application or it may be determined specifically for the application of interest in the process of running the model itself.

The most common example of a semiempirical method is the Gaussian plume treatment of dispersion from a continuous source as described by Turner (1969). This particular approach involves the assumption that the horizontal crosswind pollutant distribution from such a source may be

described, on average, by a Gaussian function and that, except for the effects of the ground, so can the vertical distribution. The only parameters beside the wind speed which appear explicitly in these functions and which reflect the prevailing meteorological conditions are the horizontal and vertical standard deviations, or dispersion coefficients, corresponding to the assumed horizontal and vertical Gaussian distributions.

Another example of a semiempirical model is the simple box model, which assumes a spatially uniform pollutant distribution within some region. Dispersion is not explicitly treated in such a model, but additional assumptions are implicitly being made. If the pollutant distribution is taken to be uniform in the vertical direction up to some specified height, the process of vertical dispersion is implicitly being assumed fast enough to justify that treatment over the time scale of the problem. The assumption of uniformity in the horizontal crosswind direction is often used and is justified if the distribution of emissions is relatively uniform; this approximation, when used in conjunction with the determination of pollutant levels due to area source emissions, is called the narrow-plume approximation. A type of narrow-plume approximation may also be used for treating point sources in climatological models and will be discussed in that context later in this section.

Dynamic Treatments

This category includes all methods in which the concentration is predicted explicitly as a function of time. Treatments in which one or more trajectories of pollutant releases are calculated from wind field data, or are simply assumed on any reasonable basis, are also included under the definition of dynamic models followed in this workbook. Dynamic treatments may be either numerical or semiempirical in nature.

Dynamic models must be able to properly handle situations involving changing meteorological conditions and the resulting changes in the rate of dispersion. There is usually no difficulty in doing this in numerical models, but if a time-dependent generalization of a semiempirical steady-state method is used, problems can arise in making sure that the model parameters which describe the extent of dispersion at any given time are continuous functions of time. For example, if the horizontal crosswind pollutant distribution

about some trajectory is assumed to be Gaussian, the horizontal standard deviation should be a continuous function of time. Most commonly used formulae or graphs give the standard deviation as a function of downwind distance or travel time only for the case in which the meteorological conditions are constant, and are not directly applicable under changing conditions. A treatment which uses a description of the rate of change of the standard deviation as a function of meteorological conditions is usually preferable for dynamic models.

Examples of numerical/dynamic treatments are 1) those using the numerical solution to the full time-dependent three-dimensional advection-diffusion equation and 2) those using the narrow-plume approximation for a grid of area sources over which a trajectory is calculated and treating vertical dispersion by numerically solving the one-dimensional (vertical) time-dependent diffusion equation. An example of a semiempirical/dynamic treatment would be one in which a trajectory originating at the location of a point source is calculated and the pollutant distribution about the trajectory is assumed to be Gaussian. Gaussian puff models, in which a plume is treated as a series of puffs which follow their own trajectories, are also semiempirical/dynamic models.

Steady-State Treatments

This category includes all methods in which temporal variations of all relevant quantities are ignored and in which the treatment of advection uses only the mean wind speed and direction for the averaging time of interest. This type of treatment predicts the average concentration as a function of position only. Steady-state methods may be either numerical or semiempirical in nature. The most familiar example of a semiempirical/steady-state treatment is the basic Gaussian plume model and an example of a numerical/steady-state treatment is one in which the time-independent version of the advection-diffusion equation is solved numerically.

Climatological Treatments

This category includes methods which predict the average pollutant distribution for long averaging times, typically a month, season, or year, using a joint frequency distribution which gives the probability of simultaneously observing specified wind speed, wind direction, and other meteorological

variables. In this approach, more information about the wind field than just the mean wind speed and direction over the desired averaging time is used in order to avoid treating variations which occur over time scales less than the averaging time as part of the horizontal dispersion process. Climatological models may in principle use either a numerical or semiempirical approach for the individual calculations, although in practice semiempirical/steady-state treatments are almost always used.

A.4.2.2 Benefits and Limitations

Numerical Methods

The main benefit to be gained by using a numerical approach is flexibility in the specification of the wind field and the meteorological variables determining atmospheric turbulence levels as functions of position and time and in the specification of boundary conditions. In principle, numerical methods allow the description of dispersion for a realistic wind field in complex situations. They are also, in principle, capable of treating the spatial distribution and temporal behavior of chemically reactive pollutants.

The main technical limitation is one of spatial resolution. Numerical methods calculate concentration values at only a finite number of points in space, normally corresponding to some conveniently defined grid, and the resolution which can be achieved is fixed by the grid spacing. In addition, the grid spacing should not be considered arbitrary, since it may be determined to a large extent by the way the wind field is determined (see Appendix A.3). Variations in the concentration distribution, in the wind speed and direction, and in the emissions themselves which occur over distances smaller than the grid spacing cannot be resolved. This lack of resolution has several consequences:

- Emissions from point or line sources into a specific grid cell are in effect dispersed instantaneously within the cell, rather than described in terms of a sub-grid scale distribution;

- The value of the eddy diffusivity must reflect the intensity of turbulent fluctuations up to the size of the grid spacing and is therefore partially determined by that spacing; and

- Pollutant concentrations cannot be predicted at arbitrary receptor locations, except by interpolation from concentration values at grid points.

The seriousness of these consequences depends on the specific application, and on the existance of practical limits to the amount of computational effort required and to the computer storage requirements. In general, however, the numerical approach is inappropriate for the treatment of dispersion when the size of the emission being dispersed is smaller than the grid spacing.

Another way of stating this conclusion is that the numerical approach using the eddy diffusivity concept is inappropriate when the size of the pollutant distribution being dispersed is smaller than or comparable to the size of any turbulent eddies contributing significantly to the dispersion. As a result, the eddy diffusivity approach is not fundamentally suitable for describing horizontal dispersion, and in particular the meandering contribution, but because of constraints on the size of vertical fluctuations due to the presence of boundaries at the ground and at the mixing height, can be justified for the treatment of vertical dispersion from ground level sources or from elevated sources after the plume has reached the ground. Treatments of horizontal dispersion using the eddy diffusivity approach do exist, however, in spite of the physical fact that dispersion by meandering cannot be considered a gradient-transfer process. Such treatments describe horizontal dispersion in a phenomenological way, rather than in a manner which reflects the basic physical processes, and the selection of an appropriate value for the horizontal eddy diffusivity must be based on more empirical grounds than is the case for the vertical diffusivity. (See the discussion of parameterization in numerical models later in this appendix.)

It is sometimes possible to describe the pollutant distribution on a scale smaller than the grid spacing in an empirical or theoretical way, and use the numerical approach to describe the large scale distribution. This is in fact desirable in the case of point sources in order to minimize the numerical errors resulting from the poor resolution near the source.

Another limitation in most cases is the lack of fundamental knowledge and appropriate meteorological data upon which to base the prediction of eddy diffusivity values, particularly at heights above 100 meters or so. This means that further assumptions must be made regarding the appropriate values to use in a model.

Semiempirical Methods

The principal technical benefit gained in this type of approach is that the assumed shape of the pollutant distribution may be based upon actual observational data. Furthermore, the distribution observed experimentally may be assumed to be the same under similar meteorological and topographical conditions, thus eliminating the need for new observations for each new application. In some cases, the assumed distribution may be derived on the basis of theoretical considerations.

The semiempirical approach has two advantages over the numerical approach from a technical point of view:

- Better spatial resolution can often be achieved in practice and
- The effect of meandering may be treated in a more appropriate way.

The general limitation on this type of approach is that it should not be used in situations in which there is insufficient observational data or theoretical results from which to determine the proper functional form. If the assumed shape is derived theoretically, its suitability depends on the nature of the assumptions made in the derivation. These may not be appropriate for the real situation.

As indicated above, the most common example of this type of approach is the Gaussian plume treatment of continuous emissions. In their basic form, Gaussian-plume based methods are inherently restricted to:

- Flat or gently rolling terrain for a considerable distance upwind and downwind of the source,
- Primary pollutants, and
- Conservative pollutants, i.e., no significant physical or chemical sinks.

It is possible to extend the utility of Gaussian models to applications involving complex terrain by making various assumptions regarding the extent to which the plume follows the terrain and by making modifications to the basic formulae. These models all fall within the category of semiempirical models and in view of the wide range of possible modifications and interpretations expert advice may be required in making a comparison. The only general guideline that can be given is that the basis or justification for the assumed

pollutant distribution should be scientifically sound. Ideally, modifications to the basic Gaussian distribution should be based on appropriate observational data, often in combination with theoretical considerations. If no information is available regarding the basis for any particular assumed pollutant distribution, it is impossible to accurately assess its validity except through an appropriate field measurement program.

It should be point out that, given certain approximations, the standard Gaussian plume formula represents the steady-state solution to the advection-diffusion equation for a single point source. The conditions which have to be met are that 1) the wind field must be uniform, constant, and have no vertical component, 2) the rate of pollutant dispersion along the direction of the wind must be negligible compared to the rate of pollutant transport by advection, and 3) the horizontal and vertical eddy diffusivities must also be uniform and constant. The extent to which the application of interest deviates from these assumptions determines the need for modifications to the formula or for a different modeling approach, e.g., a numerical model.

It is also possible to extend the basic Gaussian model to non-conservative pollutants. (See Appendices A.5 and A.6 for discussions of possible treatments.)

Limitations to the basic Gaussian plume model also exist because of the steady-state nature of the model. These are discussed in the subsection on dynamic treatments.

The narrow plume approximation mentioned earlier deserves further comment at this point. This approximation can be used for either point or area sources, although its use for point sources is restricted to climatological models except for the short-term mode of the Valley Model. For area sources, the narrow plume approximation amounts to the assumption that emission rates from nearby sources are sufficiently similar that the pollutant distribution may be assumed to be horizontally uniform. In the narrow plume approximation, pollutant concentrations along some well-defined trajectory are functions of height above ground and possibly travel time but not of horizontal crosswind position. The narrow plume approximation may be used in either a steady-state or a dynamic approach and the trajectory may be a straight line, a constant path determined, for example, by topography, or it may be determined from actual wind field data. The accompanying treatment of vertical dispersion may be either semiempirical or numerical.

Dynamic Treatments

The main benefits are:

- The ability to describe the temporal variation of the pollutant concentration and
- The ability to treat the effects of time variations in and correlations between emissions, meteorological parameters, and removal processes.

Technical limitations depend upon how the time dependence is handled. Time dependence may be incorporated in an empirical or ad hoc way, in which case the suitability of the treatment in a given application depends on the observational or theoretical basis for that particular treatment, as with the empirical methods discussed above.

Time dependence is more commonly treated by dividing the total period of interest into a number of sequential time steps. The variation of some quantity such as an emission rate is then simulated by prescribing a sequence of values, one for each time step. Such an approach predicts the concentration at a finite number of points in time and the temporal resolution of the method is determined by the size of the time step. Time variations more rapid than the time step cannot be resolved.

Steady State Treatments

No significant technical benefits are gained by using a steady-state model in preference to a dynamic approach. Steady-state models are generally simpler and easier to use, however, and the decision to use such an approach is based on these considerations as well as on the fact that the most widely used semiempirical approach, the Gaussian plume method, is a steady-state method.

Limitations include the assumptions of a constant emission rate and a constant level of atmospheric turbulence. The specified averaging time should be greater than the source-receptor travel time, as pointed out in the general discussion, so that the effect of meandering is properly treated. The assumption of constant emission rate guarantees that the duration of the release is longer than the averaging time, and the steady-state approach is clearly limited to the treatment of those sources which satisfy this requirement. Instantaneous or very short releases must be treated using dynamic

methods. Within its limitations, the steady-state approach is just as applicable as the dynamic approach for the calculation of average concentration values.

Climatological Treatments

This type of approach is used in practice only for the calculation of long-term average concentrations, the principal benefit being one of convenience compared with the alternatives of using a dynamic model or a sequence of a large number of steady-state calculations.

A calculation is done for each set of meteorological conditions which is represented in the joint distribution being used, and the average pollutant distribution is obtained with the contribution from each set of conditions being weighted by its probability of occurrance.

Limitations of the method may be divided into two categories:

- Limitations of the model used to do each separate calculation, and
- Limitations of the climatological approach, per se.

The former are described in other parts of this section and the only additional remark that needs to be made here is that the model used must be of sufficiently general applicability to be able to handle the variety of meteorological conditions represented in the climatological frequency distribution. The latter include the approximations incurred by representing the wide range of conditions that occurs in nature by a finite number of specific situations, by the suitability of those situations which are used, and by the omission of meteorological variables such as precipitation and mixing height from the joint frequency function.

In the treatment of dispersion, at least one of the parameters defining the frequency function should be a measure of the level of atmospheric turbulence. The measure of turbulence most commonly used in climatological models is the Pasquill stability classification, although others could be used. It is also common to use the narrow plume approximation for point sources. This approximation requires an assumption that the crosswind or angular distribution of pollutant from a point source over a sufficiently long period of time is given simply by the frequency distribution of the wind direction. This

assumption is reasonable if the variation in the wind direction frequency function is negligible over an angular interval corresponding to the angular width of the plume. Since the wind direction frequency function takes the form of probabilities of observing wind from within well defined sectors (commonly 10° or 22.5° wide), this approach is also referred to as "sector averaging."

A summary of the different general types of treatment is given in Table 5.7. It should be pointed out that in any given model, horizontal and vertical dispersion may be treated in completely different ways (although both will be either dynamic or steady-state) and the treatments in any case should be evaluated separately. In Table 5.7, the treatments are ranked in order of decreasing level of detail, but the user is cautioned that in the cases of horizontal and vertical dispersion the relative level of detail of two treatments is not by itself a reliable indication of their relative technical performance. As discussed above, there are limitations on the applicability of certain approaches, and the user must determine for his specific application if these are violated. If they are, those approaches should not be used. If the two models being compared use the same, or two equally applicable approaches, the relative level of detail may be used as a valid indicator.

A.4.2.3 Parameterization

Atmospheric dispersion models are generally designed for use in a variety of conditions, each characterized by a different level of atmospheric turbulence and consequently different rates of dispersion. Various meteorological conditions are handled within a given model by using different numerical values for the relevant model parameters such as eddy diffusivities or Gaussian standard deviations. The determination of the appropriate values from meteorological and other data is an important part of the total procedure by which predictions of pollutant concentrations are made. In an evaluation, the user should take into account any constraints on these parameters that are inherent in or built into the model, particularly if they clearly preclude the use of the correct values. An example of such a constraint is a built-in eddy diffusivity or standard deviation value which is not appropriate for the user's application and which the user cannot conveniently modify. The determination

of the appropriateness or correctness of any such specific parameter value may require expert assistance but a general guideline is that the value in question should be obtained from observations or theoretical analysis as closely associated as practicable with the specific location and meteorological conditions of interest. If sufficient information about the source of the values used in a given model is available, the appropriateness of those specific parameter values should be considered in making the evaluation. Table 5.10 provides a list of some of the possibilities for both numerical and semiempirical models.

Some general remarks regarding the way in which atmospheric stability and surface roughness are treated by various types of models are in order here.

Numerical Models

Confining our attention to gradient-transfer models only, the horizontal and vertical eddy diffusivities are the parameters through which the influences of stability and surface roughness on dispersion are manifested.

As indicated above, the eddy diffusivity approach is not in general appropriate for the treatment of horizontal dispersion. For this reason, the basis for choosing a specific value of the horizontal diffusivity needs to be considered further. It is possible, by appropriate selection of the time or space dependence of the horizontal diffusivity, to force a numerical model to reproduce approximately the results of a more sophisticated calculation, or of a semiempirical model. If this is the case, the parameterization of the horizontal diffusivity needs to be judged on the basis of the treatment being reproduced.

In general, the horizontal diffusivity may be expected to be roughly independent of horizontal position except when significant terrain features are present.

The vertical diffusivity near the ground may be reasonably estimated in terms of the wind speed, surface roughness (given in terms of a parameter called the "roughness length", see Slade (1968) or Pasquill (1974) for the definition and estimates for different situations), and parameters which determine the rate of heat-exchange between the earth's surface and the air. An expert should be consulted for the details of the formulation.

At higher altitudes, there is very limited data and the exact parameterization of the vertical diffusivity is a subject of current research. Consequently, any parameterization must be based on further assumptions and it is not uncommon to simply use a convenient functional form having the desired qualitative behavior and having the correct behavior near the ground.

Semiempirical Models

Since the Gaussian plume model is by far the most common example, the discussion will be restricted to this case. The user should be able to follow a similar line of thought for other treatments. In the Gaussian plume approach as described by Turner (1969), the horizontal and vertical standard deviations need to be parameterized. Atmospheric stability is divided into several discrete classes and the stability class to be used in a given situation is determined from the wind speed, solar angle, and the extent of cloud cover. The horizontal and vertical standard deviations are then prescribed functions of the stability class and downwind distance from the source. The effects of surface roughness may be accounted for in the nature of the prescribed functions or by additional modification of the basic standard deviation or may not be treated explicitly.

Tables 5.8 and 5.9 list various treatments of atmospheric stability and surface roughness, respectively. Tables B.8 and B.9 list treatments of horizontal and vertical dispersion, respectively, used by suggested reference models.

A.5 CHEMISTRY AND REACTION MECHANISM

A.5.1 General

There are two common situations in which chemistry plays a role in determining atmospheric pollution levels. On one hand, the pollutant of interest may undergo chemical reaction with some other atmospheric component; that is, a chemical sink exists for that pollutant and it is referred to as being reactive. (If the pollutant undergoes no reaction, it is called inert.) On the other hand, the pollutant of interest may be produced in the atmosphere by chemical reactions involving other pollutants (precursors); such a substance is called a secondary pollutant. (If the pollutant is directly emitted by

sources, it is called primary.) Clearly, in each case the chemical reactions involved affect the concentration of the pollutant of interest. In the first case they provide a process for the removal of that pollutant and serve to decrease its ambient concentration, while in the second case they serve to generate the pollutant and increase its concentration. Examples of primary reactive pollutants are the hydrocarbon precursors of photochemical smog. Examples of secondary, relatively inert materials are sulfate and photochemical aerosol. A pollutant may be both secondary and reactive; examples are nitrogen dioxide (NO_2) and ozone (O_3). If the pollutant of interest is both primary and inert, the element of atmospheric chemistry is irrelevant and does not need to be considered.

As pointed out in Section 3.3, the decision to regard a pollutant as being either reactive or inert depends upon the effective rate of reaction compared to the length of time that the pollutant spends within the region of interest. If the user is interested in a short-range application involving a slowly reacting material, that pollutant may be regarded as effectively inert for the application even though over a longer range this would be a poor approximation. An example of such a pollutant is sulfur dioxide (SO_2).

In the case of a secondary pollutant, some treatment of the chemical reactions which produce that pollutant will be required. Otherwise, the connection between precursor emissions and the concentration of the pollutant of interest is completely lost.

The subject of atmospheric chemistry encompasses an extremely wide range of topics and only those very basic or general aspects that are directly relevant can be described in this workbook. If atmospheric reactions play a significant role in the user's application, the advice of an expert should be sought regarding the level of detail with which the particular set of chemical reactions used by the model represents the system to be simulated.

This discussion will refer primarily to reactions between gaseous materials. The extent to which atmospheric particulate matter actually participates in chemical reactions with gaseous components is not at present well understood but if this possibility exists, the advice of an expert should again be sought. However, many of the same considerations apply as in the completely gaseous case.

The basic problem in modeling the dispersion of reactive systems is to describe the rates of production and removal of various pollutants. Equally as important is the interaction between the chemical reaction processes and the dispersion process. In order to assess the treatment of chemical reactions by a model, the user must consider two different aspects of that treatment:

- The level of detail with which the chemical reaction mechanism is described, and
- The manner in which the effects of spatial inhomogeneity on the average rates of change of the pollutant concentrations are treated.

It will be useful for the user to understand a few basic facts regarding the general nature of chemical reaction rates. The rate of a chemical reaction may be defined with sufficient precision for the purpose of this workbook as the magnitude of the time rate of change of the concentration of a reactant or product of the reaction in question. (The reactants are the chemical species actually undergoing reaction.) The reaction rate depends on the concentrations of all of the atmospheric components participating in the reaction.

Reactions can be classified as either elementary or complex. An "elementary reaction" is one in which the chemical reaction as written reflects the true sequence of events on the molecular level. For example, an important reaction in photochemical smog is that between ozone and nitric oxide (NO). This reaction involves the collision of a molecule of NO with a molecule of O_3, followed by a reaction and the separation of the products, one molecule each of NO_2 and oxygen (O_2). The most important property of elementary reactions is that the rate of such a reaction is a predictable, simple function of the reactant concentrations. In the example above, the rate of the reaction is simply equal to a constant (the rate constant) times the product of the ozone and nitric oxide concentrations. On the other hand, a "complex reaction" is essentially a statement of the net effect of some (possibly large) number of elementary reactions operating simultaneously, with only the initial reactants and final products being explicitly written. In general, the rate at which the initial reactants disappear is not equal to the rate at which the final products appear. Neither rate is a predictable function of the concentrations of only the initial and final chemical species. The sequence of elementary reactions whose net

effect is of interest forms what is called the "reaction mechanism" and the description of the pollutant concentrations as functions of time must usually be made in terms of what is known about the reaction mechanism. It should be pointed out that, in addition to the main reactants and products of interest, the mechanism of a complex reaction usually involves the existence of other chemical species that should also be treated.

An extreme example of a complex reaction is the generation of photochemical smog from nitric oxide and hydrocarbons under the action of sunlight. In this case the reaction mechanism involves literally hundreds or even thousands of reactions.

As mentioned above, the expression for the rate of an elementary reaction can be predicted in an a priori way. In practice only three cases need to be considered; these three cases are outlined in Table A.6, in which the "order" of each type of reaction is also defined. The constant appearing in the rate expression for a given reaction is called the rate constant for that reaction.

The most important feature in Table A.6 of which the user should be aware is that the rate of a first-order reaction is a <u>linear</u> function of the pollutant concentration. The rates of second and third-order reactions are <u>nonlinear</u> functions of the pollutant concentrations. This fact has significant consequences when the spatial distribution of reactive pollutants is of interest.

Table A.6. Elementary Reaction Rate Expressions

Rate Expression	Reaction Order
(constant) x (the concentration of one single reactant)	First
(constant) x (the product of the concentrations of two reactants)	Second
(constant) x (the product of the concentrations of three reactants)	Third

In order to describe the evolution of a complex reacting system, it is normally necessary to know the reaction mechanism. This mechanism consists of a set of (elementary) reactions whose rates are known functions of the pollutant concentrations. If the initial pollutants are uniformly mixed within some closed volume, their concentrations as functions of time may be predicted by numerical solution of a set of coupled ordinary, non-linear differential equations derived from the reaction mechanism. In practice, a simplified mechanism may be used in which many of the reactions of lesser importance have been omitted. Also the net effect of many reactions may have been expressed in terms of a few characteristic reactions using some kind of average or composite rate constant. The level of detail with which the reaction mechanism is treated affects the accuracy of the results and the mechanism being used should be justified by comparison with experimental studies.

Knowledge of the reaction mechanism includes not only knowledge of the reactions which can occur but also knowledge of the values of the rate constants of these reactions. The appropriate values are normally supplied with the model so that the user generally does not need to supply them. However, there is often considerable uncertainty in the experimental measurement of rate constants and the values of constants important in atmospheric chemistry are continually being redetermined. Obviously, in a practical application the values used should be as up-to-date as possible. In addition, rate constants depend on temperature. In some cases it may be important to use values appropriate for the ambient temperature in the user's specific application.

Further complications arise when dispersion is considered. It is important to emphasize at this point that chemical reactions are <u>local</u> phenomena in the sense that the rate of an elementary reaction at some point in space depends upon the reactant concentration(s) <u>at that point</u>. Thus, the rate of a given reaction is in general a function of position and time, reflecting the spatial and temporal variation in reactant concentrations. For most reactions of interest, the rate expression is a nonlinear function of pollutant concentrations, because most reactions of interest happen to be second-order. This implies that in most cases of interest the <u>average</u> rate of a given reaction within some finite volume of interest <u>cannot</u> be obtained from the rate expression simply by inserting the <u>average</u> reactant concentrations, unless all reactants are uniformly mixed within this volume. In this case, there is no spatial variation in the

reactant concentrations and hence no spatial dependence of the reaction rate. The only other situation in which the average reaction rate is given by the rate expression using the average pollutant concentration is that of a first-order reaction. In most cases of interest spatial inhomogeneity in the reactant concentrations causes the chemical and dispersion processes to be coupled in a very complicated way.

The nature of turbulent dispersion and the small size of most real emission sources guarantee that in applications of practical interest there are significant variations in the concentrations of reactive pollutants over distances much smaller than the spatial resolution of most current models. The degree of inhomogeneity depends on the level of atmospheric turbulence and on the spatial distribution of the sources. In principle, the effect on the average reaction rate of this inevitable inhomogeneity at distance scales below the resolution of the model should be taken into account. In practice, however, this has proved to be a difficult problem and is still fundamentally unsolved.

A.5.2 Treatment of Chemistry and Reaction Mechanism

It is convenient to divide the discussion of treatments into two separate parts, the first dealing with the special case in which all relevant reactions are first-order reactions, the second with the more general situation.

As pointed out in the general discussion, most chemical reactions of importance in air pollution are second-order reactions. This being the case, it may seem unrealistic to consider an application in which all the reactions of interest are first-order. There are two situations, however, in which only first-order reactions need be considered. The first involves the treatment of radioactive rather than chemical transformations; radioactive decay is rigorously a first-order process. The second arises as a result of approximating the disappearance of one pollutant and the appearance of its reaction products as a first-order process with some empirically derived effective rate constant.

A first-order process has the property that the rate of that process is a linear function of the concentration of the reactant involved. As a result, it turns out that the effect of one or more first-order processes on

the reactant and product concentrations may be determined independently from the effect of dispersion; in other words, first-order transformation processes and the dispersion process are completely separable and any of the many treatments of dispersion may be used. Furthermore, in cases where more than one source is involved, the contribution from each may be evaluated and the total predicted concentration obtained by simply adding the individual source contributions.

The simplest case arises with a primary pollutant subject to some first-order removal process. In this case, the effect of the process is simply to cause the pollutant concentrations to decay exponentially with a half-life which may be easily determined from the rate constant for the process. Many dispersion models now in use have the capability of simulating this situation.

More often, however, the user's application involves a system of chemical reactions, most of which are second-order; the most common example is photochemical smog. In general, a numerical/dynamic model is required, since the chemical mix evolves in time in a nonlinear way. The observational basis for a semiempirical approach is not usually available, although statistical models have been developed for some limited applications.

Two aspects of the treatment by a given model should in principle be evaluated:

- The level of detail used in the reaction mechanism, and
- The treatment of the effect of inhomogeneous mixing on average reaction rates.

With regard to the treatment of reaction mechanism, little can be said in general, because so much depends on the specific details of the chemistry. The simplest case is that in which either the disappearance of a particular pollutant, or the appearance of its reaction products, or both are of interest. In this case, if the reaction time scale is rather long compared to the dispersion time scale and if the reaction products are relatively inert so that, for example, the original pollutant is not regenerated by further reaction, it may be sufficient to approximate the reaction by a first-order process using an effective rate constant determined empirically. In this approximation, all details of the actual reaction mechanism are ignored. The

conversion of sulfur dioxide to sulfate aerosol over long distances is commonly treated in this manner.

In more complex cases, such as that of photochemical smog, the mechanism should be treated at some more appropriate level of detail. The required level of detail depends on the nature of the reactions being described and the number of different chemical species involved. The user should seek expert advice in evaluating a model with respect to the mechanism being used. In any case, the assumed mechanism should be sufficiently valid so as to give reasonable agreement with experimental observations.

In the photochemical smog case, three approximations are commonly used and will be discussed briefly as examples of the possibilities that can arise.

The first deals with the treatment of highly reactive intermediates which are present in photochemical smog. These intermediate species can be treated just like any other pollutant in that their concentrations may be described explicitly as functions of time. Due to their high reactivity, however, the approximation is usually made that they exist in a steady or stationary state such that for each the rate of removal equals the rate of production. Making this approximation allows their concentrations to be expressed mathematically in terms of those of measurable pollutants and thus eliminated from the rate expressions altogether. By eliminating these species from the equations, considerable simplification occurs. This approximation, called the steady-state or stationary-state approximation, should be tested for validity in any specific case and there are indications [Farrow and Edelson (1974)] that it is not necessarily valid for the photochemical smog case even though it is commonly used. This approximation is not restricted to applications involving photochemical smog but may be used in describing any reactive system in which highly reactive intermediate species are present.

A second and less detailed treatment is sometimes used when the reaction mechanism may be approximated by a small number of fast reactions such that each one in the set is accompanied by its reverse reaction. For example, over a short period of time the photochemical smog system may be approximated by a mechanism consisting of only two reactions: 1) the photolysis (absorption of light, followed by chemical reaction) of NO_2 to produce NO and O_3 and 2) the reverse reaction of NO and O_3 to produce NO_2. If each reaction in the set is fast enough, the entire system responds very rapidly to changes in composition

brought about by dispersion, and the chemical composition of the pollutant mixture at any point may be predicted by assuming the system of chemical reactions to be in equilibrium. This approximation, called the equilibrium approximation, is equivalent to the assumption that the rate of removal equals the rate of production for every chemical species present, not just the reactive intermediates. The equilibrium approximation is valid when the reaction time for each reaction in the system is much shorter than the time required for significant concentration changes resulting from dispersion processes.

The equilibrim approximation may be used in steady-state as well as dynamic models. It allows the prediction of the chemical composition of the pollutant mixture at a given point given (1) the composition of the original pollutant emission, (2) the composition of the surrounding air into which that emission is being dispersed, and (3) the concentrations predicted on the basis of the dispersion model alone.

The third approximation deals with the very large number of hydrocarbons which are actually present in the polluted atmosphere, all of which participate in the formation of photochemical smog. As a practical matter it is impossible to model the concentration of each even if their emission rates were known, which they are not in general. The approximation is made that classes of hydrocarbon may be defined such that all members of a given class share some desirable property, such as having similar reaction rates or reaction products. The total concentration of all members of each class is then modeled using a simplified reaction mechanism involving the use of average class rate constants. This technique is termed "lumping" of hydrocarbons. The validity of the procedure should be determined by comparison of predictions with observations from experiments.

For the purpose of comparing two models it should be assumed that, all other things being equal, it is better to treat reactive intermediates explicitly than to employ the steady-state approximation. The more accurate the reaction mechanism being used the better.

If the detailed spatial and temporal evolution of a dispersing reactive system is to be described, the system of chemical reactions should be treated in some detail. For other purposes, particularly involving secondary pollutants, experimental and/or observational data may be used to provide the necessary link

between the concentration of the pollutant of interest and the precursor levels at an earlier time. This may be especially useful for cases in which not enough is known about the reaction mechanism or in which only a maximum concentration regardless of location is desired.

The other aspect that needs to be evaluated is the way in which the rates of change of the average pollutant concentrations are evaluated. Dispersion models for reactive pollutants generally attempt to predict the average concentrations of all relevant pollutants within some suitably defined volumes or cells as functions of time. Thus these models should be able to evaluate the time rates of change of these quantities. As discussed earlier, if the pollutants are uniformly distributed within a given cell, the appropriate rates of change may be calculated from the elementary reaction rate expressions using the average concentrations appropriate to the given cell. Errors will be introduced if this procedure is used in cases in which spatial inhomogeneities exist in the pollutant concentrations over distances smaller than the cell size. At present, this effect is generally not treated at all. This is not to imply that modelers are unaware of the effect, but the problem of providing an adequate general treatment is still essentially unsolved.

In summary, most dispersion models for reactive pollutants use elementary reaction rate expressions which are truly valid only in homogeneous regions and make no attempt to account for imperfect mixing at sub-grid distances. If the user is confronted with a model which does in fact treat the effect of inhomogeneities in some fashion, expert advice should be sought on the manner of treatment before making an evaluation. However, in general, any reasonable treatment would be better than none at all. Table 5.12 gives the treatments of chemistry and reaction mechanism that have been discussed. No table of treatments of the effect of spatial inhomogeneities on the rate of change of average pollutant concentrations is provided. At this writing no practical general treatments exist except in models developed solely for the purpose of doing basic research. Table B.10 gives the treatments of chemistry and reaction mechanism used by suggested reference models.

A.6 PHYSICAL REMOVAL PROCESSES

A.6.1 General

The two major physical removal processes which affect ambient atmospheric pollution levels are dry deposition and precipitation scavenging. In identifying them as physical processes, the intention is to distinguish them from the chemical processes discussed in Appendix A.5, even though on a fundamental level there are chemical aspects to each. After defining these elements, each will be discussed in turn. For a more technical discussion the user is referred to the article by Hidy (1973) as well as the proceedings of the symposia on precipitation scavenging [Engelmann and Slinn (1970)] and on atmosphere-surface exchange of particulate and gaseous pollutants [Engelmann and Sehmel (1976)]. Technical but still introductory discussions are also given by Van der Hoven and Engelmann in Slade (1968).

Dry deposition is defined as the removal of a gaseous or particulate pollutant at the earth's surface by any of the several processes, including impaction, absorption, and chemical reaction. The important point is that this process occurs only at the surface.

Precipitation scavenging is defined as the removal of a gaseous or particulate pollutant by precipitation. In the past, the distinction has been made between the absorption or other collection of pollution by cloud droplets before precipitation actually occurred (denoted by the term "rainout") and the scavenging of pollutant by the precipitation itself as it falls through the polluted air (denoted by the term "washout"). For purposes of this workbook, this distinction will not be emphasized but the user should be aware of its existence.

Dry Deposition

The rate of removal of an atmospheric pollutant per unit area of ground surface is called the deposition rate (dimensions: mass/time/area). It depends upon

- The nature of the mechanism by which the pollutant, once transported to the ground, interacts with and is removed at the ground surface and
- The rate of vertical transport of that pollutant.

The pollutant is removed from the air near the ground, thereby creating a non-zero vertical concentration gradient near that surface. Vertical dispersion processes tend to smooth out this gradient by transporting pollutants downwards, thereby providing more for possible removal. The ambient pollutant concentration near the ground is lower than it would be otherwise, with the magnitude of the depletion depending on the relative rate of removal at the surface. A corresponding net decrease per unit downwind distance in the total amount of pollutant being advected by the wind is also observed.

The deposition rate depends on the nature of the interaction between pollutant and ground surface and as such depends on a wide variety of pollutant and surface characteristics. Although these are highly dependent on the specific application of interest, a few general statements can be made. The deposition of gaseous pollutants, for example, increases as the solubility or reactivity of the gas increases. The deposition of airborn particulate matter is highly dependent on particle size. If the pollutant of interest is found predominantly greater than a certain size range, this added factor should be taken into account in the treatment, as discussed below.

The deposition rate also depends strongly on the rate of vertical transport and therefore on the same factors as does vertical dispersion. (See Appendix A 4 for a discussion of these factors.)

With regard to the deposition of particulate matter, these remarks on deposition refer primarily to particles smaller than approximately 10 microns in size. Particles larger than this are sufficiently massive that gravitational settling becomes significant and these particles simply drift downward at a rate dependent on their size and weight. This deposition mechanism is very different from that described so far and in general must be treated differently; see for example the discussion in Slade (1968). Particulate matter smaller than 10 microns behaves much like a gas in many respects and gravitational settling is usually negligible.

If the removal is efficient enough, a significant fraction of the pollutant may be removed before it is transported out of the region of interest and ambient atmospheric concentrations can be significantly affected. In some application, the deposition rate or the total deposition within a given area over some specified period of time may be of interest, in addition

to or instead of the actual ambient concentration. In either case, dry deposition is an important phenomenon.

Precipitation Scavenging

This term includes processes which take place within clouds, such as the formation of cloud droplets about pollutant particles which serve as condensation nuclei and the absorption of pollutants into existing droplets, as well as the scavenging action of precipitation falling through polluted air. The importance of each of these processes depends strongly on the characteristics of the pollutant, as in the case of dry deposition, and again only very general comments can be made. For gaseous pollutant, the solubility in water is the most important factor and this often depends to a significant extent on the presence of other dissolved material in the precipitation. The solubility of sulfur dioxide, for example, decreases as the acidity of the precipitation increases. The particle size is again the most important factor for the scavenging of aerosols. The rate of pollutant removal by falling precipitation is also determined to a significant extent by the size of the falling drops and the rainfall rate.

A.6.2 Treatment of Dry Deposition

As indicated above, the removal of pollutant at the ground surface has two major effects on ambient pollutant concentrations:

- A depletion of the mass of pollutant being advected by the wind, resulting in lower concentrations than would otherwise be expected, and
- A reduction of ground level concentrations compared to those at higher elevations, resulting in a non-uniform vertical distribution.

All treatments of dry deposition that are used in practice describe the first effect but not all describe the second.

The net downward pollutant flux resulting from removal at ground level is commonly assumed proportional to the pollutant concentration at ground level, the proportionality constant actually being dependent on a variety of factors such as:

- The nature of the pollutant,
- The nature of the ground surface, and
- The prevailing meteorological conditions, particularly the atmospheric stability near the ground.

The proportionality constant is called the "deposition velocity" and its value in any given situation determines the significance of the effect of dry deposition on pollutant concentration. Theoretical procedures exist whereby appropriate values may be estimated for a specific application but their accuracy is uncertain and values derived from field observations are nearly always used in practice.

Assuming that the downwind flux of pollutant may be parameterized in this way, the problem of treating dry deposition becomes one of describing its effect on atmospheric pollutant concentrations and of calculating the amount of pollutant deposited in the area of interest. Different types of models treat these effects in different ways, depending specifically on the way vertical dispersion is treated and on the way the dependence of the pollutant concentration on height above ground is predicted.

Since pollutant removal occurs at the ground surface, the best treatment of dry deposition is to mathematically specify the appropriate boundary condition at the earth's surface and to determine or describe the corresponding effects numerically or analytically. The mathematical statement of the boundary condition, which is used in models which treat vertical dispersion by a numerical method, involves both the vertical eddy diffusivity and the deposition velocity and defines the relationship between the pollutant concentration and the concentration gradient at the ground. Numerical solution of the diffusion equation in the vertical direction then determines the predicted pollutant concentration as a function of height as well as the predicted rate of pollutant deposition on the ground. This procedure may be used in either dynamic or steady-state models.

Models which treat vertical dispersion by a semiempirical method do not necessarily handle dry deposition in a less appropriate way than do numerical models. If, for example, the assumed form for the vertical concentration distribution is based on suitable analytic solutions of the vertical diffusion equation obtained using the correct boundary conditions, the treatment may be as appropriate as any other. Normally, however, semiempirical models incorporate

certain assumptions which are to some extent invalid for the treatment of dry deposition.

Most semiempirical models incorporate the perfect reflection boundary condition, as discussed in Appendix A.7. Mathematically, this corresponds to the assumption that there is no net vertical pollutant flux and no net removal of pollutant from the atmosphere at the ground. An additional result is that the pollutant concentration is nearly independent of height near the ground. This also corresponds to the special case of a zero value for the deposition velocity. A model incorporating the perfect reflection boundary condition cannot treat the effect of dry deposition on the vertical concentration profile. If this approximation is used in a model, as it is in most Gaussian plume models, but it is still desirable or necessary to allow for the depletion of the plume as it is advected along, a time or downwind distance-dependent factor may be applied to the concentration value calculated by the basic semiempirical formula. This factor serves to simulate a reduction in the total mass of pollutant in the plume and to model pollutant removal by dry deposition. In essence, this type of treatment involves the determination of an effective source strength which is a decreasing function of travel time or downwind distance. The simplest example of this treatment is the use of an exponential decay factor in several currently available models. By appropriate choice of the value of the decay constant, it is possible to simulate crudely the effect of the removal of pollutant. An implicit assumption in this treatment is that the shape of the vertical concentration distribution is unaffected by the removal process. This assumption is valid only if the rate of vertical mixing is large compared to the rate of pollutant removal.

A somewhat more detailed treatment, described in Slade (1968), involves the assumption that the pollutant is removed at a rate proportional to the ground level concentration. However, this concentration is given by the Gaussian plume formula with perfect reflection, modified by a factor to account for that mass of pollutant already lost. The effective source strength as a function of downwind distance must be determined by quadrature for the specific parameter values involved and presented for use in graphical or tabular form. As in the simpler and less detailed exponential decay treatment, the implicit assumption is made that the shape of the vertical pollutant distribution is unaffected.

The special case of particulate matter for which gravitation settling is important is generally treated by what has come to be known as the tilted plume approximation. The vertical pollutant distribution is determined as a function of time or downwind distance using whatever model is appropriate. A downward motion with a velocity equal to the appropriate settling velocity is added to whatever other motion has been predicted for the distribution. For steady-state models, the effect is to tilt the plume centerline downwards with a slope determined by the ratio of the settling velocity to the horizontal wind speed. One should in principle use a different settling velocity, and hence a different slope, for particulate matter in different size ranges.

Table 5.13 lists possible treatments of dry deposition. Table B.11 lists the treatments used by suggested reference models.

A.6.3 Treatment of Precipitation Scavenging

The various processes whose net effect is called precipitation scavenging are not usually modeled individually except perhaps in specialized research-level models. Instead, the total effect is generally treated in an approximate way.

Both the removal of pollutants in clouds and the scavenging by falling precipitation are usually considered to be exponential processes. This may not be strictly true in all cases. For example, the uptake of SO_2 by cloud droplets is not really an exponential process because of chemical reactions which occur in the droplets themselves. Precipitation falling through a polluted layer may take up a soluble gas at one height and release it at a lower height because of evaporation of the drops exposed to a clean atmosphere. These effects must be modeled on an individual case-by-case basis.

If removal in clouds is treated as an exponential process, the decay constant is called the rainout coefficient. If removal by falling precipitation is treated as an exponential process, the decay constant is called the washout coefficient. These coefficients in principle depend on a wide variety of drop and pollutant characteristics. Empirical values are often used and it is often assumed that the relationship between the washout coefficient and the total rainfall rate may be expressed by a power law. The washout coefficient is a function of drop size. A more detailed treatment would take this into

account and determine the total rate of pollutant removal by integrating over an assumed drop size distribution function. This is rarely done in practice.

If the rainfall rate is variable, so is the washout coefficient. The pollutant concentration then decreases in a manner reflecting this variability, the decrease is not represented by simple exponential decay. For the purpose of describing the effect of rainfall on pollutant concentrations, the washout coefficient must be known or assumed, including any time variation due to variations in the rainfall rate.

If the application involves an averaging time sufficiently long that more than one rainfall occurrence needs to be treated, even simpler methods are often used. For example, the assumption may be made that every time it rains the ambient pollutant level is decreased by some constant factor which may be empirically derived or estimated from the average duration of rainfall in the area. If a climatological model is being used, the correlation between frequency of rainfall and other meteorological parameters, particularly wind direction, should be taken into account. Ignoring this correlation represents an even less detailed treatment and corresponds to simply superimposing total rainfall contours on calculated concentration contours to estimate the effect on [illegible] average concentration values. This correlation is most simply handled in climatological models by [illegible]

[illegible]

which are within the [illegible] region. [illegible] treatments used by suggested reference models.

A.7 BACKGROUND, BOUNDARY AND INITIAL CONDITIONS

A.7.1 General

An air pollution model describes the pollutant distribution within a limited volume of space for a limited period of time. This volume is bounded on the bottom by the earth's surface, on the sides by the perimeter of the region of interest, and on the top by the upper limit to vertical dispersion. Even for models which calculate only ground level concentrations explicitly, the three dimensional nature of dispersion is accounted for through inclusion of such parameters as stack height, plume rise, or mixing height. In any case, treatments of the following four aspects of the given application are required:

- Effects due to the existence of a finite upper limit to dispersion,
- The effect of the earth's surface as a barrier to dispersion and as a potential sink for atmospheric pollutants,
- The contribution to pollutant levels within the volume of interest from upwind sources not included in the model, and
- The initial concentrations throughout the volume of interest at the beginning of the time period of interest.

Numerical and semiempirical models treat the first three aspects in different ways; dynamic and steady-state models treat the last aspect in different ways.

The first two aspects are generally called boundary conditions in both numerical and semiempirical models, because they relate to effects at well defined physical boundaries. The upper limit to dispersion is commonly treated as an absolute barrier which keeps pollutants above it from entering the modeled volume and which prevents pollutants dispersing upward within the modeled volume from going any higher. In such cases, there is no net flux of pollutant through the boundary. This condition is called the perfect reflection boundary condition and is a common assumption used for the upper boundary; other assumptions regarding the upper boundary condition are less common. However, there are circumstances in which pollutants may enter the modeled region through the upper boundary. For example, pollutants lying above the mixing layer can be entrained within the modeled volume as the mixing height increases in the morning as a result of solar heating. In practice, only numerical/dynamic models treat

such situations in detail. A great deal of imprecision exists in specifying the flux (or flow) of pollutant across the upper boundary due to the lack of reliable estimates of such transfer in real situations. Even when perfect reflection is assumed, the exact value of the mixing height is generally subject to error, being based on extrapolations from measurements made at different locations or times than those being modeled.

Two effects determine the nature of the lower boundary condition:

- The behavior of the earth's surface as a barrier to downward dispersion, and
- The rate of removal of the pollutant at that surface.

These two effects are usually assumed to be related, because the rate of removal is proportional to the ground-level concentration. Various processes determine the degree of absorption and which are most important depends upon the particular situation. For example, large particles can settle out (be perfectly absorbed) under the influence of gravity. Sulfur dioxide can be absorbed by vegetation and ozone can react chemically with various materials on the earth's surface. The ground is also [illegible] pollutants e.g., for example [illegible]

[illegible]

It should also be noted that numerical models generally treat at least some fraction of the emissions or pollutants by specifying the appropriate flux through the lower boundary as part of the lower "boundary condition." In this discussion, the "boundary condition" refers to what happens to pollutants

already emitted; emissions treated as occurring at the boundary should be considered as aspects of source location and emission rate (Appendix A.1).

The third aspect, advection of pollutants into the volume of interest, is related to the concept of a background level. Such concentrations are due to natural and man-made sources not being modeled, because they are outside the modeled region. This definition of background differs from another sometimes used in which the background level is taken as the concentration which would exist if all sources in the modeled inventory ceased to emit. The latter definition would include contributions from sources within the modeled region but not included in the inventory. In the sense used here, background might be defined operationally as the pollutant concentration measured just outside the upwind boundary of the region of interest. Such a concentration would frequently depend on the direction of the wind, the location of the measurement, or the time when the measurement was made. For non-conservative pollutants, this concentration would be expected to change as the air is advected through the study region due to the operation of various removal mechanisms. For secondary pollutants, the incoming fluxes of precursors must also be taken into account, because they will generally interact significantly with emissions within the region and greatly affect the predicted levels of the pollutant of interest.

Ozone, which is both reactive and secondary, illustrates the situation well. "Background" ozone concentrations measured just upwind of urban areas are frequently reduced within these areas due to the initial scavenging of ozone by precursor nitric oxide emissions. Downwind of the urban area, the precursors react and ozone concentrations rise again to high levels. Background is thus usually not a simple additive term but is a function of position and time within the region of interest. A single, additive background number can be defined only for primary conservative pollutants. Otherwise, the flux of pollutant and/or precursors into the study region at the vertical boundaries must be known. Even for primary conservative pollutants, the incoming flux must be known as a function of position and time if significant variations occur over time or distance scales small compared with the averaging time and the size of the region of interest. Rural SO_2 or sulfate levels provide examples of situations in which a single, additive background level is likely to be appropriate.

It has been assumed in this discussion of background and the side boundary conditions that the study region has been chosen carefully to include all important sources. It would be improper, for example, to estimate the total 24-hour maximum SO_2 concentration in the vicinity of a power plant while treating the contribution of a nearby plant as a background value. Both plants would need to be included in the study region and modeled. The second plant could be excluded only if the contribution of the first plant alone, rather than the total concentration, were desired.

One other point needs to be made about background. Circumstances may arise in which background is negligible, any background concentration being small in comparison to the concentration of interest. For example, in cases where the maximum short-term concentrations near a large, relatively isolated source are being estimated, background can usually be ignored. In such cases, models ignoring background are applicable. The user must consider the application carefully when making such a determination.

The last aspect covers the initial conditions, those concentrations existing throughout the study region at the beginning of the time period of interest. These concentrations are not treated explicitly in steady-state models but must be specified in order to solve the equations used in dynamic models. Initial concentrations may be included implicitly in steady-state models when background levels are estimated. They are likely to be most important for short-term averages for which the initial concentrations can constitute a substantial part of the final time-averaged concentration. This situation would occur most frequently when the initial concentrations are large and travel time across the region of interest is equal to or greater than the averaging time of interest. As noted in Appendix A.4, this type of situation calls for a dynamic, rather than a steady-state, treatment. The concentrations of secondary and reactive pollutants are particularly sensitive to the initial concentrations and distributions of precursors and potential reactants, respectively. Initial conditions are thus important for such pollutants and a dynamic approach is better suited to their treatment. This is particularly true when short-term concentrations are desired as is the case, for example, with ozone.

A.7.2 Treatment of Background, Boundary and Initial Conditions

Since numerical and semiempirical models treat dispersion from different points of view, they employ different methods for handling background and boundary conditions. Initial conditions are treated differently by dynamic and steady-state models. The user should be aware that both "boundary conditions" and "initial conditions" signify two related but not entirely equivalent concepts. First, they mean a set of mathematical expressions required to solve the partial differential equations used in numerical models and second, the physical conditions being modeled. The mathematical expressions are the representations of the physical conditions in a form suitable for numerical models. Semiempirical models must treat the same physical conditions, still often referred to as the boundary conditions, using different methods. The discussion is conveniently divided by considering first the treatments of background and boundary conditions by numerical and semiempirical models and then the treatments of initial conditions by dynamic and steady-state models.

Background and Boundary Conditions

Part of the difference between the treatments of background and boundary conditions by numerical and semiempirical models is simply a difference in the methodologies used to express the same physical condition. As will be seen, however, the numerical approach generally provides a more detailed and flexible treatment of these conditions. At this point, the user should keep in mind that applicability of both approaches to the application as discussed in Appendix A.4.

As noted above, many processes can take place when a pollutant contacts the earth's surface. Perfect reflection or absorption are generally approximations to the real situation. The appropriateness of the approximation being used must be assessed by the user when comparing models. Numerical models treat perfect reflection mathematically by requiring that the vertical gradient of pollutant concentration be zero at the surface, that is, what comes down must go back up. Perfect absorption corresponds to the requirement that the concentration be zero at the boundary. Perfect reflection is normally assumed because it is usually a much better approximation to the real situation than is perfect absorption. Both of these situations may also be handled easily by semiempirical models. Semiempirical models treat perfect reflection

at the lower boundary by including an "image source" equivalent to the real source but located like its mirror image with the earth's surface as the mirror. The "method of images" is the technique employed in the most widely used forms of the Gaussian plume model and can only be used to handle perfect reflection or absorption.

Partial reflection at the earth's surface is treated in numerical models by using the concept of a "dry deposition velocity." This parameter is a measure of the rate of pollutant removal at the earth's surface. In essence, the mathematical formulation allows part of the incoming pollutant to be absorbed so that the total amount being dispersed is depleted after reflection. Most semiempirical models developed to date cannot treat partial reflection as a boundary condition. An approximate treatment of dry deposition as a pollutant removal process by assuming an exponential decay of the pollutant is frequently used. This is discussed in more detail in Appendix A.6. Dry deposition could also be treated as a boundary condition by semiempirical models if the assumed functional form of the pollutant distribution were based upon analytical solutions of the diffusion equations subject to the appropriate boundary condition. Numerical models can also change the amount of absorption to represent different conditions throughout the study region; semiempirical models can usually only deal with one overall average dry deposition rate throughout the region of interest.

At the mixing height, perfect reflection is generally assumed. Numerical models use the same form of mathematical boundary condition as at the surface but apply it at the height corresponding to the top of the mixing layer, which can vary with location and time. These models could also be used in principle to cover the case of partial penetration of the mixing layer (partial reflection) simply by altering the boundary condition as is done to treat dry deposition at the surface. They can also account for the transfer of pollutants into the region of interest by suitable modifications of the upper boundary conditions and thus treat fumigation or entrainment. It should also be noted that numerical models require a finite upper limit to dispersion in order to solve the relevant equations.

As at the ground, semiempirical models generally treat only the case of perfect reflection. Two methods are commonly used. The first is the method of images in which image sources are added above the mixing height to account

for the reflections from that barrier, which is generally assumed to have a constant elevation. It turns out that an infinite number of images are required to account for the multiple reflections from the ground and the mixing height [see Turner (1969)] and the result is expressed as an infinite sum. In most cases only the first few terms of the sum contribute significantly and the sum may be evaluated easily to sufficient accuracy. A more common treatment relies upon the observation that near the source the plume is not affected by conditions at the top of the mixing layer and that far enough downwind, the pollutant is uniformly mixed within the entire mixing layer. Between the distance at which the plume first feels the effects of the finite mixing height and the distance at which the vertical profile becomes uniform, the concentration is obtained by interpolation [see Turner (1969)]. A variation of this treatment used in some Gaussian plume models treats the effect of the mixing height implicitly by limiting the vertical spread of the plume by requiring that σ_z remain constant after the vertical spread of the plume (σ_z) exceeds some fraction of the mixing height. Pasquill (1976) discusses the limitations of the undisturbed and uniform mixing approximations and has presented a table for use in interpolating results in cases where the sum must be evaluated. [See also Yamartino (1977)]. Evaluating the sum will generally give more accurate results than interpolation. The gain in accuracy is slight considering the magnitude of other inaccuracies in modeling treatments and interpolation is used more frequently. Semiempirical models can also, in essence, ignore the upper boundary condition by using a functional form for the vertical concentration profile that places no limits on the height to which pollutants can disperse. This may be an appropriate representation of the real situation of the large mixing heights at short distances from the source. Semiempirical models can be modified to account for fumigations by using equations (functional forms) for predicting concentrations during the time of the fumigation. (See, for example, the equations in the appropriate references cited in Appendix A.2.)

Numerical models treat the conditions at the sides of the region as mathematical specifications of the pollutant flux into the region. As noted above, this is the most fundamental way of treating background levels. Semiempirical models cannot treat these as boundary conditions and "background" can only be treated as a general additive term. This term may be a function of location within the region but is generally treated as a single constant value thus ignoring directional dependence and spatial variations. Any temporal variation is also generally ignored.

Initial Conditions

As pointed out previously, initial conditions are treated explicitly only by dynamic models. Any contributions to the concentrations due to pollutants initially present would be handled as part of the additive background level by steady-state models. As such they would be indistinguishable from the concentrations assumed to be advected into the region as "true" background. In dynamic treatments, more detail is available when the initial conditions can be arbitrary functions of location than when single uniform values must be assumed throughout the region of interest.

A final word is in order about climatological models and temporal variations. As noted in Appendix A.4, this approach can make use of any of the basic types of models discussed although a steady-state method is most often used. Thus, the treatment of background, boundary and initial conditions by climatological models will depend upon the nature of the model used for the dispersion calculations. Both dynamic and sequential steady-state models can, of course, account for temporal variations in background and boundary conditions. Dynamic models usually allow important parameters to change relatively smoothly over time; sequential steady-state models allow parameters to assume new values at the beginning of each new time interval over which a steady-state is assumed to hold. Dynamic models most frequently treat the amount of material advected or entrained into the region of interest or the mixing height as time dependent; sequential steady-state models most frequently treat only temporal variations in the mixing height.

The ranking of treatments of background, boundary, and initial conditions is given in Table 5.14. In treating these elements, almost any combination of types of treatments at the various boundaries can occur. In rating a model, the user should rate the model's treatment of each element separately and combine them to arrive at an overall rating. Table B.12 lists the treatments of background, boundary and initial conditions used by suggested reference models.

A.8 TEMPORAL CORRELATIONS

A.8.1 General

As noted in previous subsections, many of the elements or quantities used to parameterize an element treated by a model can vary with time. The

variations of these quantities about their mean values are frequently correlated in the situation being modeled. For example, the application may involve a source with a diurnally varying emission rate and meteorology with the typical diurnal variations in atmospheric stability described in Appendix A.4. When such correlations occur it is usually important that the model correlate the time-dependent quantities, that is, treat them in such a way that concentration estimates are made on the basis of values which do occur together in the application of interest.

Implicit in the last statement is a realization that the treatment of correlations is closely related to the degree of temporal resolution obtainable in the model. In particular, the resolution time for the correlated quantities must be less than the time over which the variations can occur. For example, if two correlated quantities vary hourly, the model must treat each of them with a time resolution of one hour or less for the treatment of correlations to be possible.

As pointed out previously, there is a limit, frequently based on practical considerations or data availability, to the resolution time and hence to times over which correlations can be considered. The limiting factor is that element or quantity with the minimum degree of time resolution among those elements which are important to the particular application and which exhibit sufficiently large temporal variability to affect the model results. The primary interest is generally in correlating emission rates, meteorological parameters, and rates of removal and transformation processes. Of course, in applications where emission rates are almost constant, correlations involving them are small and may be ignored. Generally speaking, the correlations between the various meteorological parameters also need to be treated.

Dynamic and sequential models handle temporal correlations automatically within the time resolution used by the model. These models generally allow the values of most important parameters to be changed at each time step and since the data for each step are generally input as a unit by the user, they are automatically correlated. Steady-state models which treat one or several specific sets of emission and meteorological data treat correlations which occur on a time scale longer than the averaging time of the data automatically and ignore those which occur over shorter times. The correlations are implicit in the structure of the input data as in the dynamic case. This type of treatment is frequently encountered in models which estimate short-term concentration

On the other hand, climatological models use statistical wind roses and hence the only correlations inherent in this approach are between those parameters upon which the wind rose is based, typically atmospheric stability, wind speed, and wind direction. A three-hour resolution is typical of wind roses. All other correlations, particularly those involving emissions, must be treated separately.

Two factors should be considered when evaluating the treatment of correlations:

- The magnitude of the variations in the given application over time scales less than the averaging time, and
- The importance to the application of the quantities involved.

The first factor has been discussed above. As for the second, simply correlating many time-dependent quantities may be less important than correlating a few critical quantities, e.g., wind direction and emission rate when the effect of a peaking power plant at a specific location is desired.

A.8.2 Treatment of Temporal Correlations

Beginning with the most detailed, there are basically three levels at which temporal correlations can be treated:

- Sequential and fully correlated,
- Non-sequential with limited correlation, and
- Not treated explicitly.

The first type of treatment is found in dynamic models or in sequential models. In these models, the correlations are treated automatically. The second type of treatment is exemplified by climatological models. Although some statistical models may <u>implicitly</u> treat correlations by their choice of variables, they are classified here as using the third type of treatment and are discussed in Section 7.

Within the first two treatments there is a variation in the level of detail depending on:

- The degree of temporal resolution and
- The quantities allowed to vary.

The determinants and importance of these aspects have been discussed in the general discussion in Appendix A.8.1.

Table 5.15 lists the treatments of temporal correlations and the treatments by suggested reference models are given in Table B.13.

A.9 IMPORTANCE RATINGS FOR APPLICATION ELEMENTS

Source - Receptor Relationship

The source-receptor relationship is assumed to be of at least medium importance in all applications. Many factors influencing transport and dispersion depend on the source-receptor separation and orientation. The relationship is somewhat more important for secondary pollutants, because of the need for a detailed description of the mixing of various precursors. For similar reasons, it is also somewhat more important when chemical sinks are involved. Short-term concentrations are more sensitive to this relationship than long-term concentrations, since changing meteorological conditions tend to average differences in concentrations from point to point. The concentration distribution in situations involving limited numbers of sources depends heavily on the source-receptor relationship. In situations involving multiple sources where small inaccuracies in one relationship are likely to be balanced by inaccuracies in another, this relationship is less important. Area source applications require a little less detail than point or line applications, because the spatial extent of an area source makes an error in the source-receptor relationship less significant in affecting concentration estimates. The importance of this element is somewhat enhanced in complex geographic situations which place considerable importance on the precise relationship between source, receptor, and geography. Short-range applications are more sensitive to the source-receptor relationship than long-range applications. At long distances emissions have usually become relatively uniformly mixed and a change in separation or orientation that would be critical at short range produces only a negligible effect. The importance of the source-receptor relationship to each of the applications is given in Table 4.2.

Emission Rate

Other things being equal, concentrations of primary pollutants are proportional to emission rates. For secondary pollutants, the relative

concentrations of the precursors are very important factors in determining concentrations. Emission rates were thus always rated as of at least medium importance to all applications, and as somewhat more important for secondary than for primary pollutants. The same consideration applies to reactive pollutants, making emission rate slightly more important when chemical sinks are involved than when only physical sinks or inert pollutants are modeled. Emission rates must generally receive more attention in short-term or short-range applications than in long-term or long-range applications where other factors such as changing meteorology and removal processes normally can assume greater importance for determining concentrations. Emission rates are rated as somewhat more important in situations involving a limited number of sources, because of the likelihood of compensating errors in the multiple source case. No distinction is made between different source geometries nor between the importance of emission rates in simple and complex geographic situations. Ratings of the importance of emission rates to the various applications are given in Table 4.3.

Composition of Emissions

This discussion deals only with the chemical composition of emissions. If the user's application requires the specification of a size distribution for particulate matter, the importance ratings in Table 4.4 should be reconsidered. No general statements can be made in this case, and the user should consult an expert to determine importance ratings appropriate to the application of interest.

Chemical composition of emissions is critically important when secondary pollutants or chemical sinks are involved and of little importance when dealing with primary pollutants and either no sinks, or physical sinks only. No difference in importance between long-term and short-term applications is assumed. A slight extra importance is assigned to applications involving multiple sources or long-range transport, because of the increased possibility for chemical reactions when many different emissions are mixed or a long time is allowed for reactions to occur. The importance in simple and complex geographic situations is the same. The importance ratings for the chemical composition of emissions are given in Table 4.4.

Plume Behavior

Table 4.5 gives the importance of plume behavior to each of the indexed applications. Plume behavior is equally important for both primary and secondary pollutants but is rated more important in cases where physical sinks are present than when chemical or no sinks are present. This is because the plume behavior determines how easily the plume contacts the ground, allowing the physical removal process to operate. Chemical removal can occur throughout the entire volume of mixing. Plume behavior is also rated more important in short-term than in long-term averages, because over short-time spans small variations masked by averaging over long time spans, may be significant. The greater spatial inhomogeneities associated with point sources make plume behavior more important for point sources than for line sources. Similarly, it is somewhat more important for line than for area sources. In complex geographical situations, plume behavior is important in determining whether the plume will be affected by the complex situation or rise above its influence. At long range, vertical mixing tends to become uniform and hence plume behavior is relatively unimportant.

Horizontal Wind Field

The horizontal wind field is generally an important element in any application, because advection is the principal process for pollutant transport. It is considered somewhat more important when chemical reactions are important and when short-term rather than long-term averages are desired, because of the need to know the wind field more precisely. The determination of the horizontal wind field is more important in complex terrain due to the channeling of the wind and other effects. The horizontal wind field is somewhat more important in limited point or line source cases than in area or multiple source cases. Finally, the horizontal wind field is considered to be very important in those situations in which the actual trajectory of a parcel of air must be determined, because the temporal and spatial variation must be reproduced. This is the case for long range transport and for very short release times (puffs). Table 4.6 gives the importance rating of horizontal wind field for each application.

Vertical Wind Field

The vertical wind field is considered generally unimportant in many cases of interest, because it is nearly zero on average. Vertical wind field is important in situations requiring the estimation of concentrations at moderately short ranges in regions containing complex terrain due to the effect of the terrain on the (three-dimensional) wind field. Vertical wind field is considered slightly more important in applications involving chemistry than those in which chemistry is unimportant due to the need for a more accurate description of the wind field. Vertical wind field is also considered more important in estimating short-term rather than long-term estimates. No distinction was made for different source geometries or numbers. Table 4.7 gives the importance ratings of vertical wind field for the indexed applications.

Horizontal Dispersion

Table 4.8 gives the importance rating of horizontal dispersion for each of the indexed applications. Horizontal dispersion is considered to be of at least medium importance in every application. Horizontal dispersion is more important at short range than at long range, because the dispersion process is the most rapid and produces the greatest changes in concentration estimates at short ranges. Horizontal dispersion is considered less important for area sources than for line sources, and less for line than for point sources due to the emission size effect. In the case of secondary pollutants and/or the case of chemically reactive pollutants, it is very important to be able to describe the mixing of emissions with the ambient air, since chemical reaction rates are sensitive to local concentrations, therefore horizontal dispersion is considered quite important in these cases. Similarly, if physical sinks are present, it is generally more important to handle horizontal dispersion properly, depending on the nature of the removal process. The importance of horizontal dispersion is considered to be higher for short-term averages than for long-term, because the averaging which can occur over long times generally allows simpler treatments to be adequate. Finally, horizontal dispersion is considered to be equally important in either simple or complex terrain.

Vertical Dispersion

Table 4.9 gives the importance rating of vertical dispersion for each of the indexed applications. Vertical dispersion is given at least a medium

rating for every application. Its importance is considered independent of averaging time, and approximately independent of the type of terrain. Vertical dispersion is considered much more important at short range than at long range [illegible] more important for secondary pollutants [illegible] of removal processes [illegible] primarily for secondary pollutants [illegible] operative. Finally [illegible] is considered to be relatively unimportant for source type [illegible].

Chemistry and Reaction Mechanism

The importance of chemistry and its treatment is determined primarily by the chemical nature of the pollutants involved and to some extent by the travel distance; no other characteristics of the application need be considered. Chemistry is irrelevant for primary inert pollutants, is of importance for primary reactive or secondary inert pollutants, and is of even more importance for secondary reactive pollutants. The importance of chemistry is rated lower for primary reactive and secondary inert pollutants than for secondary reactive pollutants. If chemical reactions provide both a source and a sink for a given pollutant, chemistry is more important than if they provide either source or sink, but not both. This is a somewhat arbitrary ranking; the real importance of a detailed treatment of chemistry depends on the complexity of the system of reactions and the number of pollutants involved. Chemistry is considered slightly more important for long-range than for short-range applications due to the longer travel time and greater opportunity for reactions to occur. Table 4.10 gives the list of importance ratings of chemistry and reaction mechanism for each of the indexed applications.

Physical Removal Processes

We consider two processes in this category: dry deposition and precipitation scavenging. Physical removal is important, by definition, in those applications for which the user has taken the physical or chemical/physical sink branch on the Application Tree. Physical removal is also slightly more important for pollutants with chemical sinks than conservative ones. Physical removal is more important for long-range than for short-range applications, because of the cumulative effects of the process. Its importance is considered roughly independent of source type and averaging time. Physical removal is

considered slightly more important in complex rather than simple terrain, due to the increased surface roughness. It should be pointed out that the importance of precipitation scavenging, as a removal process, depends primarily on the fraction of the time during which precipitation occurs in the application of interest. Thus, for short-term applications precipitation scavenging may usually be neglected, while for long-term, or possibly long-range, applications a convenient measure of its importance is the rainfall probability. Table 4.11 lists the importance ratings of physical removal for the indexed applications.

Background, Boundary and Initial Conditions

The importance ratings of background, boundary and initial conditions to the indexed applications are given in Table 4.12. These conditions were rated as highly important for secondary pollutants where precursor background levels can significantly influence the pollutant concentrations in the region of interest and for applications involving sinks where the advected concentrations might be significantly depleted during transit. These elements are crucial for applications involving reactive pollutants where the details of the pollutant mix must be known. These elements are equally important for short and long-term averaging times and for short and long-range transport. They are independent of the specific source characteristics and geography and are assumed to be of at least medium importance to all applications.

Temporal Correlations

Temporal correlations relate the time variations of the other application elements in their proper sequence. The importance of temporal correlations to the indexed applications is given in Table 4.13. They are rated more important for secondary than for primary pollutants, because the exact sequence and correlation of emissions and meteorology determine whether the pollutants are brought into contact so that reactions can occur. The ambient concentration is less sensitive to correlations for primary pollutants. Similarly, when physical and chemical sinks are involved, it is important to treat correlations. When treating short-term averages, it is generally important to know the detailed short-term fluctuations in the relevant factors and to correlate them properly; such detail is usually unnecessary when treating long-term averages. Thus, correlations are more important in short-term than in long-term applications. No distinctions are made between the various source types. More importance is

associated with temporal correlations in complex geographic situations. Here correlations between emissions and dispersion factors can determine whether a particular emission passes within the perturbing influence of the complex geography. Short-range applications usually require more attention to temporal correlations. At short range, rapid changes normally occur in plumes whereas at long range these changes are slower and require less detail to treat adequately.

APPENDIX B

BACKGROUND MATERIAL ON SUGGESTED REFERENCE MODELS

Appendix B. BACKGROUND MATERIAL ON SUGGESTED REFERENCE MODELS

Appendix B is divided into two parts. The first, Appendix B.1, consists of Table B.1 which provides the classification of each suggested reference model, and Tables B.2-B.13 which provide the treatment of each of the twelve application elements used by these models. The second part, Appendix B.2, provides abstracts of and the working equations used by the suggested reference models. A glossary of symbols is provided at the end of Appendix B.2.

CONTENTS OF APPENDIX B

B.1. REFERENCE MODEL TREATMENTS OF APPLICATION ELEMENTS

This appendix provides the classification of each suggested reference model in Table B.1 and the treatment used by each model of the twelve application elements in Tables B.2-B.13.

Table B.1. Reference Model Classification

Suggested Reference Model	Classification
APRAC-1A	Semiempirical/Sequential (steady-state)
ATM	Semiempirical/Climatological (steady-state)
CDM	Semiempirical/Climatological (steady-state)
Single Source (CRSTER)	Semiempirical/Sequential (steady-state)
DIFKIN	Numerical (vertical)/Semiempirical (horizontal)/ Dynamic
HIWAY	Semiempirical/Steady-state
RAM	Semiempirical/Sequential (steady-state)
SAI	Numerical/Dynamic
STRAM	Semiempirical/Dynamic
Valley (short-term)	Semiempirical/Steady-state
(long-term)	Semiempirical/Climatological (steady-state)

Table B.2. Treatment of Source-Receptor Relationship by Reference Models

a. Horizontal Source and Receptor Location

Reference Model	Source Geometry	Method of Treatment
APRAC-1A	Line and area	User specifies line sources (traffic links) with arbitrary locations and lengths. Area sources (off link traffic) allocated to 2 mi x 2 mi grid. For each receptor both are aggregated onto wedge-shaped areas of a polar grid centered on a receptor (a different grid is used for each receptor) such that: 1) Radii of circular boundaries increase in geometric progression. 2) Radial boundaries are 22.5° beyond 1000 m and 45° under 1000 m from receptor. (3,3 for area, line)[a] Up to 10 arbitrarily located receptors. (1)[b] Street canyon submodel: Four internally located receptors on each user-designated street. (2 for line)[a] (4)[b]
ATM	Point, area, and line	Arbitrary location for all sources. (1 for all source types)[a] Areas should be roughly square or circular. Arbitrary receptor location. (1)[b] Assumes flat terrain; elevation not treated. Treats multiple point, area, and line sources. Treats up to ten receptors.
CDM	Point and area	Arbitrary location for point sources. (1 for point)[a] Area sources are squares of uniform size in user-defined grid; user may specify sources which are integer multiples of the grid size, but these must be superimposable directly on the grid. (2 for area)[a] Receptors located arbitrarily. (1)[b]
Single Source[g] (CRSTER)	Point	Up to 19 sources all assumed to be located at same user-specified, arbitrary position. (1-2)[a] Receptor locations restricted to 36 azimuths (every 10°) and five user-specified radial distances. (3)[b]
DIFKIN	Point and area	All sources aggregated to square 2 mi x 2 mi grid cells in an array 25 cells x 25 cells. (2,2 for point, area)[a] Sources classified as points (power plants, refineries), distributed stationary, and mobile. Receptors located arbitrarily within boundaries of emission grid. (2)[b]
HIWAY	Line	Straight finite line segments (will treat up to 24 parallel segments), arbitrarily located. (2)[a] Arbitrarily located receptors. (1)[b] Cut section mode: Emissions treated as coming from 10 lines at top of cut. (2-3)[a] Receptors cannot be in cut. (2)[b]

Table B.2 (Cont'd)

a. (Cont'd)

Reference Model	Source Geometry	Method of Treatment
RAM	Point and area	Arbitrary location for point sources. (1 for point)[a] Receptors may be: 1) Located arbitrarily, (1)[b] 2) Located internally near individual source maxima, (4)[b] 3) Located on internally generated hexagonal grid to give good coverage in user-defined portion of region of interest. (4)[b] Area sources are multiples of unit squares on a grid; user controls scale of grid. (2 for area)[a]
SAI	Point and area	All sources aggregated to square grid of arbitrary spacing and up to 25 x 25 cells. (2,2 for point, area)[a] Sources classified as points (power plants), distributed stationary and mobile. Multiple receptors located arbitrarily within boundaries of emission grid. (2)[b] Concentrations also calculated in each grid cell (up to 25 x 25 x 5 estimates).
STRAM	Point	Arbitrary location for each source. (1)[a] Up to 10 arbitrarily located receptors plus receptors at intersections of a grid of up to 13 x 13 equally spaced boundaries. (1,3)[b]
Valley	Point and area	Arbitrary location and elevation for each point source. (1 for point)[a] Arbitrary location, elevation, and size for square area sources. (1 for area)[a] Must be less than 51 sources. Receptors (112) on 16 direction radial grid; relative radial distances fixed internally; scale and origin of grid defined by user. (3)[b]

b. Release and Receptor Heights

Reference Model	Source Geometry	Method of Treatment
APRAC-1A	Line and area	Sources assumed at ground level. (3,5 for line, area)[c] Receptors assumed at ground level. (7)[d]
ATM	Point, area and line	Arbitrary release height for each source. (2,3,2 for point, line, area)[c] Receptors at ground level. (7)[d]
CDM	Point and area	Assumes flat terrain; arbitrary stack height for each source. (2,3 for point, area)[c] Chooses larger of input stack height or 1 m. Receptors at ground level. (7)[d]
Single Source[g] (CRSTER)	Point	Arbitrary stack height for each source. (1)[c] Unique topographic elevation for each receptor: must be less than each stack height. Receptors must be at ground level. (combination of 2,7)[d]

Table B.2 (Cont'd)

b. (Cont'd)

Reference Model	Source Geometry	Method of Treatment
DIFKIN	Point and area	Emissions treated as upward pollutant fluxes at ground surface. (5,5 for point, area)[c]
		Receptors at equally spaced heights from the ground to the mixing height. (4)[d]
HIWAY	Line	Arbitrary release heights. (2)[c]
		Arbitrary receptor heights. (1)[d]
RAM	Point and area	Arbitrary release height for each point source. (2 for point)[c]
		Up to three effective release heights (appropriate for 5m/sec winds) may be specified for area sources. (2 for area)[c]
		Value for a particular area must be one of these three.
		Receptors all of same height at or above ground level; flat terrain assumed. (7)[c]
SAI	Point and area	Arbitrary release height for point sources (power plants). (1 for point)[c]
		Point source emissions assumed uniformly mixed throughout vertical column in which emission takes place.
		Other emissions treated as upward fluxes at ground surface; arbitrary topographic elevation. (Combination of 1,3 for area)[c]
		Receptors at ground level. (7)[d]
STRAM	Point	Arbitrary release height for each source. (2)[c]
		Receptors at ground level; flat terrain assumed. (7)[d]
Valley	Point and area	Arbitrary release height for each source. (1, combination of 1, 3 for point, area)[c]
		Receptors at ground level at any elevation on existing topographic features. (combination of 7)[d]

c. Downwind/Crosswind Distances[e]

Reference Model	Source Geometry	Method of Treatment
APRAC-1A	Line and area	Uses exact downwind distances to the two radial boundaries of each gridded area source. (1 for area)
ATM	Point, area	Unique downwind and crosswind distances for each point source-receptor pair, for three points within each area source, and for nine points along each line source. (1 for all source types)
CDM	Point and area	Calculates unique downwind distance for each point source-receptor pair. Calculates representative distances for area source-receptor pairs. (1, 2 for point, area)
Single Source[g] (CRSTER)	Point	Calculated from source to each receptor location. (1)
DIFKIN	Point and area	Not applicable. Distance traveled along computed trajectory not used explicitly.
HIWAY	Line	Precise downwind and crosswind distances for each point along line. (1)

Table B.2 (Cont'd)

c. (Cont'd)

Reference Model	Source Geometry	Method of Treatment
RAM	Point and area	Unique downwind and crosswind distances for each point source-receptor pair. (1 for point) Downwind distance calculated for points along rays which intersect area sources. (1 for area)
SAI	Point and area	Not applicable.
STRAM	Point	Not applicable; concentration calculated at each receptor based upon distance along and distance from trajectory centerline.
Valley	Point and area	Exact downwind distance calculated for each point-source receptor pair. (1 for point) Single representative downwind distance used for area sources. (2 for area)

d. Orientation[f]

Reference Model	Source Geometry	Method of Treatment
APRAC-1A	Line and area	Traffic links (lines) may have arbitrary horizontal orientation but this detail is lost when links are gridded onto the receptor-centered polar grid. (2,2 for area, line)
ATM	Point, area and line	Orientation of areas not treated explicitly. (3 for area) Lines horizontal, arbitrary orientation. (2 for lines)
CDM	Point and area	Sides of areas must lie along grid directions.
Single Source[g] (CRSTER)	Point	Not applicable.
DIFKIN	Point and area	Areas oriented by fixed grid boundaries. (2)
HIWAY	Line	Line assumed horizontal with arbitrary orientation. (2)
RAM	Point and area	Sides of areas must lie along grid directions. (2)
SAI	Point and area	Areas oriented by fixed grid boundaries. (2)
STRAM	Point	Not applicable.
Valley	Point and area	Area sources assumed oriented with one side parallel to wind direction. (Somewhat less detailed than 2)

[a]Numbers in parentheses refer to treatments of horizontal source location for the appropriate source type as given in Table 5.1 a.

[b]Numbers in parentheses refer to treatments of receptor location as given in Table 5.1 e.

[c]Numbers in parentheses refer to treatments of release height for the appropriate source type as given in Table 5.1 b.

[d]Numbers in parentheses refer to treatments of receptor height as given in Table 5.1 f.

[e]Numbers in parentheses refer to treatments of downwind/crosswind distances for the appropriate source type as given in Table 5.1 c.

[f]Numbers in parentheses refer to treatments of source orientation for the appropriate source type as given in Table 5.1 d.

[g]CRSTER should be used only when the receptor is below stack height.

Table B.3. Treatment of Emission Rate by Reference Models

Reference Model	Source Geometry	Method of Treatment	
		Spatial Variation[a]	Temporal Variation[b]
APRAC-1A	Line and	Arbitrary line source emissions aggregated onto grid described under source-receptor relationship (Table B.2). Arbitrary off-link grid squares assumed uniform and aggregated to same grid. Area source contributions from grid obtained by numerical integration of narrow plume approximation formulae; contributions calculated from all upwind sources located within the wedge-shaped grid. (2 for gridded area sources)	Daily trafic volume for each link and off-link grid square is input and modified to produce hour-by-hour emissions. (Equivalent to 2b) Street canyon submodel: Hourly emission rate for link of interest is input by user. (5)
ATM	Point, area, and line	Arbitrary rate for each point, line and area source. Area sources transformed into polar areas each of which is represented by three effective point sources; shape of area depends upon angle subtended by area at each receptor. Total area source contribution estimated as a sum of individual contributions. Line sources treated as ten effective points. Areas and lines assumed uniform. (1, modified 4,4 for point, area, line) Treats "windblown" source as an area source of TSP with emission rate determined by user input values of type of material, density, saltation diameter, and suspension diameter appropriate to each source and the wind speed. ("Windblown" source: modified 4)	Constant emission rates. (5)
CDM	Point and area	Arbitrary emission rate for each point and area source. Area sources assumed uniform. Area source contributions integrated numerically one 22.5° sector at a time, based on sampling points located at specific angular and radial intervals on a polar grid centered at receptor. (1, 3 for point, area)	Day/night variations in emissions; same variation for all sources. (2b)
Single Source[c] (CRSTER)	Point	Arbitrary emission rate for each source. (1)	Monthly variation in emission rate allowed. (3)
DIFKIN	Point and area	Emissions treated as upward pollutant fluxes at ground surface. Individual rate for each 2 mi x 2 mi grid square: Rates for mobile sources determined from user-supplied emission factors and traffic data. Rates for stationary sources input by user. Calculates contributions from grid squares along trajectory. (1, modified 3 for point, area) Program option allows user to input directly arbitrary surface pollutant fluxes for up to three pollutants (not necessarily photochemically reactive).	Sequence of hourly average rates for mobile sources. Stationary source rates assumed constant. (1,3)

Table B.3 (Cont'd)

Reference Model	Source Geometry	Method of Treatment	
		Spatial Variation[a]	Temporal Variation[b]
HIWAY	Line	Uniform emission rate for each traffic lane. Each lane integrated numerically to obtain contribution. (3)	Constant emission rates. (5)
RAM	Point and area	Arbitrary emission rate for each point and area source. Area source contributions obtained by numerical integration along upwind distance of narrow-plume approximation formulae for area source with given effective release height. Includes only those areas intersected by the upwind ray. (1 for point; 4,5 for area)	Constant emission rates. (5)
SAI	Point and area	Point source emissions distributed homogeneously throughout entire vertical column above grid square containing the source; emission rates supplied by user. Other emissions treated as upward pollutant fluxes at ground surface. Rates for mobile sources determined from user-supplied emission factors and traffic data. Rates for stationary sources input by user. (Modified 1,3 for point, area)	Sequence of hourly average rates for mobile sources. Stationary source rates assumed constant. (1,3)
STRAM	Point	Arbitrary emission rate for each source. (1)	Constant emission rates. (5)
Valley	Point and area	Arbitrary rate for each point and area source. Area sources treated as single effective point sources. Total area source contribution estimated as a sum of individual contributions. (1,4 for point, area)	Constant emission rates. (5)

[a] Numbers in parentheses refer to treatments of spatial variation as given in Table 5.2.

[b] Numbers in parentheses refer to treatments of temporal variation as given in Table 5.2.

[c] CRSTER should be used only when the receptor is below stack height.

Table B.4. Treatment of Composition of Emissions by Reference Models

Reference Model	Method of Treatment: Chemical Composition	Method of Treatment: Size Distribution
APRAC-1A	Not applicable; model designed for primary, unreactive pollutant.	Not applicable; model designed for gaseous pollutants.
ATM	Not applicable; model designed for primary, unreactive pollutant.	User inputs single particle size (and density) for use in calculating terminal velocity for particulates. Treats three types of sand (uniform, naturally graded, wide size range) and single saltation and suspension diameters (and single density) for windblown sources. (4)[b]
CDM	Not applicable; model designed for primary pollutants.	Not treated explicitly. (7)[b]
Single Source[c] (CRSTER)	Not applicable; model designed for primary, unreactive pollutant.	Not treated explicitly. (7)[b]
DIFKIN[d]	Treats emissions of CO, NO, and reactive hydrocarbons. Emissions of NO_x in inventory assumed to be entirely NO_2; converted internally entirely into NO. Hydrocarbons in inventory assumed to be total hydrocarbons; reactive fraction of mobile source hydrocarbon emissions assumed to be 70.4% by weight. Stationary source hydrocarbons assumed to be 100% reactive. (4,5)[a] Program option: User directly input fluxes up to three arbitrary pollutants (for applications not involving photochemical smog). (Not applicable: chemical reaction not treated.)	Not applicable; model designed for gaseous pollutants.
HIWAY	Not applicable; model designed to treat primary, unreactive pollutant.	Not applicable; model designed for gaseous pollutants.
RAM	Not applicable; model designed to treat primary, unreactive pollutant.	Not treated explicitly. (7)[b]

Table B.4 (Cont'd)

Reference Model	Method of Treatment: Chemical Composition	Method of Treatment: Size Distribution
SAI[d]	Treats emissions of reactive hydrocarbons, unreactive hydrocarbons, NO, NO_2, and CO. User imputs mobile source emissions of hydrocarbons, NO_x, and CO. Mobile source hydrocarbon emissions split internally into 67.4% (mole fraction) reactive fraction and 32.6% unreactive fraction. Mobile source NO_x emissions assumed to be 99% NO_2; converted internally to NO. User inputs stationary source (both point and area) emissions of reactive hydrocarbons, unreactive hydrocarbons, NO, NO_2 and CO. (4,5)[a]	Not applicable; model designed for gaseous pollutants.
STRAM	Treats two compounds; one is assumed to be SO_2 the other, sulfate ($SO_4^{=}$). (4)[a]	Not treated explicitly. (7)[b]
Valley	Treats only one compound. Capable of treating at most one compound or a single representative compound in cases where chemical reactions occur. (6)[a]	Not treated explicitly. (7)[b]

[a]Numbers in parentheses refer to treatments of chemical composition in Table 5.3.

[b]Numbers in parentheses refer to treatments of size distribution in Table 5.3.

[c]CRSTER should be used only when receptor height is below stack height.

[d]Designed specifically to treat photochemical oxidants.

Table B.5. Treatment of Plume Rise by Reference Models

Reference Model	Treatment of Plume Rise[a]	Treatment of Downwash/Fumigation
APRAC-1A	Not treated explicitly. (5)	Does not treat either.
ATM	For each point source, user inputs a value representing the product of plume rise with 1) wind speed and 2) the cube root of the wind speed for neutral and stable conditions, respectively. Maximum effective stack height limited to 1500 m. (Modified 4b) No plume rise for area and line sources; a constant value could be included in user-supplied release height. (4e,5) Uses "tilted plume" approximation to treat deposition of particulates (see Table 5.13).	Does not treat either.
CDM	Briggs' 2/3 (1971) neutral/unstable formula used for point sources. If (stack height) + (plume rise) exceeds mixing height, ground level concentrations are assumed equal to zero. (Modified 4a) As an alternative to Briggs', the user may input a value of the product of plume rise and wind speed for each point source. (Alternative : 4e) No plume rise calculated for area sources; a constant value could be included in user-supplied release height. (4e,5)	Does not treat either.
Single Source[b] (CRSTER)	Briggs' (1971, 1972) final plume rise formulas; plume rise not treated as a function of downwind distance. If plume height exceeds mixing height, concentrations further downwind assumed equal to zero. (4a)	Does not treat either.
DIFKIN	Not treated explicitly. (5)	Does not treat either.
HIWAY	Not treated explicitly but could be included in release height. (4e,5)	Does not treat either.
RAM	Uses Briggs' (1971, 1972) downwind distance dependent plume rise formulae for point sources. If plume height exceeds mixing height, ground level concentrations assumed zero. (Modified 4a) No plume rise calculated for area sources; could be included in release height. (4e,5)	Does not treat either.
SAI	Uses Briggs' formulae (1971) for point sources (power plants only) to determine if plume penetrates inversion. If plume height exceeds mixing height, emissions from source are not treated. Other power plant emissions included in ground level flux. (4a) Treats emissions as ground level fluxes; plume rise not treated explicitly. (5)	Does not treat either.
STRAM	Not treated explicitly; could be included in release height for each source. (4e,5)	Does not treat either.
Valley	Uses Briggs' (1971, 1972) plume rise formulae for both point and area sources. Option: A single constant plume rise value may be input for any or all sources. (Option: 4e) If plume height exceeds mixing height: A. For long-term calculations, ground level concentrations assumed equal to zero. B. For short-term calculations, maximum plume height is limited to the mixing height. (Modified 4a)	Does not treat either.

[a]Numbers in parentheses refer to treatments as given in Table 5.4.

[b]CRSTER should be used only if receptor height is below stack height.

Table B.6. Treatment of Horizontal Wind Field by Reference Models

Reference Model	Method of Treatment[a]
APRAC-1A	Constant, uniform wind speed and direction assumed for each of a sequence of hours.
	Wind speed, direction values input by user. (4,7,2)
	Street canyon sub-model: specific positional and height dependence built in; constant in time. (3,5,4)
ATM	Constant, uniform wind speed and direction.
	Climatological treatment with sixteen wind sectors, 8 wind speed classes used. (4,7,3)
CDM	Constant, uniform wind speed and direction.
	Wind speed is estimated value at release height, correction from value at reference height (10m) dependent only on stability class.
	Climatological treatment with sixteen wind sectors, 6 wind speed classes used. (4,6,3)
Single Source[b] (CRSTER)	Constant, uniform wind speed and direction assumed for each of a sequence of hours.
	Wind speed, direction values input by user;[c] speed corrected for release height depending on stability class. (4,7,2b)
DIFKIN	Trajectory model.
	Wind speed and direction specified for each of a sequence of time steps at point on a horizontal grid, interpolated from nearest 1, 2, or 3 surface measurements.
	Discrete user-specified number (n) of wind directions allowed, $4 \leq n \leq 99$;
	Arbitrary wind speed values allowed.
	Wind speed, direction independent of height. (2,7,2b)
	Program option allows direct user input of trajectory.
HIWAY	Constant, uniform wind speed and direction.
	Wind speed, direction values input by user for the hour of interest. (4,7,4)
RAM	Constant, uniform wind speed and direction assumed for each of a sequence of hours.
	Wind speed, direction values input by user.[c]
	Wind speed is modified to correspond to value at release height, modification dependent only on stability class. (4, modified 6,2b)
SAI	Fixed grid model.
	Wind speed and direction specified for each of a sequence of hours at point on a horizontal grid, interpolated from surface measurements.
	Arbitrary wind speed, direction values allowed.
	Wind speed, direction independent of height. (2,7,2b)

Table B.6 (Cont'd)

Reference Model	Method of Treatment[a]
STRAM	Trajectory model. Wind speed and direction specified at 12-hour intervals on a horizontal grid, interpolated from radiosonde measurements. Wind speed and direction interpolated in time between measurements. Arbitrary wind speed, direction values allowed. Wind speed, direction independent of height. (2,7,2a)
VALLEY	1. Long-term calculations: Constant, uniform wind direction and speed, except for stable conditions over complex terrain for which implicit treatment of locational height dependencies is implemented - effect of plume deflection by terrain is accounted for by linear interpolation of centerline concentrations between 10-m value at impingement point and zero at 400 m above impingement point. (6,8,5) Climatological treatment with 16 wind sectors, 6 wind speed classes. Wind speed class values input by user, used without correction for height. (4,7,3) 2. Short-term techniques: Same as long-term except primary intent is for use where terrain elevations approach or exceed plume height. In such cases, intent is for user to input single wind speed, e.g. 2.5 mps, for typically one wind direction(and stability).

[a]Numbers in parentheses refer to the dependence on horizontal location, height above ground, and time as given in Table 5.5.

[b]CRSTER should be used only if the receptor height is less than the stack height.

[c]Assumes wind directions given to nearest 10^{o}, randomizes wind direction by addition of the amount $(n-4)^{o}$ where n is a random number between 0 and 9.

Table B.7. Treatment of Vertical Wind Field by Reference Models

Reference Model	Method of Treatment[a]
APRAC-1A	Assumed equal to zero. (4b,4b,3) Street canyon sub-model: specific positional and height dependence built in, assumed constant in time. (3,3,3)
ATM	Assumed equal to zero. (4b,4b,3)
CDM	Assumed equal to zero. (4b,4b,3)
Single Source[b] (CRSTER)	Assumed equal to zero. (4b,4b,3)
DIFKIN	Assumed equal to zero. (4b,4b,3)
HIWAY	Assumed equal to zero. (4b,4b,3)
RAM	Assumed equal to zero. (4b,4b,3)
SAI	Vertical wind speed specified for each of a sequence of hours at points on a three-dimensional grid. Values assumed linearly increasing functions of height, values near surface determined from horizontal wind speed and directions using mass consistency requirements. (2,3,2b)
STRAM	Assumed equal to zero. (4b,4b,3)
Valley	1. Long-term calculations: Assumed equal to zero for stable atmospheric conditions, except for implicit treatment of deflection by terrain above impingement elevation as noted in Table B.6. Implicit treatment for neutral and unstable conditions: plume assumed to remain at a constant height above terrain. No time dependence (4a,4a,3) 2. Short-term calculations (24-hour maximum only): as in long-term calculations for stable conditions. (4b,4b,3)

[a]Numbers in parentheses refer to the dependence on horizontal location, height above ground, and time as given in Table 5.6.

[b]CRSTER should be used only if the receptor is less than the stack height.

Table B.8. Treatment of Horizontal Dispersion by Reference Models

Reference Model	Classification	Method of Treatment
APRAC-1A	Semiempirical/sequential (steady-state)	Sector averaging (narrow plume approximation) 45.0° less than 1 km. 22.5° beyond 1 km. Atmospheric stability not treated explicitly. Surface roughness not treated explicitly. (4b,3,3,na)[a]
ATM	Semiempirical/climatological (steady-state)	Uniform horizontal distribution assumed within each of 16 22.5° sectors (sector averaging). Atmospheric stability not treated explicitly. Surface roughness not treated explicitly. Averaging time assumed long enough for sector averaging to be valid. (5c,3,2a,na)[a]
CDM	Semiempirical/climatological (steady-state)	Uniform horizontal distribution assumed within each of 16 22.5° sectors (sector averaging). Atmospheric stability not treated explicitly. Surface roughness not treated explicitly. Averaging time assumed long enough for sector averaging to be valid. (5c,3,3,na)[a]
Single Source[c] (CRSTER)	Semiempirical/sequential (steady-state)	Gaussian plume function assumed. Atmospheric stability divided into seven classes. Surface roughness not explicitly treated. One hour averaging time used. (4a,2b,3,3)[a]
DIFKIN	Numerical (vertical)/ Semiempirical (horizontal)/dynamic	Narrow plume approximation about calculated trajectory. (3c,3,3,na)[a]
HIWAY	Semiempirical/steady-state	Gaussian plume function assumed for each point along line; numerical integration along line. Atmospheric stability divided into six (Pasquill-Gifford) classes. Dispersion coefficients from Zimmerman and Thompson (1975) less than 100m, from Turner (1969) beyond 100m. Level grade mode - initial value of dispersion coefficient set at 3.0 m. Cut section mode - initial value of dispersion coefficient an empirical function of wind speed. Surface roughness not treated explicitly. One hour averaging time used. (4a,2b,3,3)[a]
RAM	Semiempirical/sequential (steady-state)	Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes. Dispersion coefficients from Turner (1969) or McElroy and Pooler (1968) at user option. Surface roughness not treated explicitly. One hour averaging time used. Point sources: (4a,2b,3,3)[a]; Area sources: (4b,3,3,na)[a]

Table B.8 (Cont'd)

Reference Model	Classification	Method of Treatment
SAI	Numerical/dynamic	Numerical solution of advection-diffusion equation in three dimensions. Horizontal eddy diffusivity value assumed uniform and constant and is fixed in the code. (1b,3,3,3)[a],(4,4,3)[b]
STRAM	Semiempirical/dynamic	Crosswind distribution about calculated trajectory assumed Gaussian. Atmospheric stability divided into six (Pasquill-Gifford) classes. Same stability class assumed to hold over entire region of interest. Surface roughness not treated explicitly. Dispersion coefficients determined by integration of expressions for rates of change; based on Turner (1969) up to 100km, Heffter and Ferber (1975) beyond 100 km. Averaging time specified by user. (3b,2b,3,3 and 5)[a]
Valley	Semiempirical/climatological (steady-state)	Long-term calculations: Uniform horizontal distribution assumed within each of 16 22.5° sectors (sector averaging). Atmospheric stability not treated explicitly. Surface roughness not treated explicitly. Averaging time assumed long enough for sector averaging to be valid. (5c,3,3,na)[a]
	Semiempirical/steady-state	Short-term calculations (24-hour maximum only): Uniform horizontal distribution assumed within each of 16 22.5° sectors (sector averaging). Atmospheric stability not treated explicitly. Surface roughness not treated explicitly. Averaging time: 24 hours. (5c,3,3,na)[a]

[a] Numbers in parentheses refer to treatments listed in Tables 5.7, 5.8, 5.9 and 5.10 respectively. The user should refer to the appropriate section (numerical or semiempirical) of Table 5.10 according to the model classification.

[b] Numbers in parentheses refer to the dependence of the horizontal eddy diffusivity on horizontal location, height above ground, and time as given in Table 5.11.

[c] CRSTER should be used only when the receptor is below stack height.

Table B.9. Treatment of Vertical Dispersion by Reference Models

Reference Model	Classification	Method of Treatment
APRAC-1A	Semiempirical/sequential (steady-state)	Gaussian plume function assumed. Atmospheric stability divided into six (modified Pasquill-Gifford) classes. Dispersion coefficient modified from McElroy and Pooler (1968). Surface roughness not treated explicitly. Downwind distance dependence of dispersion coefficient assumed ax^b for purposes of doing analytic integration. In street-canyon submodel, semiempirical function of wind speed, street width, and direction is used. (4a,2b,3,3)[a]
ATM	Semiempirical/climatological (steady-state)	Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes. Dispersion coefficients from Turner (1969) or Hosker (1973). (user option). Surface roughness characterized by a user-specified roughness parameter (Hosker dispersion coefficients only) (4a,2b,2a,3)[a]
CDM	Semiempirical/climatological (steady-state)	Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes, with neutral stability divided into day and night cases. Stability class decreased by one class (more unstable) for area sources. Surface roughness not treated explicitly. Dispersion coefficients from Turner (1969). (4a,2a,3,3)[a]
Single Source[c] (CRSTER)	Semiempirical/sequential (steady-state)	Gaussian plume function assumed. Atmospheric stability divided into seven (P-G) classes. Surface roughness not treated explicitly. Dispersion coefficients from Turner (1969). (4a,2b,3,3)[a]
DIFKIN	Numerical (vertical)/ Semiempirical (horizontal)/ dynamic	Numerical integration of diffusion equation in vertical direction. Vertical eddy diffusivity values specified hourly by user at user-defined discrete heights above ground. (1b,2a,3,2)[a], (4,3,2b)[b]
HIWAY	Semiempirical/steady-state	Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes. Dispersion coefficient from Zimmerman and Thompson (1975) less than 100m, from Turner (1969) beyond 100m. Level grade mode - initial dispersion coefficient set at 1.5m. Cut section mode - initial dispersion coefficient an empirical function of wind speed. (4a,2b,3,3)[a]

Table B.9 (Cont'd)

Reference Model	Classification	Method of Treatment
RAM	Semiempirical/sequential (steady-state)	Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes. Dispersion coefficients from Turner (1969) or McElroy and Pooler (1968) at user's option. Surface roughness not treated explicitly. (4a,2b,3,3)[a]
SAI	Numerical/dynamic	Numerical solution of advection-diffusion equation in three dimensions. Vertical eddy diffusivity an empirical function of wind speed and height above ground. (1b,3,3.2)[a], (4,3,2b)[b]
STRAM	Semiempirical/dynamic	Two options are available to the user: 1) Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes. Same stability class assumed to hold over entire region of interest. Surface roughness not treated explicitly. Dispersion coefficients determined by integration of expressions for rates of change; based on Turner (1969) up to 100 km, Heffter and Ferber (1975) beyond 100 km. 2) Uniform vertical distribution up to mixing height assumed. (3b or 3d,2b,3,3)[a]
Valley[a]	Semiempirical/climatological (steady-state)	Long-term calculations: Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes. Surface roughness not treated explicitly. Dispersion coefficients from Turner (1969). (4a,2b,3,3)[a] All input stable conditions are treated as neutral in urban option.
	Semiempirical/steady-state	Short-term calculations (24-hour maximum only): Gaussian plume function assumed. One stability class (stable: Pasquill-Gifford "F") used when terrain elevation approaches or exceeds stable plume height. Surface roughness not treated explicitly. Dispersion coefficients from Turner (1969). (4a,2c,3,3)[a] All input stable conditions are treated as neutral in urban option.

[a]Numbers in parentheses refer to treatments listed in Tables 5.7, 5.8, 5.9 and 5.10, respectively, The user should refer to the appropriate section (Numerical or Semiempirical) of Table 5.10 according to the model classification.

[b]Numbers in parentheses refer to the dependence of the vertical eddy diffusivity on horizontal location, height above ground and time is given in Table 5.11.

[c]CRSTER should be used only when the receptor is below stack height.

Table B.10 Treatment of Chemistry and Reaction Mechanism by Reference Models

Reference Models	Method of Treatment[a]
APRAC-1A	Not treated explicitly. (7)
ATM	Not treated explicitly. (7)
CDM	Treats only first-order removal processes: exponential decay. Single, constant user-supplied halflife used. (6)
Single Source[b] (CRSTER)	Not treated explicitly. (7)
DIFKIN	Photochemical smog system: (4) Sixteen reactions involving 10 chemical species (NO, Hc, NO_2 O_3, HNO_2, NO_3, N_2O_5, OH, RO_2, CO). Lumping approximation for 2 species (Hc, RO_2). Steady-state approximation for 4 species (NO_3, N_2O_5, OH, RO_2). User specifies NO_2 photolysis rate constant as function of time (up to 300 sequential values). No adjustment made for effects of imcomplete turbulent mixing below the resolution of the grid. Program option allows user to prescribe arbitrary chemical reaction mechanism (up to 20 chemical species, up to 20 reactions).
HIWAY	Not treated explicitly. (7)
RAM	Treats only first-order removal process: exponential decay. Single, constant user-supplied halflife used. (6)
SAI	Photochemical smog system: (4) Fifteen reactions involving 10 species (NO, NO_2, O_3, Hc, O, OH, HO_2, RO_2, NO_3, HNO_2). Lumping approximation for 2 species (Hc, RO_2). Steady-state approximation for 6 species (NO_3, O, RO_2, OH, HO_2, HNO_2). NO_2 photolysis rate calculated internally as a function of time. No adjustments made for the effects of incomplete turbulent mixing below the resolution of the grid.
STRAM	SO_2-sulfate aerosol system: SO_2 to sulfate conversion approximated by a first-order process with internally defined value of the rate constant. (6)
Valley	Treats only first-order removal processes: exponential decay. Single, constant user-supplied halflife used. (6)

[a] Numbers in parentheses refer to treatment numbers in Table 5.12.

[b] CRESTER should be used only if receptor height is less than stack height.

Table 3.11. Treatment of Physical Removal Processes by Reference Models

Reference Model	Method of Treatment
APRAC-1A	Not treated explicitly. (4,5)[a]
ATM	Dry deposition: (2a)[b]
	Pollutant removal simulated by effective source treatment.
	Multiplicative factor determined by downwind integration of removal rate.
	Rate of removal determined from ground-level pollutant concentration and a constant deposition velocity.
	Deposition velocity (gases) adjusted within internally defined range of values by user-supplied measure of surface roughness, related to extent and type of vegetation cover.
	Effect of atmospheric stability not treated explicitly.
	Deposition velocity (particulate matter) is the greater of the gravitational settling velocity or 0.01 m/sec.
	Tilted plume approximation used for particulate matter if gravitational settling velocity is greater than 0.01 m/sec. (3)[b]
	Effect on vertical concentration profile not treated explicitly except in tilted plume case.
	Precipitation scavenging: (2)[c]
	Exponential decay with constant washout coefficient.
	Removal occurs only for fraction of time equal to frequency of occurrence of rainfall (input by user); not correlated with any other meteorological variables.
	Washout coefficient calculated internally from user supplied mean rainfall rate.
CDM	Treats only first-order removal processes; exponential decay.
	Single, constant user-supplied halflife used. (2b,5)[a]
Single Source[d] (CRSTER)	Not treated explicitly. (4,5)[a]
DIFKIN	Not treated explicitly. (4,5)[a]

Table B.11 (Cont'd)

Reference Model	Method of Treatment
HIWAY	Not treated explicitly. (4,5)[a]
RAM	Treats only first-order removal processes: exponential decay. Single, constant user-supplied halflife used. (2b,5)[a]
SAI	Not treated explicitly. (4,5)[a]
STRAM	Dry deposition: (2a)[b] Pollutant removal simulated by effective source treatment. Multiplicative factor determined by downwind integration of removal rate. Rate of removal determined from ground-level pollutant concentration and constant deposition velocity. Deposition velocities for SO_2, sulfate aerosol are fixed in the program at 1.0 and 0.1 cm/sec., respectively. Effects of surface roughness or atmospheric stability not treated explicitly. Effects on vertical concentration profile not treated explicitly. Precipitation scavenging: (5)[c] Not treated explicitly.
Valley	Treats only first-order removal processes: exponential decay. Single, constant user-supplied halflife used. (2b,5)[a]

[a]First number refers to treatments of dry deposition in Table 5.13, second number refers to treatments of precipitation scavenging in Table 5.13.

[b]Numbers refers to treatments of dry deposition in Table 5.13.

[c]Numbers refers to treatments of precipitation scavenging in Table 5.13.

[d]CRSTER should be used only if receptor height is less than stack height.

Table B.12. Treatment of Background, Boundary and Initial Conditions by Reference Models

a. Background[a]

Reference Model	Classification	Method of Treatment
APRAC-1A	Semiempirical/sequential (steady-state)	Value calculated for each receptor; box model used to estimate contributions from upwind sources beyond 32 km based on wind speed, mixing height and annual fuel consumption. (2) In street canyon sub-model, contribution from other streets is included in the background. (2)
ATM	Semiempirical/climatological (steady-state)	Not treated explicitly. (3)
CDM	Semiempirical/climatological (steady-state)	Single constant input values for each pollutant. (2)
Single Source[g] (CRSTER)	Semiempirical/sequential (steady-state)	Not treated explicitly. (3)
DIFKIN	Numerical (vertical)/ Semiempirical (horizontal)/dynamic	Not applicable.
HIWAY	Semiempirical/steady-state	Not treated explicitly. (3)
RAM	Semiempirical/sequential (steady-state)	Not treated explicitly. (3)
SAI	Numerical/dynamic	(Treated as a boundary condition on flux at vertical boundaries.)
STRAM	Semiempirical/dynamic	Not treated explicitly. (4)
Valley	Semiempirical/climatological (steady-state)	Long-term calculations: Not treated explicitly. (3)
	Semiempirical/steady-state	Short-term calculations (24-hour maximum only). Not treated explicitly. (3)

b. Upper Boundary Condition (at Mixing Height)[b]

APRAC-1A	Semiempirical/sequential (steady-state)	Perfect reflection: ignores effect until concentration equals that calculated using box model; uses box model (uniform vertical distribution) thereafter. (Intermediate between 2-3) Mixing height determined from morning radiosonde data and during day, surface temperature variations: Midnight to dawn: constant at pre-dawn value obtained using minimum urban temperature; Dawn to sunset: afternoon maximum temperature used to obtain maximum height; hourly values obtained from surface temperature variations; Sunset to midnight: linear interpolation over time.

Table B.12 (Cont'd)

b. (Cont'd)

Reference Model	Classifications	Method of Treatment
ATM	Semiempirical/climatological (steady-state)	Treated implicitly by limiting vertical dispersion coefficient to be no larger than mixing height. (4)
CDM	Semiempirical/climatological (steady-state)	Perfect reflection: no effect until vertical dispersion coefficient equals 0.8 of the mixing height, uniform vertical mixing assumed thereafter. (2)
Single Source[g] (CRSTER)	Semiempirical/sequential (steady-state)	Perfect reflection: method of multiple images treated by summation of series until vertical dispersion coefficient = 1.6x (mixing height); uniform vertical mixing thereafter. (1) Mixing height for a given hour obtained by interpolation of radiosonde data (see Appendix B.4 for algorithm).
DIFKIN	Numerical (vertical)/ Semiempirical (horizontal)/dynamic	Perfect reflection: flux required to be equal to zero at boundary. (3) Mixing height can change at hourly intervals.
HIWAY	Semiempirical/steady-state	Perfect reflection: 1) Stable conditions or mixing height greater than 5000m: assume no effect (treats only reflection from ground); (3) 2) Neutral or unstable conditions with mixing height less than 5000m: method of multiple images treated by summation of infinite series until vertical dispersion coefficient > 1.6 × (mixing height); uniform vertical distribution thereafter. (1)
RAM	Semiempirical/sequential (steady-state)	Perfect reflection: 1) Neutral and unstable conditions: method of multiple images treated by summation of infinite series until σ_z = 1.6×(mixing height); uniform mixing assumed thereafter; (1) 2) Stable conditions: mixing height assumed to have no effect. (3) Mixing height for a given hour obtained interpolation of radiosonde data (see Appendix B.8 for algorithm).
SAI	Numerical/dynamic	Perfect reflection for pollutants within region of interest (turbulent diffusive flux = 0). Allows for entrainment of pollutants from above mixing layer. (1)
STRAM	Semiempirical/dynamic	Two options: 1) Uniform mixing (perfect reflection) (4) or 2) Mixing height assumed to have no effect. (3)
Valley	Semiempirical/climatological (steady-state) and Semiempirical/steady-state	Perfect reflection: 1) Neutral and unstable conditions: perfect reflection; method of multiple images treated by summation of infinite series; (1) 2) Stable conditions: ignores effect of upper boundary, except all input stable conditions treated as neutral in urban option. (3) 3) Input afternoon mixing height internally adjusted according to stability

Table B.12 (Cont'd)

Reference Model	Classification	Method of Treatment
		c. Lower Boundary Condition (at Earth's Surface)[c]
APRAC-1A	Semiempirical/sequential (steady-state)	Perfect reflection; single image source.[f] (Intermediate between 3-4).
ATM	Semiempirical/climatological (steady-state)	Perfect reflection; single image source.[f] (4)
CDM	Semiempirical/climatological (steady-state)	Perfect reflection; single image source.[f] (3)
Single Source[g] (CRSTER)	Semiempirical/sequential (steady-state)	Perfect reflection in plane at same height as receptor; multiple image sources.[f] (2)
DIFKIN	Numerical/(vertical)/ Semiempirical (horizontal)/ dynamic	Emissions treated as upward fluxes at the ground. Implicit perfect reflection; no adjustment made to fluxes to account for removal. (3)
HIWAY	Semiempirical/steady-state	Perfect reflection by method of multiple images.[f] (2)
RAM	Semiempirical/sequential (steady-state)	Perfect reflection by method of multiple images.[f] (2)
SAI	Numerical/dynamic	All non-point source (power plant) emissions treated at upward fluxes at ground. Implicit perfect reflection; no adjustment made to fluxes to account for removal. (3)
STRAM	Semiempirical/dynamic	Perfect reflection by method of single image source.[f] (4).
Valley	Semiempirical/climatological (steady-state) and Semiempirical/steady-state	Perfect reflection by method of single image source in stable cases and multiple image source in neutral and unstable cases.[f] (stable: 4; other: 2).
		d. Boundary Condition at Vertical Sides[d]
APRAC-1A	Semiempirical/sequential (steady-state)	Not applicable; treated as background.
ATM	Semiempirical/climatological (steady-state)	Not applicable; treated as background.
CDM	Semiempirical/climatological (steady-state)	Not applicable; treated as background.
Single Source[g] (CRSTER)	Semiempirical/sequential (steady-state)	Not applicable; treated as background.

Table B.12 (Cont'd)

Reference Model	Classification	Method of Treatment
		d. (Cont'd)
DIFKIN	Numerical (vertical)/ Semiempirical (horizontal)/ dynamic	Not treated explicitly; horizontal uniformity assumed. (5)
HIWAY	Semiempirical/steady-state	Not applicable; treated as background.
RAM	Semiempirical/sequential (steady-state)	Not applicable; treated as background.
SAI	Numerical/dynamic	Treated as a function of position and elevation; total flux normal to side of region required to be continuous across boundary at each point. (1)
STRAM	Semiempirical/dynamic	Not applicable; treated as background.
Valley	Semiempirical/climatological (steady-state) and Semiempirical/steady-state	Homogeneously mixed across 2π/16-radian sector; linear interpolation than effected between adjacent sector centerlines.
		e. Initial Conditions[e]
APRAC-1A	Semiempirical/sequential (steady-state)	Not applicable.
ATM	Semiempirical/climatological (steady-state)	Not applicable.
CDM	Semiempirical/climatological (steady-state)	Not applicable.
Single Source[g] (CRSTER)	Semiempirical/sequential (steady-state)	Not applicable.
DIFKIN	Numerical (vertical)/ Semiempirical (horizontal)/ dynamic	User specifies arbitrary initial concentrations for all species not treated by steady-state assumption (all but NO_3, N_2O_5, RO_2, OH) at each discrete height above ground. (1)
HIWAY	Semiempirical/steady-state	Not applicable.
RAM	Semiempirical/sequential (steady-state)	Not applicable.
SAI	Numerical/dynamic	Mean initial concentrations of 6 species (reactive HC, NO, O_3, NO_2, CO, unreactive Hc) specific for each grid cell. (1)
STRAM	Semiempirical/dynamic	Not applicable.
Valley	Semiempirical/climatological (steady-state) and Semiempirical/steady state	Not applicable.

Table B.12 (Cont'd)

[a]Numbers in parentheses refer to treatments of background given in Table 5.14a for models having the same classification as the reference model.

[b]Numbers in parentheses refer to treatments of the upper boundary condition (at the mixing height) given in Table 5.14b for models having the same classification as the reference model.

[c]Numbers in parentheses refer to treatments of the lower boundary condition (at the earth's surface) given in Table 5.14c for models having the same classification as the reference model.

[d]Numbers in parentheses refer to treatments of the boundary condition at vertical sides given in Table 5.14d for models having the same classification as the reference model.

[e]Numbers in parentheses refer to treatments of initial conditions given in Table 5.14e for models having the same classification as the reference model.

[f]See also the description of the treatment of the upper boundary condition.

[g]CRSTER should be used only when the receptor height is below the stack height.

Table B.13 Treatment of Temporal Correlations by Reference Models

Reference Model	Type of Treatment	Degree of Temporal Resolution and Quantities Correlated[a]
APRAC-1A	Sequential; correlations automatic.	Emissions a function of hour of the day and day of the week. Wind speed, direction, stability and mixing height are functions of hour of the day. (1a)
ATM	Non-sequential (climatological); limited correlation between some meteorological parameters.	Wind speed, wind direction, stability correlated via stability wind rose. Emission rates constant, not correlated with other parameters. Mixing height correlated with stability class through limits on σ_z, different limit for each class. (2b)
CDM	Non-sequential (climatological); limited correlation between total emission rate and meteorological parameters.	Wind speed, wind direction, stability correlated via stability wind rose. Mixing height adjusted according to stability class: Class A--1.5 x (afternoon climatological value). Class D (night)--average of morning and afternoon climatological values. Class E--Morning climatological value. Class B, C, D (day)--Appropriate climatological value. Emission rates: day-night variations allowed; all sources vary by same factor. (2b)
Single Source[b] (CRSTER)	Sequential; correlations automatic for meteorological parameters.	User supplies hourly values of wind speed, wind direction, mixing height, and other meteorological variables required for determining stability class and plume rise. Monthly emission variation allows limited emission-meteorology correlations. (1c)
DIFKIN	Sequential treatment up to 24 hours; correlations automatic.	Parameters updated each hour: mobile emissions from each grid square, wind speed and direction (trajectory); vertical diffusivity values at each height, mixing height, NO_2 photalysis rate constant. Update based on user input values. (1b)
HIWAY	Not applicable.	Not applicable; user inputs specific parameter values for the hour of interest.
RAM	Sequential treatment; correlations automatic for meteorological parameters.	User supplies hourly values of wind speed, wind direction, mixing height, and other meteorological variables required for determination of stability class and plume rise. Emission rates constant, not correlated with other parameters. (1c)
SAI	Sequential treatment up to 24 hours; correlations automatic.	Parameters updated every hour: mobile source emission for each ground-level grid square, point source (power plant) emissions, wind speed and direction, mixing height at every vertical column of grids, vertical eddy diffusivity at every vertical interface of grid cells, incoming fluxes at boundaries, NO_2 photalysis rate constant. Update based on user input values. (1a)
STRAM	Sequential treatment; correlations automatic for meteorological variables.	Stability class and mixing height changed each hour based on user-input values. Horizontal components of windfield updated at 12 hour intervals based on radiosonde data; changed each hour by interpolation between updates. Emission rates constant; not correlated with other parameters. (1c)
Valley	Non-sequential (climatological); limited correlation for meteorological variables.	Wind speed, direction, stability correlated via stability wind rose. Emission rates constant; not correlated with other parameters.

Table B.13 (Cont'd)

Reference Model	Type of Treatment	Degree of Temporal Resolution and Quantities Correlated[a]
Valley (Cont'd)		Mixing height adjusted according to stability class: (2b) •Long-term mode Class A: 1.5x (afternoon value) Class B,C: Afternoon value. Class D(day): Afternoon value for 60% of cases. Class D(night): Urban--0.5x((afternoon value) + (nighttime value)) for 40% of cases. Rural--0.5x(afternoon value for 40% of cases. Class E,F: Urban--nighttime mixing height (dispersion treated as Class D). Rural--No limit. •Short-term mode Class A,B,C,D: Afternoon value. Class E,F: Same as long-term mode.

[a]Numbers in parentheses refer to treatment numbers in Table 5.15.

[b]CRSTER should be used only when receptor height is below stack height.

B.2 REFERENCE MODEL ABSTRACTS AND EQUATIONS

This appendix provides abstracts and working equations for each reference model identified and suggested for use with this workbook. A glossary of symbols is given at the end of this appendix.

B.2.1 CDM

Reference: Busse and Zimmerman (1973), Brubaker, et. al. (1977).

Abstract: The Climatological Dispersion Model (CDM) is a climatological steady-state Gaussian plume model for determining long-term (seasonal or annual) arithmetic average pollutant concentrations at any ground level receptor in an urban area.

A statistical model based on Larsen (1968) is used to transform the average concentration data from a limited number of receptors into expected geometric mean and maximum concentration values for several different averaging times.

Equations:

$$\chi_{point} = \frac{16}{2\pi} \sum_{n=1}^{N} \sum_{\ell=1}^{6} \sum_{m=1}^{6} Q_n \, \phi_{k_n \ell m} \, S_{\ell m}(\rho_n)/\rho_n$$

$$\chi_{area} = \frac{16}{2\pi} \int \left[\sum_{k=1}^{16} q_k(\rho) \sum_{\ell=1}^{6} \sum_{m=1}^{6} \phi_{k\ell m} \, S_{\ell m}(\rho) \right] d\rho$$

$$\text{with } q_k(\rho) = \int_{\text{Sector k}} Q(\rho,\theta) d\theta$$

$$S_{\ell m}(\rho) = \frac{2}{\sqrt{2\pi}\, \sigma_z \, u_\ell} \exp\left[-\frac{1}{2} \left(\frac{H}{\sigma_z} \right)^2 \right] \exp\left[-\frac{0.692\rho}{u_\ell \, T_{1/2}} \right] \text{ for } \sigma_z \leq 0.8L$$

$$S_{\ell m}(\rho) = \frac{1}{u_\ell L} \exp\left[-\frac{0.692\,\rho}{u_\ell T_{1/2}} \right] \text{ for } \sigma_z > 0.8L$$

$\sigma_z = a\rho^b$; a, b = functions of stability class (m) and downwind distance (ρ) - three ranges of distance used: 100 - 500, 500 - 5000, 5000 - 50000 m

Calibration: $\chi_{calibrated} = \chi_{background} + A + B\,\chi_{uncalibrated}$

with $\chi_{uncalibrated} = \chi_{point} + \chi_{area}$

Statistical transformation of averaging times for 1-24 hour averages.

B.2.2 RAM

Reference: Hrenko and Turner (1975).

Abstract: RAM is a steady state Gaussian plume model for estimating concentrations of relatively stable pollutants for averaging times from an hour to a day in urban areas from point and area sources. Level or gently rolling terrain is assumed. Calculations are performed for each hour.

Equations:

Contribution from single upwind area source

$$\chi_A = \frac{Q}{u} \int_{x_1}^{x_2} f \, dx, \quad \text{integral evaluated numerically}$$

x_1, x_2 = points of intersection of ray from receptor through area source in question.

Stable conditions: $f = \frac{1}{\sqrt{2\pi}\,\sigma_z} g_2$

$$\chi_{point} = \frac{Q}{2\pi u \sigma_y \sigma_z} g_1 g_2$$

Neutral or stable conditions with $\sigma_z \leq 1.6L$

$$f = \frac{1}{\sqrt{2\pi}\,\sigma_z} g_3$$

$$\chi_{point} = \frac{Q}{2\pi u \sigma_y \sigma_z} g_1 g_3$$

Neutral or unstable conditions with $\sigma_z > 1.6L$

$$f = \frac{1}{L}$$

$$\chi_{point} = \frac{Q}{\sqrt{2\pi}\, uL\sigma_y} g_1$$

In which

$$g_1 = \exp\left[-\frac{1}{2} \left(\frac{y}{\sigma_y} \right)^2 \right]$$

$$g_2 = \exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]$$

$$g_3 = \sum_{n=-\infty}^{+\infty}\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H+2nL}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+H+2nL}{\sigma_z}\right)^2\right]\right\}$$

Mixing Height Algorithm:

Two different mixing heights can be calculated. One is for basically rural surroundings; the other is for urban locations. The user is given the option to specify which he wants to use. The way in which hourly mixing heights are determined from maximum mixing heights (MXDP) for yesterday (i-1), today (i) and tomorrow (i+1) and minimum mixing height (MNDP) for today (i) and tomorrow (i+1) is depicted in Figure B.1.

For urban mixing height, between midnight and sunrise; if the stability is neutral interpolate between $MXDP_{i-1}$ and $MXDP_i$ (1), if stability is stable use $MNDP_i$ (2). For hours between sunrise and 1400, if the hour before sunrise was neutral, interpolate between $MXDP_{i-1}$ and $MXDP_i$ (3). For sunrise to 1400, if the hour before sunrise was stable, interpolate between $MNDP_i$ and $MXDP_i$ (4). For 1400 to sunset, use $MXDP_i$ (5). For hours between sunset and midnight; if stability is neutral interpolate between $MXDP_i$ and $MXDP_{i+1}$ (6), if stability is stable interpolate between $MXDP_i$ and $MNDP_{i+1}$ (7).

For rural mixing height between midnight and sunrise, interpolate between $MXDP_{i-1}$ and $MXDP_i$ (8). For hours between sunrise and 1400, if the hour before sunrise was neutral interpolate between $MXDP_{i-1}$ and $MXDP_i$ (9). For sunrise to 1400, if the hour before sunrise was stable, interpolate between 0 and $MXDP_i$ (10). For 1400 to sunset, use $MXDP_i$ (11). For sunset to midnight, interpolate between $MXDP_i$ and $MXDP_{i+1}$ (12).

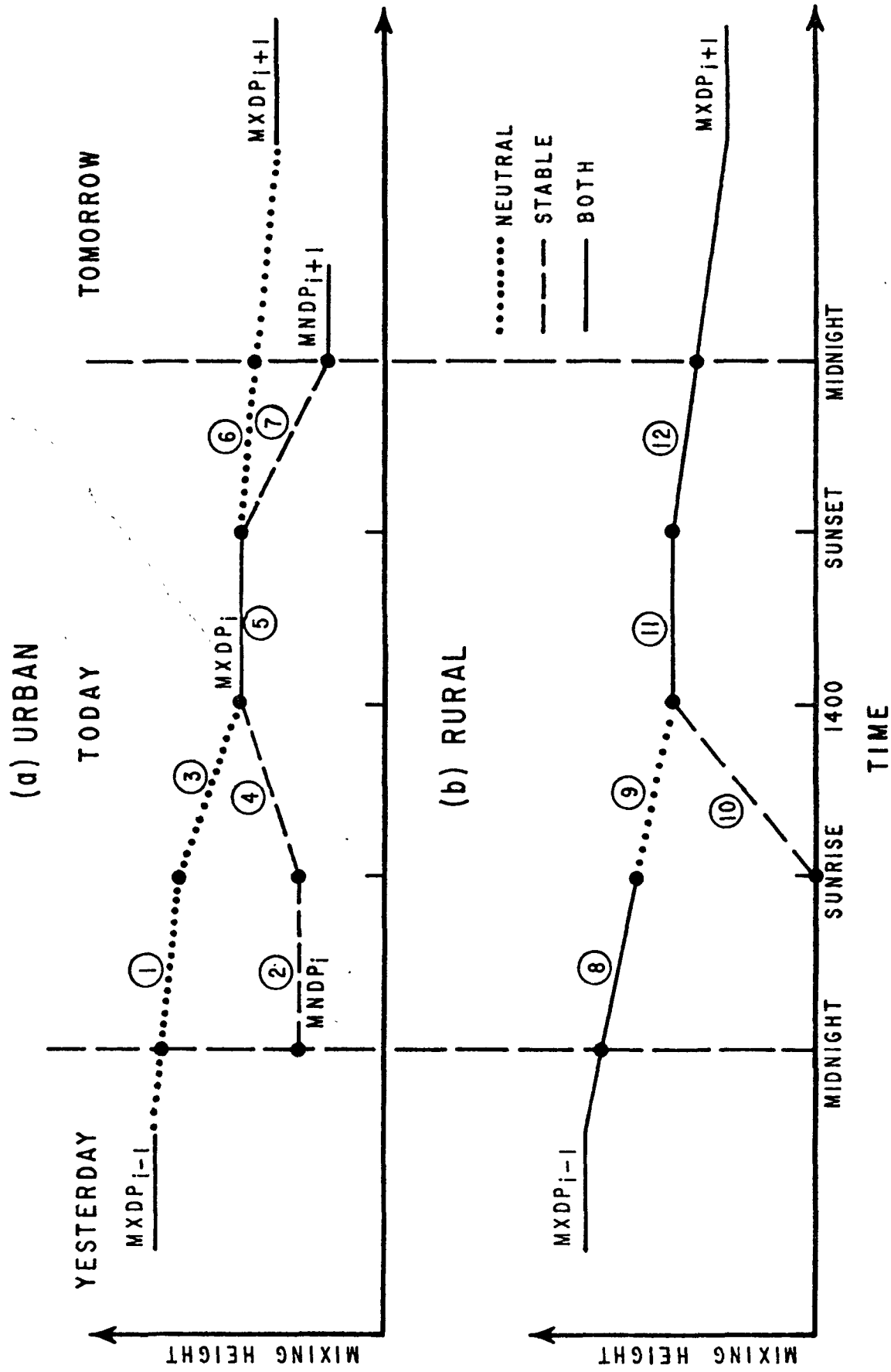


Figure B.1. Mixing Height Algorithm Used in RAM

B.2.3 Single Source (CRSTER)

Reference: EPA (1977).

Abstract: Single Source (CRSTER) is a steady state Gaussian plume technique applicable where terrain elevation does not exceed physical stack height. The purposes of the technique are: 1) to determine the maximum 24-hour concentration from a single point source of up to 19 stacks for one year, 2) to determine the meteorological conditions which cause the maximum concentrations, and 3) to store concentration information useful in calculating frequency distributions for various averaging times. The concentration for each hour of the year is calculated and midnight-to-midnight averages are determined for each 24-hour period.

Equations:

$$\chi = \frac{Q}{2\pi u \sigma_y \sigma_z} g_1 g_3 \qquad \text{for } \sigma_z \leq 1.6L$$

$$\chi = \frac{Q}{2\pi u L \sigma_y} g_1 \qquad \text{for } \sigma_z > 1.6L$$

$\chi = 0$ (stability class 7)

L = constant, independent of downwind distance

D = (stack height + plume rise) - (difference in elevation between receptor and base of stack)

$$g_1 = \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]$$

$$g_3 = \sum_{n=-\infty}^{+\infty}\left\{\exp\left[-\frac{1}{2}\left(\frac{2nL-D}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2nL+D}{\sigma_z}\right)^2\right]\right\}$$

Mixing Height Algorithm:

Two different mixing heights can be calculated. One is for basically rural surroundings, the other is for urban locations. The user is given the option to specify which he wants to use. The way in which hourly mixing heights are determined from maximum mixing heights (MXDP) for yesterday (i-1), today (i) and tomorrow (i+1) and mimimum mixing height (MNDP) for today (i) and tomorrow (i+1) is depicted in Figure B.2.

For urban mixing height between midnight and sunrise; if the stability is neutral interpolate between $MXDP_{i-1}$ and $MXDP_i$ (1), if stability is stable use $MNDP_i$ (2). For hours between sunrise and 1400, if the hour before sunrise was neutral, interpolate between $MXDP_{i-1}$ and $MXDP_i$ (3). For sunrise to 1400, if the hour before sunrise was stable, interpolate between $MNDP_i$ and $MXDP_i$ (4). For 1400 to sunset, use $MXDP_i$ (5). For hours between sunset and midnight; if stability is neutral interpolate between $MXDP_i$ and $MXDP_{i+1}$ (6), if stability is stable interpolate between $MXDP_i$ and $MNDP_{i+1}$ (7).

For rural mixing height between midnight and sunrise, interpolate between $MXDP_{i-1}$ and $MXDP_i$ (8). For hours between sunrise and 1400, if the hour before sunrise was neutral interpolate between $MXDP_{i-1}$ and $MXDP_i$ (9). For sunrise to 1400, if the hour before sunrise was stable, interpolate between 0 and $MXDP_i$ (10). For 1400 to sunset, use $MXDP_i$ (11). For sunset to midnight, interpolate between $MXDP_i$ and $MXDP_{i+1}$ (12).

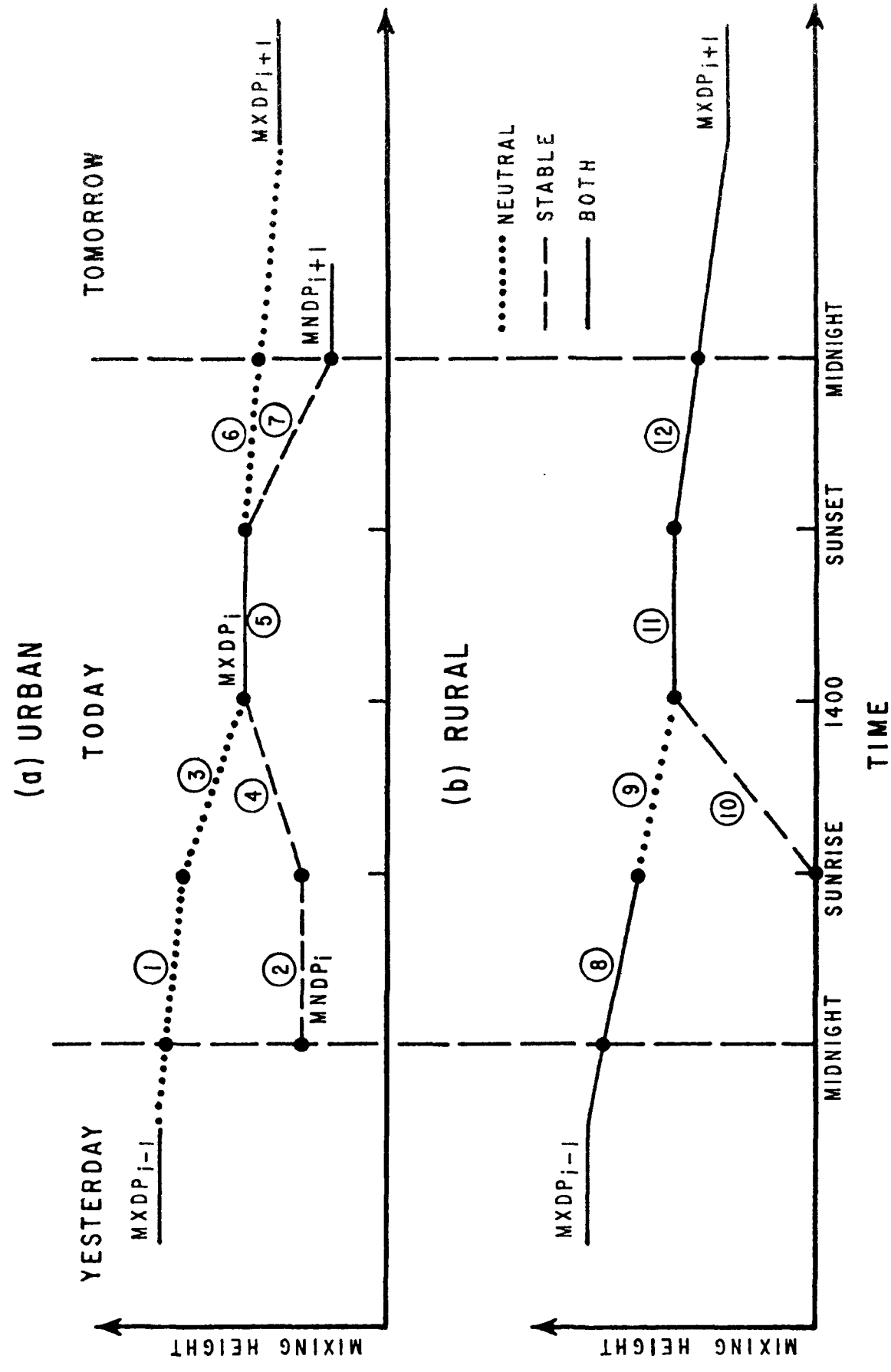


Figure B.2. Mixing Height Algorithm Used in CRSTER

B.2.4. Valley

Reference: Burt (1977).

Abstract: Valley is a climatological, Gaussian model whose primary intended use is the estimation of the maximum 24-hour SO_2 and TSP concentrations at ground level from single facilities in rural complex terrain, although annual average SO_2 and TSP concentrations may also be estimated and flat terrain applications are possible.

Equations:

- Long-term calculations:

$$\chi = \sum_{n=1}^{N} \chi_n \quad \text{,where}$$

$$\chi_n = \sum_{k=1}^{16} \sum_{\ell=1}^{6} \sum_{m=1}^{6} \phi_{k\ell m}\, \theta_{km}\, \chi_{k\ell mn} \quad \text{, where } \theta_{kn} \text{ is a function of}$$

crosswind distance of the receptor from the mean position of the plume from source n for direction k, and where for:

Neutral or unstable conditions -

$$\chi_{k\ell mn} = \frac{16}{2\pi\rho_n} \frac{Q_n}{u_\ell} g_3 \exp -\left[\frac{0.693\rho_n}{u_\ell T_{1/2}}\right]$$

$$g_3 = \frac{2}{\sqrt{2\pi}\,\sigma_{zm}} \sum_{i=-5}^{5} \exp\left[-\frac{1}{2}\left(\frac{2iL_m + H_{\ell m \rho u_\ell}}{\sigma_{zm}}\right)^2\right]$$

for $\sigma_{zm} \leq 2L_m$

$$g_3 = \frac{1}{L_m} \text{ for } \sigma_{zm} > 2L_m$$

$$\chi_{k\ell mn} = 0 \text{ if } H_{\ell m \rho u_\ell} > L_m$$

Stable conditions -

$$\chi_{k\ell mn} = \frac{16}{2\pi\rho_n} \frac{Q_n}{u_\ell} \frac{2}{\sqrt{2\pi}\sigma_{zm}} \exp\left[-\frac{1}{2}\left(\frac{H_{\ell m\rho u_\ell}}{\sigma_{zm}}\right)^2\right] \exp\left[-\frac{0.693\rho_n}{u_\ell T_{1/2}}\right]$$

Define D = (stack height + plume rise) - (receptor elevation)

if $D \geq 10$ meters, set H = D

if $D < 10$ meters, set H = 10 meters and interpolate concentration linearly to zero at a height of 400 meters above (stack height + plume rise).

- Short-term calculations:

  (Maximum 24-hour concentration for a single elevated point source.)

  $$\chi = \frac{6}{24} \chi_{k\ell mn}$$

  with $\chi_{k\ell mn}$ given by the stable conditions formula on the preceding page, and with

  ℓ = wind speed class index corresponding to u_ℓ = 2.5 meter/sec, and

  m = 6 (Pasquill-Gifford "F" stability class).

  k may be assigned the full range from 1 to 16, or any part(s) thereof, depending upon the relative location of sources and receptors. If k, ℓ, m or n assumes multiple values, then a summation must be effected as in long-term concentrations above; in this case, H and σ_z should be subscripted with ℓ and/or m, as appropriate. This is not the recommended method of application.

  $H_{\ell m\rho u}$ is reassigned the value of the adjusted L_m if the calculated or assigned $H_{\ell m\rho u} > L_m$.

B.2.5. ATM

Reference: Culkowski and Patterson (1976).

Abstract: The Atmospheric Transport Model (ATM) is a climatological steady-state Gaussian plume model for use in mesoscale range (up to 50 km) modeling. This model includes the effect of surface roughness on dispersion coefficients, treats dry deposition and precipitation scavenging, and treats gravitational settling of heavy particulates using a tilted plume approximation. The model is primarily intended for calculating monthly averages but averages for other time periods can be estimated by the use of appropriate climatological data. Although the treatment of ATM is comprehensive in the Workbook, the model should only be used for point source deposition applications at this time.

Equations:

$$\chi_{point} = \sum_{n=1}^{N} \sum_{\ell=1}^{8} \sum_{m=1}^{6} \bar{Q}_{n\ell m}(\rho_n)\, \phi_{k_n \ell m}\, S_{\ell m}(\rho_n)/\rho_n$$

with $$\bar{Q}_{n\ell_m}(\rho_n) = Q_n \left[f_w \exp(-\lambda\rho_n/u_\ell) + \exp\left[-(v_g/u_\ell)\, f_m(\rho_n) \right] \right]$$

= effective source strength

= true source strength modified by depletion of pollution due to deposition and washout at distances less than ρ_n.

λ = washout coefficient

= $5.55 \left[\text{Rainfall rate (mm/hr)} \right]^{0.6}$

v_g = dry deposition velocity (meter/sec)

$$f_m(\rho_n) = \sqrt{2/\pi} \int_o^{\rho_n} \left(\frac{1}{\sigma_z} \right) \exp(-H^2/2\sigma_z^2)\, dx$$

f_w = fraction of the time washout occurs

$$S_{\ell m}(\rho_n) = \frac{2.032}{\sigma_z u_\ell} \exp(-H^2/2\sigma_z^2)$$

σ_z = vertical dispersion coefficient, a function of stability class (m) and downwind distance (ρ_n)

The equations for the emission rate from a windblown source are quite complex and will not be given here.

B.2.6. STRAM

Reference: Hales, et. al. (1977).

Abstract: STRAM (Source-Transport-Receptor Analysis Model) is a trajectory model using a Gaussian crosswind pollutant distribution designed to estimate ground-level concentrations of pollutants over source-receptor distances of up to approximately 1000 km. STRAM is designed to treat SO_2 emissions from several elevated point sources and the conversion of SO_2 to sulfate aerosol.

Equations:

(1) Unlimited mixing height case:

$$C_i = \frac{\Omega_i(x)}{2\pi\sigma_y\sigma_z u} \exp(-y^2/2\sigma_y^2)\left\{\exp\left[-\frac{(z-h)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z+h)^2}{2\sigma_z^2}\right]\right\}$$

$$\frac{d\Omega_i}{dx} = R_i - \frac{\lambda_i\Omega_i}{u} - \sqrt{2/\pi}\left(\frac{\Omega_i v_{di}}{\sigma_z u}\right)\exp(-h^2/2\sigma_z^2)$$

$\Omega_i = Q_{oi}$ = the emission rate of the ith source at x = 0.

(2) For a limited mixing height (L):

$$C_i = \frac{\Omega_i(x)}{\sqrt{2\pi}\, uL\sigma_y} \exp(-y^2/2\sigma_y^2)$$

$$\frac{d\Omega_i}{dx} = R_i - \frac{\lambda_i\Omega_i}{u} - \frac{\Omega_i v_{di}}{uL}$$

$\Omega_i = Q_{oi}$ at x = 0.

Where C_i = ground level concentration of species i.

Ω_i = total mass of species i in the plume passing a downwind plane per unit time

$$R_i = \int_0^{\infty}\int_{-\infty}^{\infty} r_i(x,y,z)\,dy\,dz$$

r_i = rate of gain (or loss) of species i by chemical reaction

λ_i = washout coefficient for species i

v_{di} = dry deposition velocity for species i.

B.2.7. APRAC-1A

Reference: Ludwig and Mancuso (1972) and Ludwig and Dabbert (1972).

Abstract: APRAC is a model which computes hourly average carbon monoxide concentrations for any urban location. The model calculates contributions from dispersion on various scales: extraurban, mainly from sources upwind of the city of interest; intraurban, from freeway, arterial, and feeder street sources; and local, from dispersion within a street canyon. APRAC requires an extensive traffic inventory for the city of interest.

Equations:

Extraurban - $\chi_e = \frac{5.15 \times 10^{-11} F}{uL}$; F = annual fuel consumption within 22.5° sector extending from 32 km to 1000 km upwind of receptor.

Intraurban - $\chi_{ij} = \frac{0.8Q_i}{ua_{ij}} \left(\frac{x_{i+1}^{1-b_{ij}} - x_i^{1-b_{ij}}}{1-b_{ij}} \right)$ until this expression equals

the "box model value" $\frac{Q_i}{uL} \left(x_{i+1} - x_i \right)$

Thereafter the box model formula is used.

i = upwind area segment label

j = stability class label

a_{ij} and b_{ij} from $(\sigma_z)_{ij} = a_{ij} x^{b_{ij}}$ for x within segment i

Street Canyon - Lee side $\chi_L = \frac{KQ_s}{(u+0.5)\ [(x^2 + z^2)^{\frac{1}{2}} + L_o]}$

Windward side $\chi_W = \frac{KQ_s\ (B-z)}{(u+0.5)\ SB}$

Intermediate wind direction $\chi_I = \frac{1}{2} (\chi_L + \chi_W)$ (less than ±30° from street direction).

In which

x = horizontal distance from traffic lane

z = height above pavement

K = constant $\simeq 7$

L_o = vehicle size $\simeq 2$ meters

u = rooftop wind speed

Q_s = CO emission rate/meter

S = street width

B = average building height $\simeq 38.8$ meters

B.2.8. HIWAY

Reference: Zimmerman and Thompson (1975).

Abstract: HIWAY is a Gaussian plume model that computes the hourly concentrations of non-reactive pollutants downwind of roadways. It is applicable for uniform wind conditions and level terrain. Although best suited for at-grade highways, it can also be applied to depressed highways (cut sections).

Equations:

$$\chi = \frac{q}{u} \int_0^D f \, d\ell$$ integral along length of line segment, evaluated using trapezoidal rule.

q = CO emission rate/unit length

for stable conditions or if mixing height $L \geq 5000$ m

$$f = \frac{1}{2\pi\sigma_y\sigma_z} g_1 g_2,$$

for neutral or unstable conditions, with $\sigma_z \leq 1.6\ L$

$$f = \frac{1}{2\pi\sigma_y\sigma_z} g_1 g_3 ,$$

for neutral or unstable conditions, with $\sigma_z > 1.6L$

$$f = \frac{1}{\sqrt{2\pi}\,\sigma_y L} g_1$$

with

$$g_1 = \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2 \right]$$

$$g_2 = 2$$

$$g_3 = 2 \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{1}{2}\left(\frac{2nL}{\sigma_z}\right)^2 \right]$$

B.2.9. DIFKIN

Reference: Martinez, et.al. (1973).

Abstract: The DIFKIN (Diffusion/Kinetics) model is a numerical/dynamic (trajectory) model for photochemical smog simulation. It determines the trajectory of an air parcel across an emission grid network and calculates pollutant concentrations as functions of time. The model obtains concentrations and fluxes at up to ten mesh points between ground level and the top of the mixing layer.

Equations:

DIFKIN numerically solves the vertical diffusion equation

$$\frac{\partial c_\ell}{\partial t} = \frac{\partial}{\partial z}\left(K_V \frac{\partial c_\ell}{\partial z}\right) + R_\ell \quad \text{for } \ell = 1, 2, \ldots, p$$

Along a trajectory determined from surface wind measurements, subject to the following initial and boundary conditions:

A. Initial Conditions

$C_\ell(z, t_{initial}) = f_\ell(z)$ = initial concentration distribution for species ℓ,

B. Boundary Conditions

(1) $z = 0$ (at ground level)

$$-K_V \frac{\partial c_\ell}{\partial z} = q_\ell(t)$$ (perfect reflection plus addition of emissions from ground level flux)

(2) $z = L(t)$ (at mixing height)

$$-K_V \frac{\partial c_\ell}{\partial z} = 0$$ (perfect reflection)

where c_ℓ = mean concentration of species ℓ

R_ℓ = rate of production (or depletion) of species ℓ through chemical reaction

K_V = vertical eddy diffusivity, a function of height z.

$q_\ell(t)$ = ground-level flux of species ℓ

B.2.10. SAI

Reference: Reynolds (1973).

Abstract: The SAI model is a numerical/dynamic model for studying the dispersion of photochemical pollutants, employing a fixed grid coordinate system and a finite difference solution of the atmospheric diffusion equation. The model calculates an emission inventory based on extensive traffic input data as well as stationary source emissions. It requires extensive meteorological data including both spatial and temporal variations and uses a kinetic mechanism for photochemical smog involving fifteen chemical reactions and ten chemical species.

Equations:

SAI numerically solves the advection-diffusion equation:

$$\frac{\partial}{\partial t}(\Delta H c_\ell) + \frac{\partial}{\partial x}(u \Delta H c_\ell) + \frac{\partial}{\partial y}(v \Delta H c_\ell) + \frac{\partial}{\partial \rho}(W c_\ell)$$

$$= \frac{\partial}{\partial x}\left(K_H \Delta H \frac{\partial c_\ell}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \Delta H \frac{\partial c_\ell}{\partial y}\right)$$

$$+ \frac{\partial}{\partial \rho}\left(\frac{K_V}{\Delta H}\frac{\partial c_\ell}{\partial \rho}\right) + R_\ell \Delta H + S_\ell \Delta H, \quad \ell = 1, 2, \ldots, p$$

where $\Delta H = H(x,y,t) - h(x,y)$ = elevation difference between the mixing height and ground level,

$W = w - \rho \frac{\partial(\Delta H)}{\partial t}$, and

$\rho = \frac{z - h(x,y)}{H(x,y,t) - h(x,y)}$

subject to the following:

A. Initial Conditions

$c_\ell(x,y,\rho,t_{initial}) = f_\ell(x,y,\rho)$ = initial concentration distribution fc species ℓ,

B. Boundary Conditions

(1) $\rho = 0$ (at ground level)

$$-\frac{K_V}{\Delta H}\frac{\partial c_\ell}{\partial \rho} = q_\ell(x,y,t)$$ (perfect reflection plus addition of emissions from ground level flux)

(2) $\rho = 1$ (at mixing height)

$$Wc_\ell - \frac{K_V}{\Delta H}\frac{\partial c_\ell}{\partial \rho} = Wg_\ell \quad \text{if } W \leq 0$$ (material from outside of region entrained if mixing height is increasing)

$$-\frac{K_V}{\Delta H}\frac{\partial c_\ell}{\partial \rho} = 0 \quad \text{if } W > 0$$ (perfect reflection with no entrainment otherwise)

(3) $x = x_E$ or x_W (along the east or west vertical boundaries)

$$uc_\ell - K_H\frac{\partial c_\ell}{\partial x} = ua_\ell \quad \text{if } \vec{U}\cdot\vec{n} \leq 0$$ (transport wind into region; material advected in from outside)

$$-K_H\frac{\partial c_\ell}{\partial x} = 0 \quad \text{if } \vec{U}\cdot\vec{n} > 0$$ (transport wind out of region)

(4) $y = y_N$ or y_S (along the north or south vertical boundaries)

Similar to (3), except involving v, the y- component of the wind.

where

$\vec{U}$ = horizontal wind vector

$\vec{n}$ = outwardly directed unit vector perpendicular to the vertical boundary

c_ℓ = mean concentration of species ℓ

p = number of species

u,v,w = components of wind in x, y, z directions

K_H, K_V = horizontal and vertical eddy diffusivities

S_ℓ = emission rate of species ℓ from elevated source

R_ℓ = production rate of species ℓ by chemical reaction

q_ℓ = ground-level flux of species ℓ

g_ℓ = concentration of species ℓ above region

ℓ = concentration of species ℓ outside region

x_N, x_S, x_E, x_W = northern, southern, eastern, western boundaries of region

$h(x,y)$ = terrain elevation

$H(x,y,t)$ = elevation of inversion base.

GLOSSARY OF SYMBOLS

A,B	Regression coefficients used in calibration procedures.
h	Stack height
$H_{\ell m p u}$	Effective stack height = (stack height) + (plume rise)
k	Wind sector index
k_n	Wind sector index corresponding to the sector containing the n-th source
ℓ	Wind speed class index
L	Mixing height (L_m if a function of stability)
m	Stability class index
n	Point and area source index
N	Total number of point and area sources
Q	Emission rate
Q_n	Emission rate for the n-th source
$T_{\frac{1}{2}}$	Pollutant half-life
u_ℓ	Representative horizontal wind speed for the ℓ-th wind speed class
u,v	Components of horizontal wind speed
w	Vertical wind speed
x	Downwind distance or distance in x-direction
y	Crosswind distance or distance in y-direction
z	Vertical distance
ρ	Downwind distance
σ_y, σ_z	Crosswind, vertical dispersion coefficients (subscripted with m if a function of stability)
$\phi_{k_n \ell m}$, $\phi_{k \ell m}$	Meteorological joint frequency function for wind in subcardinal direction k_n, k
χ	Pollutant concentration

APPENDIX C
APPLICATIONS TO SPECIFIC MODELS

APPENDIX C APPLICATIONS TO SPECIFIC MODELS

This appendix contains examples of the application of the methodology presented in this workbook to several specific atmospheric dispersion models. Each subsection deals with a different study model and illustrates the nature of the information required about a study model, the factors involved in making individual element-by-element comparisons with a reference model, and the process of arriving at a final technical evaluation. Each subsection consists of a body of text in which the reasons for obtaining the various element-by-element comparisons and the final technical evaluation are explained. In the first example, the entire procedure is illustrated. In subsequent examples, it is assumed that the first five steps in the comparison need little additional explanation and that the Application Classification Form and the Evaluation Form - Part A have been completed. In each example, the application for which the study model is considered has been chosen so that the study model is in fact applicable in order to illustrate the methodology. A complete set of forms for each example, filled out in accordance with the discussion presented in the text, is located at the end of each subsection. The user should refer to these completed forms while reading the text.

CONTENTS OF APPENDIX C

C.1 EXAMPLE 1: SCIM/1243

In this example, the application of interest involves estimating the maximum expected one-hour sulfur dioxide concentration in Sample City, a moderately sized urban area located in gently rolling terrain far from any large bodies of water. Each step in the entire methodology is illustrated. While reading the text, the user should refer to the completed forms at the end of the section.

The first step involves the classification of the application as explained in Section 3. With regard to pollutant characteristics, sulfur dioxide is a primary pollutant not subject to significant removal processes within the time scale of the application. The size of the region of interest is of the order of 50 km or less, and the residence time of a pollutant emitted within this region is less than 5-8 hours for typical wind speeds. As indicated in Table 3.1, the appropriate pollutant characteristics index number under these circumstances is one.

The averaging time is short (under 24 hours); the appropriate averaging time index number is two, as discussed in Section 3.4.

The Sample City emission inventory is assumed to contain both point and area sources and the appropriate source characteristics index number is therefore four, as explained in Section 3.5.

Finally, since the terrain in which Sample City is located is simple and the size of the region of interest is less than 100 km, the appropriate transport characteristics index number is three, as explained in Section 3.6.

The completed Application Classification Form for this example can be found at the end of this section. As indicated, the appropriate application index is 1243.

At this time, the basic information sections of the Evaluation Form - Part A are also completed by listing the reference documentation and preparing a short abstract describing SCIM's mode of operation.

This completes step 1.

The next step in the comparison involves the documentation of the study model equations. The references listed on the front of the Evaluation Form - Part A are used to determine the working equations shown on the reverse side of the form to complete step 2.

These references also indicate that SCIM selects a sample of one-hour periods from the total number in some period of record, typically one year. The sample is obtained by taking every n-th hour where n is an integer specified by the user. Having selected the sample, SCIM applies a steady-state Gaussian model separately to each hour in the sample and estimates from these results both the long term average concentration and the frequency distribution of one-hour concentrations. With this information, SCIM may be classified and its compatibility with the application of real interest checked (steps 3 and 4 in the comparison).

It is assumed, in this example, that the Sample City emission inventory is structured in a manner compatible with SCIM input requirements, specifically that all required source information is available, that area sources are defined in a suitable manner, that the number of point and area sources is within SCIM limitations, and so on. It is also assumed that the necessary meteorological and other data are available in the appropriate format.

The user has already classified the application and in the process has determined that sulfur dioxide transformation and removal are not important enough to select any other pollutant characteristics branch than number one. As a consequence, no check need be made at this point to determine whether or not SCIM incorporates treatments of these elements. Had the application index begun with number three, for example, indicating that some physical removal process is important, the user would have been required at this point to determine whether SCIM incorporates a treatment, however simplified, of that process. SCIM provides estimates of various percentile one-hour concentrations at each receptor, including the maximum expected value, and therefore does estimate precisely the quantity of interest. If the application had involved the estimation of the maximum 24-hour SO_2 concentration, SCIM would not have been found applicable, because it does not estimate this quantity directly, even though the necessary program modifications to do this calculation may be straightforward or even though the necessary calculations could easily be done by hand.

As a result of these checks and determinations, SCIM is found to be applicable to the application of interest. The "Applicable" box on Part A is checked to indicate this determination.

The description above also implies that SCIM is a simulation model and, in view of the guidelines for model classification in Section 4.3, the appropriate classification is:

Semiempirical/Sequential (Steady-State).

Step 5 simply involves referring to Table 4.1 to identify RAM as a suggested reference model for application 1243.

The next step (step 6) is to review the importance ratings of the application elements for application index number 1243 and to determine if modifications to these ratings are necessary to more accurately define the relative importance of the elements in the situation of real interest. Expert advice may be necessary in this step. It is assumed here that the importance ratings as given in Tables 4.2 - 4.13 are appropriate with the exception of those for composition of emissions and chemistry and reaction mechanism, which are modified from LOW to IRRELEVANT for purposes of this example. Notice that the rating for physical removal has not been changed from LOW to IRRELEVANT even though no physical removal process is considered important enough to affect the application classification. The distinction between LOW and IRRELEVANT is that, as explained in Section 4.4, the treatments of IRRELEVANT elements are not taken into account at all in the evaluation, while the treatments of LOW elements may be considered in certain cases. It is assumed for this example that the involvement of sulfur dioxide in atmospheric chemical reactions in and around Sample City is considered so unimportant that it should play no role at all in evaluating simulation models. Therefore, the elements "composition of emissions" and "chemistry and reaction mechanism" are in fact irrelevant. In contrast, it is assumed that dry deposition of sulfur dioxide, while not important enough to affect the application classification, nevertheless does occur and is not insignificant enough to be totally irrelevant. Thus, the importance rating of physical removal is kept at LOW. Both initial and modified importance ratings for each element are inserted in Part B of the Evaluation Form.

The next step (step 7) is the determination of the treatment by SCIM of all application elements not rated IRRELEVANT. Operating equations used by SCIM are reproduced on the reverse side of Part A of the evaluation form. Using these equations and the material in the references as sources, descriptions of the treatments by SCIM, together with the corresponding reference model treatments obtained from Tables B.2- B.13 and the importance ratings for each element, are entered on Part C of the evaluation form. The treatments by SCIM

were determined in accordance with the guidelines given in Section 5, supplemented by the discussions presented in Appendix A.

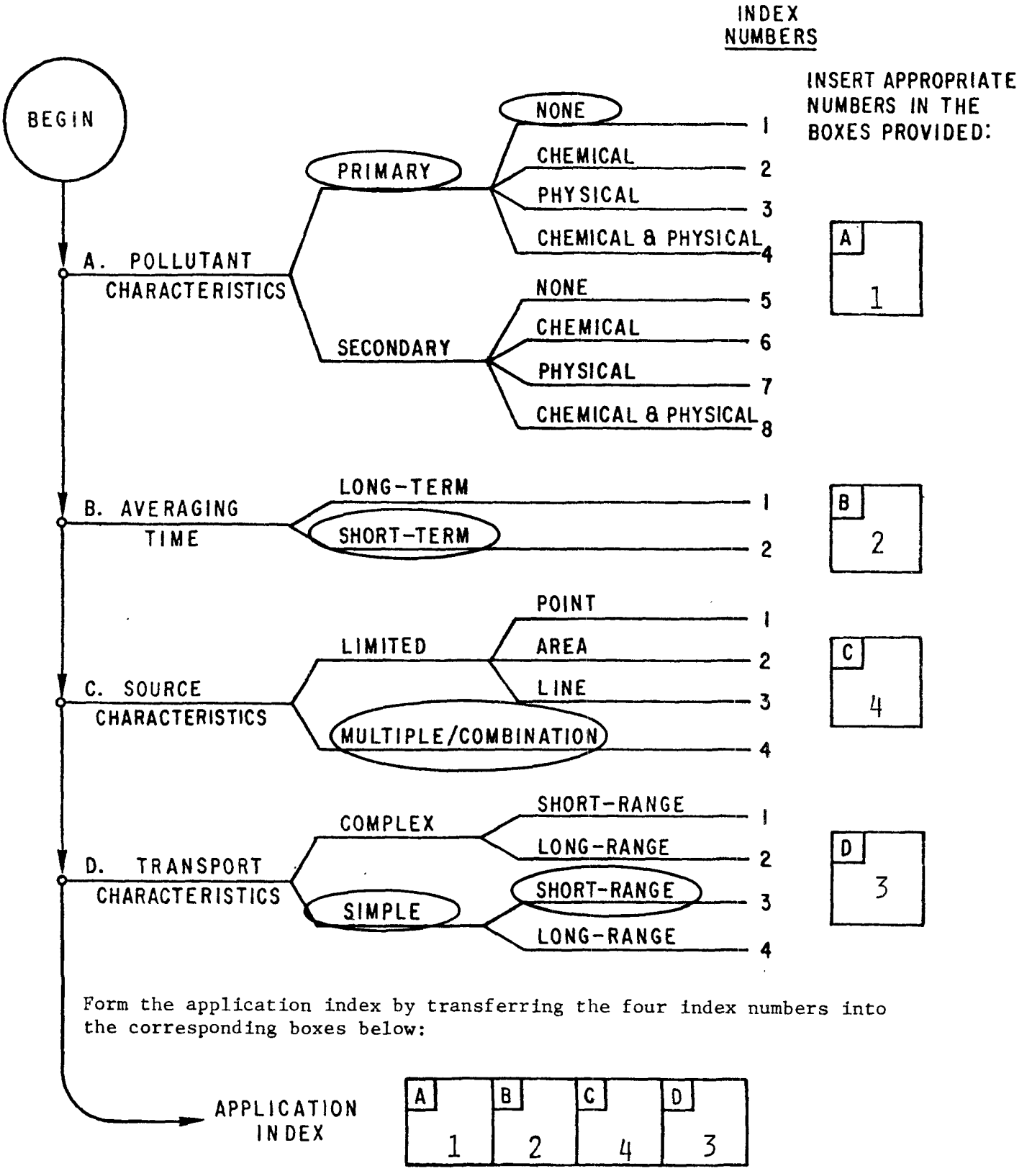
After both the study model and reference model treatments of a given element have been entered on the Evaluation Form - Part C, the comparison of these two treatments may be made using the guidelines in Section 6.2.1. The level of detail involved in each treatment is examined with reference to the relative ranking of treatments in Tables 5.1-5.15. The result of each comparison consists of the single adjective from the set BETTER, COMPARABLE, WORSE which most accurately describes the treatment used by the study model in comparison with that used by the reference model. This result is then entered in the place provided in each section of Part C.

The various treatments by SCIM and RAM of most application elements are clearly COMPARABLE, and are virtually identical in several cases. The exceptions are the elements horizontal wind field and background, boundary and initial conditions. The two treatments of horizontal wind field are basically COMPARABLE. However, SCIM does not employ a randomization procedure for wind direction and RAM does, with the result that SCIM only allows 36 different wind directions while RAM allows 360. Thus, SCIM may be somewhat WORSE in its treatment of the horizontal wind field. In cases of doubt, both results are indicated on the form; the primary evaluation as usual, followed by a secondary evaluation in parentheses (see the entries on Part C). The same situation arises for background, boundary and initial conditions. The two treatments are basically COMPARABLE, but SCIM may be a little WORSE because of its less detailed treatment of the upper boundary condition. On the other hand, SCIM allows a background value to be input. Both comparisons are indicated on Part C of the Evaluation Form.

In the cases of emission rate and temporal correlations, it is necessary to judge the importance of area source emissions in Sample City before making the comparisons because SCIM and RAM differ in the level of detail with which the temporal variation of area source emissions are described. The comparisons actually made in the example assume that area source contributions are not significant enough to justify rating the SCIM treatment BETTER. If these contributions were more important in the application, the additional detail in the SCIM treatment might justify a BETTER rating.

The synthesis of these individual comparisons into a final technical evaluation (step 9) is documented on the Evaluation Form - Part D. The guidelines in Section 6.2.2 are used to arrive at this final evaluation. In the example, there are no CRITICAL elements. Therefore, the initial evaluation is based on the comparisons for the three HIGH-rated elements. All of these comparisons are COMPARABLE, resulting in an initial comparative rating of COMPARABLE. Of the elements rated MEDIUM, all five have COMPARABLE treatments; therefore no change in the initial rating is indicated. Even if the secondary evaluations for horizontal wind field and background, boundary and initial conditions were used, they would not carry sufficient weight to alter the evaluation. Thus, the technical evaluation of SCIM for Application 1243 is that SCIM is COMPARABLE to the reference model, RAM. This evaluation is further supported by the distribution of comparisons for the LOW elements, although these would not be considered here, because the rating based upon HIGH and MEDIUM elements is unambiguous.

APPLICATION CLASSIFICATION FORM



EVALUATION FORM

Part A: Abstract and References

Study Model: Sampled Chronological Input Model (SCIM)

References: Koch, R.C. and G.H. Stadsklev, *A User's Manual for the Sampled Chronological Input Model (SCIM)*, GEOMET Report No. E-261, prepared for U.S. EPA under Contract No. 68-02-0281. (December 1974).

Koch, R.C. and S.D. Thayer, *Validation and Sensitivity Analysis of the Gaussian Plume Multiple - Source Urban Diffusion Model*, NTIS PB 206951, National Technical Information Service, Springfield, Va. 22151. (November 1971).

Abstract: The Sampled Chronological Input Model (SCIM) is a Gaussian plume-based model designed to estimate mean long-term pollutant concentrations and the frequency distribution and maximum of one-hour pollutant concentrations in an urban area.

Classification: Semiempirical/Sequential (Steady-State)

Application Index: 1243 Reference Model: RAM

Application Description: Maximum 1-hour SO_2 concentration in an urban area.

Model Applicability: Applicable [X] Not Applicable [ ]

EVALUATION FORM

Part A (reverse): Equations

Study Model: SCIM

Equations:

Point sources:

$$\chi_n = \frac{Q_n}{2\pi u \sigma_y \sigma_z} g_2 \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \exp\left(-\frac{kx}{u}\right)$$

$$\text{with } g_2(x,z;H) = \exp\left[-\frac{1}{2}\left(\frac{H-z}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{H+z}{\sigma_z}\right)^2\right]$$

Area sources:

$$\chi_A = \frac{1}{2\pi}\int_o^{x_d} \frac{\bar{q}(x)}{u\sigma_z} g_2(x,z;H) \exp\left(-\frac{kx}{u}\right) dx$$

with $\bar{q}(x) \cong q(x,o)$, $q(r,\theta)$ = emission rate per unit area at position (r,θ) from receptor

(Narrow plume approximation)

Integral evaluated using trapezoidal rule.

Total estimated concentration $\chi_{tot} = \chi_A + \sum_{n=1}^{N} \chi_n$

N = number of point sources

Vertical dispersion coefficient:

$$\sigma_z = ax^b \qquad x \leq x_1$$

$$\sigma_z = L \qquad x \geq x_2$$

$$\sigma_z = \frac{L}{2}\left(\frac{x+x_2-2x_1}{x_2-x_1}\right) \qquad x_1 < x < x_2$$

$$x_1 = \left(\frac{L}{2a}\right)^{1/b} \quad \text{and} \quad x_2 = \left(\frac{L}{a}\right)^{1/b}$$

EVALUATION FORM

Part B: Importance Ratings

Application Index: 1243

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship	M	M
Emission Rate	M	M
Composition of Emissions	L	I ✓
Plume Behavior	**H**	**H**
Horizontal Wind Field	**M**	**M**
Vertical Wind Field	L	L
Horizontal Dispersion	**H**	**H**
Vertical Dispersion	**H**	**H**
Chemistry and Reaction Mechanism	**L**	**I ✓**
Physical Removal Processes	**L**	**L**
Background, Boundary, Initial Conditions	**M**	**M**
Temporal Correlations	M	M

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element: Source-Receptor Relationship	Application Element: Emission Rate
Reference Model: RAM Treatment: Arbitrary location and release height for each point source. Flat terrain. Area sources defined as square cells (or multiples) in a rectangular array; up to three effective release heights (for u=5m/sec) user-specified. Arbitrary receptor locations - all at the same height above (or at) ground. Precise downwind, crosswind distances for each source-receptor pair. Sides of area sources must lie along grid boundary directions.	Reference Model: RAM Treatment: Arbitrary constant emission rate for each point and area source. Area source contributions obtained by numerical integration along upwind distance of narrow-plume approximation formulae for area source with given effective release height. Includes only those areas intersected by the upwind ray.
Study Model: SCIM Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE Treatment: Arbitrary location and emission height for point sources. Flat terrain. Arbitrary location and height for receptors. Area sources defined as square cells in up to three concentric arrays with user-defined grid sizes. Up to five user-defined release heights for area sources. Precise downwind and crosswind distance for each source-receptor pair.	Study Model: SCIM Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE Treatment: Arbitrary constant emission rate for each point source. Arbitrary average emission rate for each area source; area source emissions assumed functions of average emission rate, temperature and time of day. Area source contributions obtained by numerical integration along upwind distance of narrow-plume approximation formulae for area source with given effective release height; includes only those areas intersected by the upwind ray.

EVALUATION FORM

Part C : Treatment of Elements

Application Index: 1243

Application Element: Plume Behavior	Application Element: Horizontal Wind Field
Reference Model: RAM Treatment: Uses Briggs' (1971, 1972), downwind distance dependent plume rise for point sources. If plume height exceeds mixing height, ground level concentrations assumed zero. No plume rise calculated for area sources; assumed to be included in release height. Fumigation, downwash not treated.	Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Constant, uniform wind speed and direction assumed for each of a sequence of hours. Arbitrary wind speeds and direction values to 10° input by user; directions randomized by addition of $(n-4)^{o}$ with n = random integer from zero to nine. Wind speed is modified to correspond to value at release height, modification dependent only on stability class.
Study Model: SCIM Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Two step procedure using Briggs'(1969) for point sources. Not treated explicitly for area sources-assumed included in input release heights. If stack height +50% of plume rise exceeds mixing height, source is excluded. Fumigation, downwash not treated.	Study Model: SCIM Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE (WORSE) Treatment: Semiempirical/Sequential (Steady-State). Constant, uniform wind speed within each of sequence of one-hour periods. Arbitrary wind speeds and directions to 10° input by user. Wind speed modified (power law) to correspond to value at release height, modification procedure depends only on stability (unstable, neutral, stable).

EVALUATION FORM

Part C : Treatment of Elements

Application Index: 1243

Application Element: Vertical Wind Field	Application Element: Horizontal Dispersion
Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Assumed equal to zero (implicit).	Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed for point sources. Atmospheric stability divided into six (Pasquill-Gifford) classes, determined hourly. Dispersion coefficients from Turner (1969) or McElroy and Pooler (1968) at user option. Surface roughness not treated explicitly One hour averaging time used. Area sources: Narrow plume approximation.
Study Model: SCIM Importance Rating: LOW Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Assumed equal to zero (implicit).	Study Model: SCIM Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function for point sources. Atmospheric stability divided into four classes (urban) or five classes (rural), determined hourly. Dispersion coefficients: McElroy-Pooler (1968) for urban area, Pasquill-Gifford (Turner, 1969) for rural areas. Surface roughness not treated explicitly. One-hour averaging time. Area Sources: Narrow plume approximation.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element: Vertical Dispersion	Application Element: Physical Removal
Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes, determined hourly. Dispersion coefficients from Turner (1969) or McElroy and Pooler (1968) at user's option. Surface roughness not treated explicitly.	Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Exponential decay - first order (linear). Single, constant user-specified decay constant.
Study Model: SCIM Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function. Atmospheric stability divided into four classes (urban) or five classes (rural), determined hourly. Dispersion coefficients: McElroy-Pooler (1968) (urban), or Pasquill-Gifford (Turner, 1969) (rural). Surface roughness not treated explicitly.	Study Model: SCIM Importance Rating: LOW Comparative Evaluation: COMPARABLE Treatment: Exponential decay. Single, constant user-supplied decay constant.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element: Background, Boundary, Initial Conditions

Reference Model: RAM

Treatment: Background not treated explicitly. Both upper and lower boundaries - perfect reflection.

1) Neutral and unstable conditions: method of multiple images treated by summation of infinite series until σ_z = 1.6×(mixing height); uniform mixing assumed thereafter;

2) Stable conditions: mixing height assumed to have no effect.

Mixing height for a given hour obtained interpolation of radiosonde data.

Study Model: SCIM

Importance Rating: MEDIUM

Comparative Evaluation: COMPARABLE (WORSE)

Treatment: Background - Single Constant Value

Lower boundary - perfect reflection.

Upper boundary - implicit treatment; no effect until σ_z=0.5 (mixing height), maximum σ_z value = mixing height, linear interpolation on σ_z in transition region; transition distances determined using $\sigma_z = ax^b$.

Mixing height interpolated from radiosonde data.

Application Element: Temporal Correlations

Reference Model: RAM

Treatment: Sequential.

User supplies hourly values of wind speed, wind direction, mixing height, and other meteorological variables required for determination of stability class and plume rise. (Correlations automatic.)

Emission rates constant, not correlated with other parameters.

Study Model: SCIM

Importance Rating: MEDIUM

Comparative Evaluation: COMPARABLE

Treatment: Sequential.

User supplies hourly values of wind speed, direction, mixing height and other variables required for stability determination. (Correlations automatic.)

Point source emissions constant, not correlated with other parameters.

Area source emissions an empirical function of ambient temperature and hour of the day. (Correlations automatic.)

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element:	Application Element:
Reference Model:	Reference Model:
Treatment:	Treatment:
Two IRRELEVANT elements: • Composition of Emissions • Chemistry and Reaction Mechanism	
Study Model:	Study Model:
Importance Rating:	Importance Rating:
Comparative Evaluation:	Comparative Evaluation:
Treatment:	Treatment:

EVALUATION FORM

Part D: Technical Comparison

Application Index: 1243 Reference Model: RAM Study Model SCIM

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL	0	-	-	-	-
HIGH	3	0	3	0	COMPARABLE
MEDIUM	5	0	5 (3)	0 (2)	COMPARABLE
LOW[a]	2	0	2	0	
IRRELEVANT	2	XXX	XXX	XXX	
	Total 12 (Should equal 12)				

TECHNICAL EVALUATION COMPARABLE

[a]Used only in ambiguous cases.

C.2 EXAMPLE 2: AQDM/1143

The application of interest involves the estimation of long-term sulfur dioxide concentrations in Sample City, a moderately sized urban area located in gently rolling terrain, the same urban area used in Example 1, Appendix C.1. The appropriate application index is 1143 and the suggested reference model is CDM. The completed Application Classification Form and Evaluation Form for this example may be found at the end of this section.

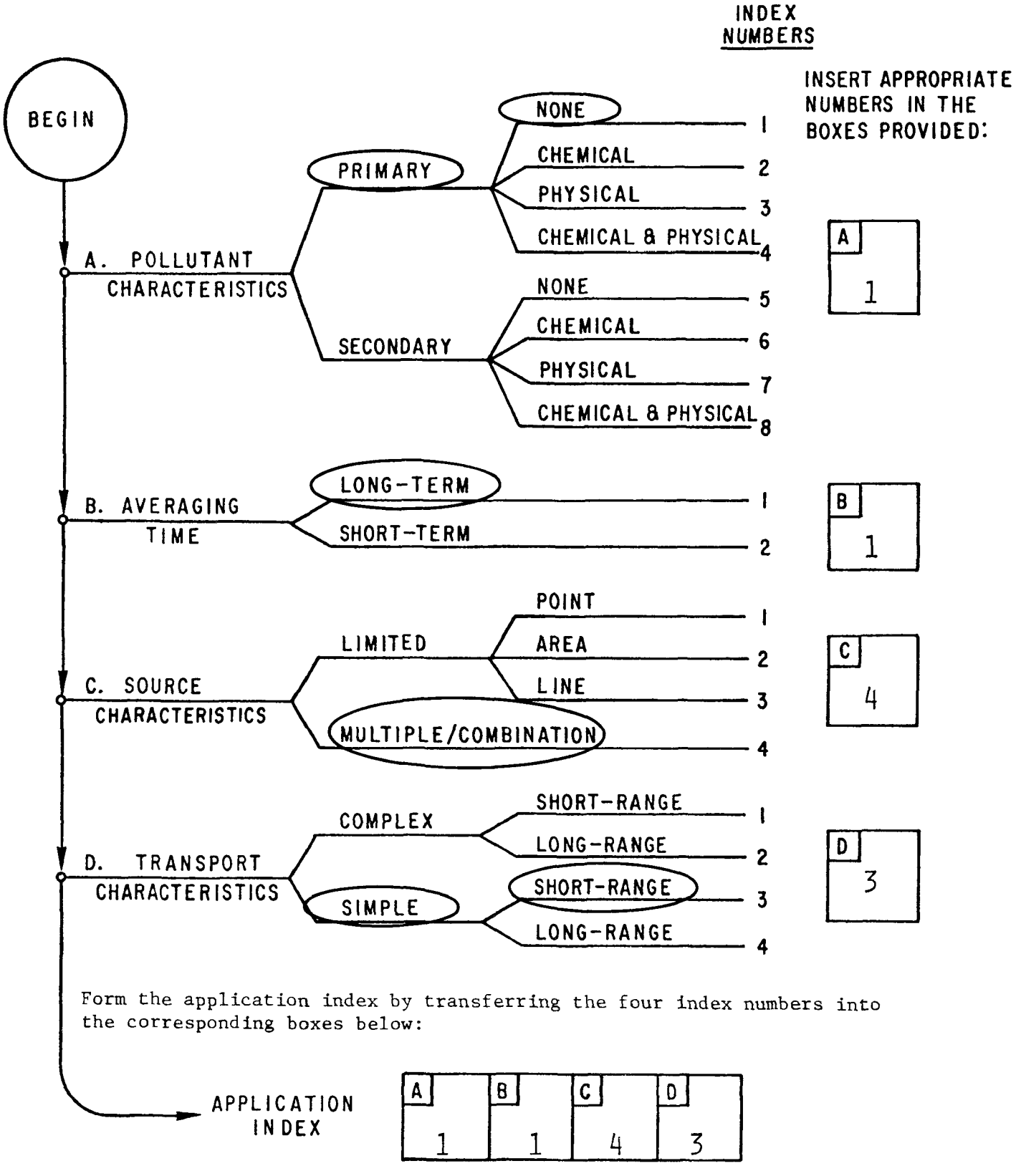
It is assumed that the user can classify AQDM, determine that AQDM is applicable, review and modify the importance ratings, determine the equations used by AQDM, and determine the treatments of the application elements by both AQDM and CDM. The classification and applicability checks are straightforward. The importance rating modifications are the same as in Example 1, specifically, that the elements composition of emissions and chemistry and reaction mechanism are rated IRRELEVANT due to the non-involvement of sulfur dioxide in atmospheric chemistry over the distances and times of interest. The determination of the equations and of the treatments are straightforward. The results are presented on the Evaluation Form-Part A(reverse) and C, respectively.

AQDM and CDM are similar in most respects and most comparisons result in COMPARABLE ratings. The two exceptions are emission rate and horizontal wind field, for both of which AQDM is rated WORSE. The AQDM treatment of emission rate is rated WORSE primarily because of the use of a single effective point source approximation for area sources instead of the more detailed numerical integration used by CDM, and secondarily because CDM allows a day/night variation in emission rates whereas AQDM allows no variation. The AQDM treatment of the horizontal wind field is rated WORSE, because CDM uses a wind speed which is corrected for emission height while AQDM does not incorporate any such variation.

With only one element rated of HIGH importance, the initial rating is the same as the rating for that element; in this case, the initial rating is COMPARABLE. The MEDIUM-rated elements, however, definitely show a bias toward a rating of WORSE. In this case, taking into account the relatively low number of HIGH-rated elements, the relatively high proportion of MEDIUM-rated elements for which AQDM uses a WORSE treatment, and the absence of any elements that are treated BETTER by AQDM, a change in the comparative rating of AQDM from COMPARABLE to WORSE is justified. Furthermore, the distribution of comparisons for

the LOW-rated elements supports this conclusion, although little weight should be given to the LOW-rated elements. Therefore, the appropriate technical evaluation for AQDM in application 1143 is WORSE.

APPLICATION CLASSIFICATION FORM



Form the application index by transferring the four index numbers into the corresponding boxes below:

EVALUATION FORM

Part A: Abstract and References

Study Model: Air Quality Display Model (AQDM)

References: TRW Systems Group. "Air Quality Display Model." Prepared for National Air Pollution Control Administration under Contract No. PH-22-68-60 (NTIS PB 189194), DHEW, U.S. Public Health Service, Washington, D.C., November 1969.

Abstract: The Air Quality Display Model (AQDM) is a climatological steady state Gaussian plume model that estimates annual arithmetic average sulfur dioxide and particulate concentrations at ground level. A statistical model based on Larsen (1969) is used to transform the average concentration data from a limited number of receptors into expected geometric mean and maximum concentration values for several different averaging times.

Classification: Semiempirical/Climatological (Steady-State)

Application Index: 1143 Reference Model: CDM

Application Description: Urban, long-term, conservative pollutants, simple terrain.

Model Applicability: Applicable [X] Not Applicable [ ]

EVALUATION FORM

Part A(reverse): Equations

Study Model: AQDM

Equations:

Point sources only.

$$\chi = \sum_{n=1}^{n} \sum_{\ell=1}^{6} \sum_{m=1}^{5} \phi_{k_n \ell m} \chi_{n\ell m}$$

N = Number of sources

with

$$\chi_{n\ell m} = \frac{16}{2\pi x} \frac{2Q_n}{2\pi\, u_\ell \sigma_z} \left(\frac{C-y}{C}\right) \exp\left[-\frac{1}{2}\left(\frac{H}{\sigma_z}\right)^2\right] \quad \text{for } x \leq x_L$$

$$\chi_{n\ell m} = \frac{16}{2\pi x} \frac{Q_n}{u\ell L} \left(\frac{C-y}{C}\right) \quad \text{for } x \geq 2x_L$$

linear interpolation for $x_L < x < 2x_L$

x_L is defined by $\sigma_z(x_L) = 0.47L$

y = crosswind distance between receptor and sector k centerline

C = sector width at receptor location

$\sigma_z(x) = ax^b + c$; a, b, c = functions of stability class (m)
a, b, c for neutral conditions split into
x > 1000m case and x ≤ 1000m case.

Calibration: $\chi_{calibrated} = A + B\left(\chi_{background} + \chi_{uncalibrated}\right)$
with $\chi_{uncalibrated}$ given by the first equation above.

Larsen (1971) statistical transformation of averaging times used for 1 - 24 hour averages.

EVALUATION FORM

Part B: Importance Ratings

Application Index: 1143

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship	M	M
Emission Rate	M	M
Composition of Emissions	L	I ✓
Plume Behavior	M	M
Horizontal Wind Field	M	M
Vertical Wind Field	L	L
Horizontal Dispersion	M	M
Vertical Dispersion	H	H
Chemistry and Reaction Mechanism	L	I ✓
Physical Removal Processes	L	L
Background, Boundary, Initial Conditions	M	M
Temporal Correlations	L	L

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Source-Receptor Relationship	Application Element: Emission Rate
Reference Model: CDM	Reference Model: CDM
Treatment: Arbitrary location for each point source. Area sources specified as integral multiples of basic grid cell size, located on user-defined grid; sides lie along grid boundary directions. Receptor location arbitrary. Arbitrary release heights for point and area sources. Precise separation for each source-receptor pair. Receptors are at ground level. No terrain differences between source/receptor.	Treatment: Single arbitrary emission rate for each point and area source. Area integrations are done numerically one 22.5° sector at a time; sampling at discrete intervals on a polar grid centered on the receptor. Day/night variations in emissions, same variation assumed for all sources.
Study Model: AQDM	Study Model: AQDM
Importance Rating: MEDIUM	Importance Rating: MEDIUM
Comparative Evaluation: COMPARABLE	Comparative Evaluation: WORSE
Treatment: Arbitrary location for each point source. Arbitrary location and size for each area source. Up to 225 receptors located on uniform rectangular grid. Up to 12 user-specified receptor locations. Arbitrary release height for each point, area source. Precise downwind and crosswind distance for each source-receptor pair. Receptors at ground level. No terrain differences between source and receptor.	Treatment: Point sources: single rate for each source. Area sources: single rate for each source. Each source treated by effective single source approximation. No temporal variation allowed.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Plume Behavior	Application Element: Horizontal Wind Field
Reference Model: CDM	Reference Model: CDM
Treatment: Briggs' 2/3 (1971) neutral/unstable formula used. If stack height + plume rise is greater than mixing height, ground level concentrations assumed equal to zero. Alternative to Briggs - input value of plume rise times wind speed for each point source. No plume rise calculated for area sources. Does not treat fumigation or downwash.	Treatment: Climatological approach. 16 wind directions. 6 wind speed classes. Wind speed corrected for release height based on power law variation, exponents from DeMarrais (1959). Constant, uniform (steady-state) wind assumed.
Study Model: AQDM	Study Model: AQDM
Importance Rating: MEDIUM	Importance Rating: MEDIUM
Comparative Evaluation: COMPARABLE	Comparative Evaluation: WORSE
Treatment: Holland (1953) formula, with adjustment for stability. No plume rise calculated for area sources. Does not treat fumigation or downwash. If stack height plus plume rise is greater than mixing height, ground level concentration assumed equal to zero.	Treatment: Climatological approach. 16 wind directions. 6 wind speed classes. No variation in windspeed with height. Constant, uniform (steady-state) wind assumed.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Vertical Wind Field	Application Element: Horizontal Dispersion
Reference Model: CDM	Reference Model: CDM
Treatment:	Treatment:
Assumed equal to zero.	Semiempirical/Climatological (Steady-State).
	Uniform distribution within each of 16 sectors (narrow-plume approximation).
	Averaging time = 1 month to 1 year.
	Surface roughness not treated explicitly.
Study Model: AQDM	Study Model: AQDM
Importance Rating: LOW	Importance Rating: MEDIUM
Comparative Evaluation: COMPARABLE	Comparative Evaluation: COMPARABLE
Treatment:	Treatment:
Assumed equal to zero.	Climatological approach. Linear interpolation between 22.5° sector centerlines; center value calculated by sector averaging procedure (narrow plume approximation).
	Averaging time = 1 month - 1 year.
	Surface roughness not treated explicitly.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Vertical Dispersion	Application Element: Physical Removal
Reference Model: CDM	Reference Model: CDM
Treatment: Semiempirical/climatological (Steady-State) Gaussian plume function assumed. 5 stability classes as defined by Turner (1964). Neutral stability split into day/night cases, giving six classes in all. Dispersion coefficients taken from Turner (1970). Area sources - stability class is decreased by 1 category from input values to account for urban effects. Neutral dispersion coefficients are used for all neutral and stable classes. No provision for variations in surface roughness.	Treatment: Dry deposition only. Effective source treatment using exponential decay (First-order process). Single constant user-supplied halflife used.
Study Model: AQDM	Study Model: AQDM
Importance Rating: HIGH	Importance Rating: LOW
Comparative Evaluation: COMPARABLE	Comparative Evaluation: WORSE
Treatment: Semi-empirical/Gaussian plume. 5 stability classes (Turner, 1964). Neutral stability split internally into 60% day, 40% night. Dispersion coefficients from Pasquill (1961) and Gifford (1961). Neutral dispersion coefficients used for all neutral and stable classes. No provision for variations in surface roughness.	Treatment: Not treated explicitly.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Background, Boundary, Initial Conditions	Application Element: Temporal Correlations
Reference Model: CDM	Reference Model: CDM
Treatment:	Treatment:
Input single constant background value for each pollutant. Lower boundary (ground): assumes perfect reflection; uses single image source. Upper boundary (mixing height): no effect until vertical dispersion coefficient equals 0.8 of mixing height, uniform vertical mixing assumed beyond this point.	Wind speed, direction, stability correlated via wind rose. Mixing height is adjusted according to stability class: Class A - 1.5 x afternoon climatological value, Class D (night) - average of morning and afternoon climatological values, Class E - morning climatological value. Emission rates: day-night variation allowed; all sources assumed to vary by same factor. Non-sequential (climatological) limited correlation.
Study Model: AQDM	Study Model: AQDM
Importance Rating: MEDIUM	Importance Rating: LOW
Comparative Evaluation: COMPARABLE	Comparative Evaluation: COMPARABLE
Treatment:	Treatment:
Input single constant background value for each pollutant. Lower boundary (ground): perfect reflection; single image source. Upper boundary (mixing ht): no effect until $\sigma_z \geq .47H$ (occurs at $x=x_L$); for $x > 2x_L$, uniform mixing; in between, linear interpolation transition region used.	Wind speed, direction, stability correlated via wind rose. Emission rate - not correlated with any other factor. Non-sequential (climatological) limited correlation. Mixing height adjusted according to stability class: Class A - 1.5 x afternoon climatological value, Class D (night, internally divided) average of 100 meters and afternoon climatological value, Class E - assumes 100 meters.

EVALUATION FORM

Part C : Treatment of Elements

Application Index: 1143

Application Element:	Application Element:
Reference Model:	Reference Model:
Treatment:	Treatment:
Two IRRELEVANT elements: • Composition of Emissions • Chemistry and Reaction Mechanism	
Study Model:	Study Model:
Importance Rating:	Importance Rating:
Comparative Evaluation:	Comparative Evaluation:
Treatment:	Treatment:

EVALUATION FORM

Part D: Technical Comparison

Application Index: 1143 Reference Model: CDM Study Model AQDM

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL	0	--	--	--	--
HIGH	1	0	1	0	COMPARABLE
MEDIUM	6	0	4	2	WORSE
LOW [a]	3	0	2	1	
IRRELEVANT	2	XXX	XXX	XXX	
Total	12 (Should equal 12)				

TECHNICAL EVALUATION WORSE

[a]Used only in ambiguous cases.

C.3. EXAMPLE 3: PTDIS/1213

The application of interest involves the estimation of ground level centerline sulfur dioxide concentrations at various distances downwind of a power plant located in relatively flat terrain. The appropriate application index is 1213 and the suggested reference model is CRSTER (Single Source). Both CRSTER and RAM are suggested as reference models for application 1213 in Table 4.1. In accordance with footnote j of that table, CRSTER has been chosen, since the application of interest involves only a single power plant. PTDIS is classified as a Semiempirical/Steady-State model and is determined to be applicable. Part A of the Evaluation Form summarizes the general information regarding this example.

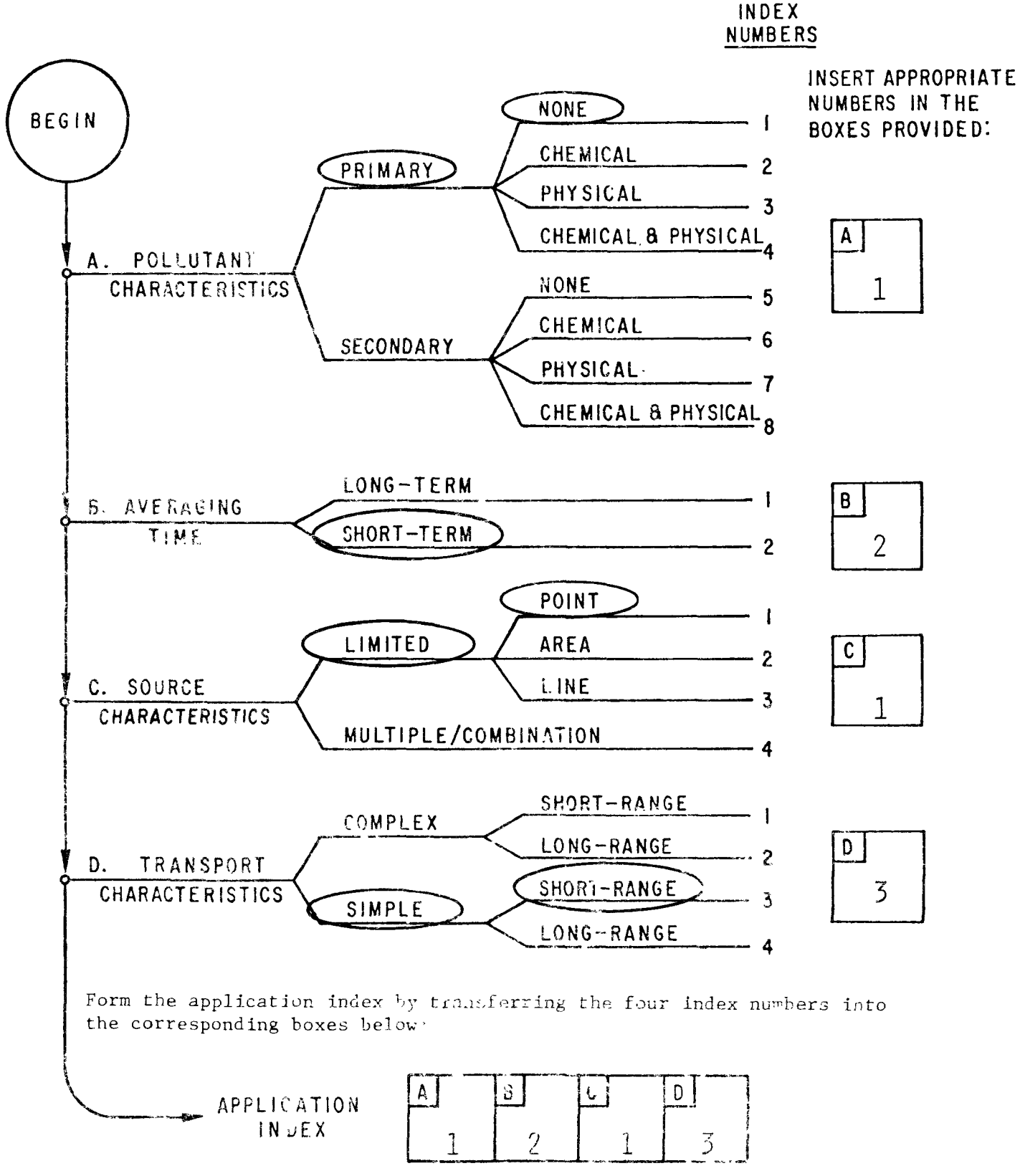
The importance ratings are given on Part B of the Evaluation Form; in this example three modifications have been made. Due to the physical and chemical characteristics of sulfur dioxide and the short range of the application the elements physical removal processes, chemistry and reaction mechanism, and composition of emissions have been rated IRRELEVANT.

The reverse side of Part A of the Evaluation Form gives the equations used used by PTDIS and Part C gives the treatments, importance ratings, and comparison results for all elements not rated IRRELEVANT. As can be seen, the treatments are very similar in all cases and in all cases a comparative rating of COMPARABLE is appropriate. For source-receptor relationship and horizontal wind field, some confusion may arise regarding the appropriate rating, the possible source of confusion being the specification in the application description on Part A that centerline ground level concentrations are desired. PTDIS is designed specifically for this application, whereas CRSTER (Single-Source) is designed to estimate concentrations at receptors on a polar grid with a 10° increment between successive radial directions. In addition, CRSTER accepts real meteorological data in which the wind direction is assumed given to the nearest 10° and randomizes this direction by the addition of an integer chosen from the values -4° to +5°. Thus CRSTER may not provide centerline concentration estimates; it was never intended to do so explicitly. CRSTER would in fact be found not applicable in this case were it the study model and PTDIS the reference model. This difference in objectives does not invalidate the use of CRSTER as a basis for comparison but implies that those aspects of source-receptor relationship and horizontal wind field which have treatments

which differ simply because of the different objectives of the two models should not be considered in making the comparisons.

The Evaluation Form - Part D summarizes the individual comparison results and shows that the technical evaluation of PTDIS for application 1213 is obviously COMPARABLE.

APPLICATION CLASSIFICATION FORM



Form the application index by transferring the four index numbers into the corresponding boxes below:

APPLICATION INDEX

A	B	C	D
1	2	1	3

EVALUATION FORM

Part A: Abstract and References

Study Model: PTDIS

References: Environmental Protection Agency, *User's Network for Applied Modeling of Air Pollution (UNAMAP)*, NTIS PB 229771, National Technical Information Service, Springfield, Va. (1974).

Turner, D.B., *Workbook of Atmospheric Dispersion Estimates*, NTIS PB 191482, National Technical Information Service, Springfield, Va.

Abstract: PTDIS is a steady-state Gaussian plume model that estimates short-term center-line concentrations directly downwind of a point source at distances specified by the user for a single user-specified set of meteorological conditions. The effect of limiting vertical dispersion by a mixing height can be included and gradual plume rise to the point of final rise is also considered. An option allows the calculation of isopleth half-widths for specific concentrations at each downwind distance.

Classification: Semempirical/Steady-State

Application Index: 1213

Reference Model: Single Source (CRSTER)

Application Description: Single elevated point source, flat terrain, sulfur dioxide, downwind centerline ground level concentrations only.

Model Applicability: Applicable [X] Not Applicable [ ]

EVALUATION FORM

Part A(reverse): Equations

Study Model: PTDIS

Equations:

$$\chi(x;0,0;H) = \frac{Q}{2\pi u \sigma_y \sigma_z} g_1 \; g_3$$

with $g_1 = 1$

and $$g_3 = \sum_{n=-\infty}^{+\infty} \left[\exp \left[-\frac{1}{2} \left(\frac{2nL-H}{\sigma_z} \right)^2 \right] + \exp \left[-\frac{1}{2} \left(\frac{2nL+H}{\sigma_z} \right)^2 \right] \right]$$

$\chi = 0$ if $H > L$

EVALUATION FORM

Part B: Importance Ratings

Application Index: 1213

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship	H	H
Emission Rate	H	H
Composition of Emissions	L	I ✓
Plume Behavior	H	H
Horizontal Wind Field	H	H
Vertical Wind Field	L	L
Horizontal Dispersion	H	H
Vertical Dispersion	H	H
Chemistry and Reaction Mechanism	L	I ✓
Physical Removal Processes	L	I ✓
Background, Boundary, Initial Conditions	M	M
Temporal Correlations	M	M

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Source-Receptor Relationship	Application Element: Emission Rate
Reference Model: Single Source (CRSTER)	Reference Model: Single Source (CRSTER)
Treatment: Up to 19 sources all assumed to be located at same position. Receptor locations restricted to 36 azimuths (every 10^{o}) and five user-specified radial distances. Arbitrary stack height for each source. Unique stack height for each source. Unique topographic elevation for each receptor: must be less than each stack height. Receptors must be at ground level. Precise downwind/crosswind distance for each source receptor pair.	Treatment: Single arbitrary value for each source. Monthly variation allowed.
Study Model: PTDIS	Study Model: PTDIS
Importance Rating: HIGH	Importance Rating: HIGH
Comparative Evaluation: COMPARABLE	Comparative Evaluation: COMPARABLE
Treatment: Single stack of arbitrary height. Up to 50 receptors, all at ground level, directly underneath plume centerline, at arbitrary user-specified downwind distances. Flat terrain assumed.	Treatment: Single arbitrary constant value.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Plume Behavior	Application Element: Horizontal Wind Field
Reference Model: Single Source (CRSTER) Treatment: Briggs' (1971, 1972) final plume rise formulas; plume rise not treated as a function of downwind distance. If plume height exceeds mixing height, concentrations further downwind assumed equal to zero. Does not treat either fumigation or downwash.	Reference Model: Single Source (CRSTER) Treatment: Semiempirical/Sequential (Steady-state) Constant, uniform wind speed and direction assumed for each of a sequence of hours. Wind speeds (arbitrary) and directions (nearest 10°) input by user; directions randomized by addition of (n-4)° with n = random integer from 0 to 9. Wind speed corrected for release height with corrections dependent only on stability class.
Study Model: PTDIS Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Briggs (1971, 1972) plume rise formulae. Alternatively, one user-supplied plume rise value can be used. Does not treat fumigation or downwash. If plume height exceeds mixing height, ground level concentration assumed equal to zero.	Study Model: PTDIS Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Steady-state) Wind directions implicit along source-receptor direction. Uses user-defined wind speed. No variation in wind speed with height. Constant, uniform (steady-state) wind assumed.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Vertical Wind Field	Application Element: Horizontal Dispersion
Reference Model: Single Source (CRSTER) Treatment: Assumed equal to zero (implicit).	Reference Model: Single Source (CRSTER) Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into seven classes (Pasquill-Gifford); class 7 - extremely stable - elevated plume assumed not to touch ground. Dispersion coefficients from Turner (1969). Surface roughness not treated explicitly. 1-hour averaging time.
Study Model: PTDIS Importance Rating: LOW Comparative Evaluation: COMPARABLE Treatment: Assumed equal to zero (implicit).	Study Model: PTDIS Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Steady-State. Gaussian plume function assumed. Calculations for a single user-specified (Pasquill-Gifford) stability class. Dispersion coefficients from Turner (1969); no adjustments made for variations in surface roughness, averaging time or travel time. Averaging time unknown, approximately 10 - 60 minutes.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Vertical Dispersion	Application Element: Background, Boundary, Initial Conditions
Reference Model: Single Source (CRSTER)	Reference Model: Single Source (CRSTER)
Treatment:	Treatment:
Semiempirical/Sequential (Steady-State).	Background not treated explicitly.
Gaussian plume function assumed.	Lower boundary: perfect reflection in horizontal plane at receptor height.
Atmospheric stability divided into seven (Pasquill-Gifford) classes; class 7 - extremely stable - elevated plume does not touch ground.	Upper boundary: perfect reflection; method of multiple images treated by summation of series until vertical dispersion coefficient = 1.6x (mixing height); uniform vertical mixing thereafter.
Dispersion coefficients from Turner (1969).	Mixing height for a given hour obtained by interpolation of radiosonde date.
Surface roughness not treated explicitly.	
Study Model: PTDIS	Study Model: PTDIS
Importance Rating: HIGH	Importance Rating: MEDIUM
Comparative Evaluation: COMPARABLE	Comparative Evaluation: COMPARABLE
Treatment:	Treatment:
Semiempirical/Steady-State.	Background not treated explicitly.
Gaussian plume function assumed.	Lower boundary: perfect reflection.
Calculations done for user-specified (Pasquill-Gifford) stability class.	Upper boundary: (neutral and unstable conditions) user-input mixing height used; perfect reflection assumed.
Dispersion coefficients from Turner (1969).	Upper boundary: (stable conditions) - concept of mixing height not employed; no upper boundary considered - given meteorological conditions implicitly assumed to extend higher than plume at all distances.
Surface roughness not treated explicitly.	Multiple reflections numerically accounted for by summation of series.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Temporal Correlations	Application Element:
Reference Model: Single Source (CRSTER) Treatment: Sequential; correlations automatic for meteorological parameters. User supplies hourly values of wind speed, wind direction, mixing height, and other meteorological variables required for determining stability class and plume rise. Monthly emission variation allows limited emission/meteorology correlations.	Reference Model: Treatment: 3 IRRELEVANT Elements: • Composition of Emissions • Chemistry and Reaction Mechanism • Physical Removal
Study Model: PTDIS Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE Treatment: User supplies appropriate values of all input variables for the hour in question; correlations automatic.	Study Model: Importance Rating: Comparative Evaluation: Treatment:

EVALUATION FORM

Part D: Technical Comparison

Application Index: 1213 Reference Model: Single Source (CRSTER) Study Model PTDIS

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL	0	-	-	-	-
HIGH	6	0	6	0	COMPARABLE
MEDIUM	2	0	2	0	COMPARABLE
LOW[a]	1	0	1	0	
IRRELEVANT	3	XXX	XXX	XXX	
	Total 12	(Should equal 12)			

TECHNICAL EVALUATION COMPARABLE

[a]Used only in ambiguous cases.

C.4. EXAMPLE 4: PTMAX /1213

The application of interest involves the estimation of maximum ground level concentrations of sulfur dioxide downwind of a single power plant located in relatively flat terrain, as well as the downwind distance to the maximum, for a variety of conditions. The appropriate application index is 1213 and the suggested reference model is Single Source (CRSTER). CRSTER is used instead of RAM because the application involves a single point source, as explained in footnote j to Table 4.1. PTMAX is classified as a Semiempirical/ Steady-State model and is determined to be applicable. Part A of the Evaluation Form summarizes the general information for this example.

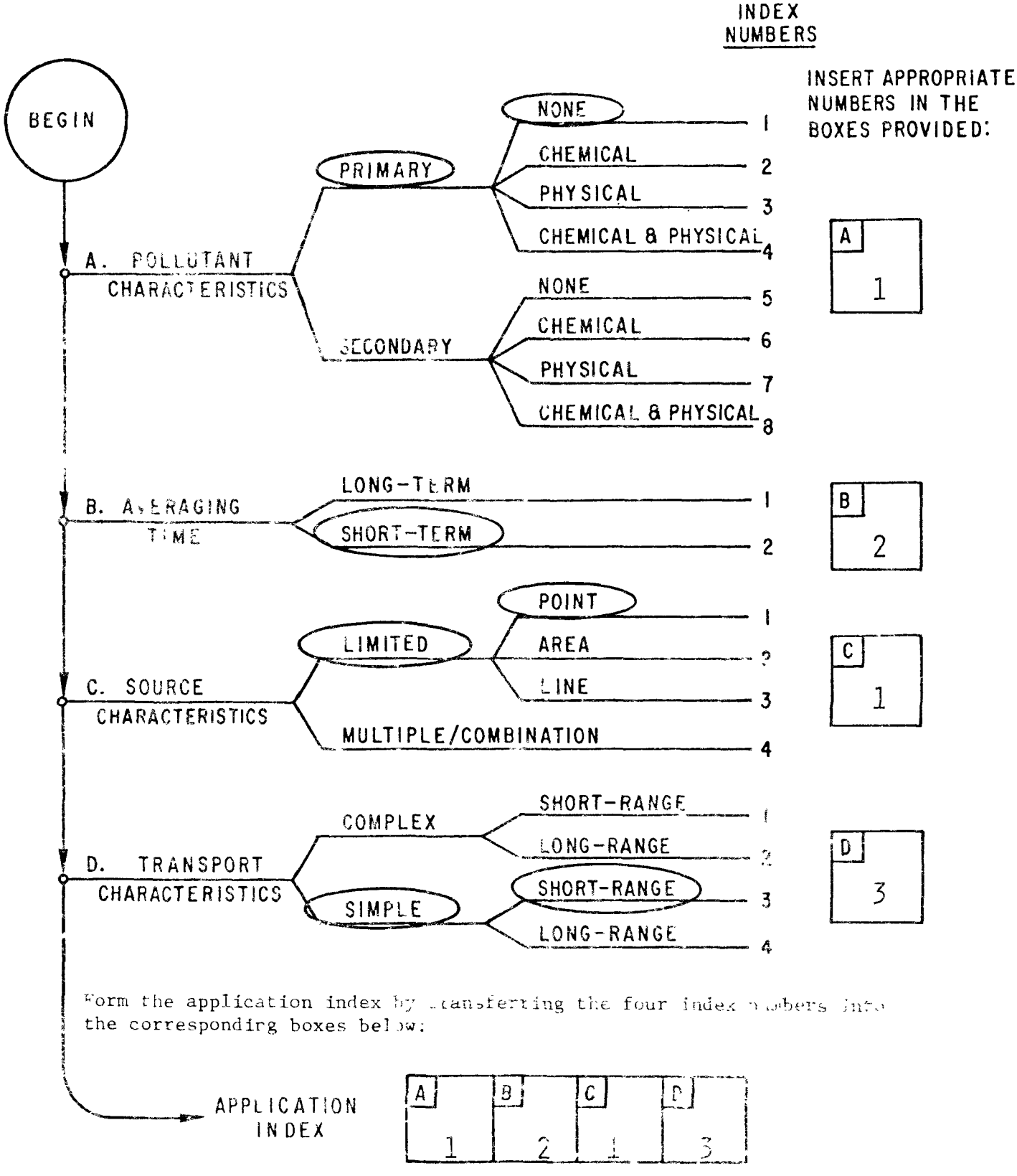
The importance ratings are given on the Evaluation Form - Part B; in this example four modifications have been made. Due to the physical and chemical characteristics of sulfur dioxide and the short range of the application the elements physical removal processes, chemistry and reaction mechansim, and composition of emissions have been rated IRRELEVANT. In addition, due to the desire on the part of the user to estimate maximum downwind concentrations under a variety of conditions, the importance rating of background, boundary and initial conditions has been modified from MEDIUM to HIGH. This modification reflects the need for treating the effects of limited mixing due to a low-lying inversion, a situation which may result in relatively high ground level concentrations.

The reverse side of Part A of the Evaluation Form gives the equations used by PTMAX and Part C gives the treatments, importance ratings, and comparison results for all elements not rated IRRELEVANT. As can be seen, the treatments are very similar in all cases and in all but one case a rating of COMPARABLE is appropriate. The one element which PTMAX does not treat in a manner comparable to that used by CRSTER is background, boundary and initial conditions, for which the treatment by PTMAX is rated WORSE. As in the previous example, PTMAX is rated COMPARABLE to CRSTER for source-receptor relationship and horizontal wind field in spite of obvious differences in the treatments of these elements, because the differences relate to aspects of each element which are not relevant to the real application of interest.

Part D of the Evaluation Form summarizes the individual comparison results. The initial technical evaluation for PTMAX is WORSE due to the worse

treatment of background, boundary and initial conditions. Specifically, the treatment used by PTMAX of the effects of the upper boundary is worse than that used by CRSTER. Since the user is particularly interested in maximum concentrations, which may result in part from a low-lying upper boundary, this single WORSE comparison is considered sufficient justification for a WORSE initial comparison. Furthermore, due to the small number of MEDIUM- and LOW-rated elements, there is no justification for modifying this initial rating. Thus, the appropriate technical evaluation for PTMAX in application 1213 is WORSE.

APPLICATION CLASSIFICATION FORM



Form the application index by transferring the four index numbers into the corresponding boxes below:

APPLICATION INDEX

A	B	C	D
1	2	1	3

EVALUATION FORM

Part A: Abstract and References

Study Model: PTMAX

References: Environmental Protection Agency, *User's Network for Applied Modeling of Air Pollution (UNAMAP)*, NTIS PB 229771, National Technical Information Service, Springfield, Va. (1974).

Turner, D.B., *Workbook of Atmospheric Dispersion Estimates*, NTIS PB 191482, National Technical Information Service, Springfield, Va. (1969).

Abstract: PTMAX is a steady-state Gaussian plume model that performs an analysis of the maximum short-term concentrations from a single point source as a function of stability and wind speed. The final plume height is used for each computation. A separate analysis must be made for each individual stack; the model cannot give the maximum concentrations from a combination of stacks.

Classification: Semiempirical/Steady-State

Application Index: 1213

Reference Model: Single Source (CRSTER)

Application Description: Maximum ground level sulfur dioxide concentrations from a single power plant in relatively flat terrain.

Model Applicability: Applicable [X] Not Applicable [ ]

EVALUATION FORM

Part A(reverse): Equations

Study Model: PTMAX

Equations:

$$\chi(x,0,0;H) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{H}{\sigma_z}\right)^2\right]$$

EVALUATION FORM

Part B: Importance Ratings

Application Index: 1213

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship	H	H
Emission Rate	H	H
Composition of Emissions	L	I ✓
Plume Behavior	H	H
Horizontal Wind Field	H	H
Vertical Wind Field	L	L
Horizontal Dispersion	H	H
Vertical Dispersion	H	H
Chemistry and Reaction Mechanism	L	I ✓
Physical Removal Processes	L	I ✓
Background, Boundary, Initial Conditions	M	H ✓
Temporal Correlations	M	M

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Source-Receptor Relationship	Application Element: Emission Rate
Reference Model: Single Source (CRSTER)	Reference Model: Single Source (CRSTER)
Treatment: Up to 19 sources all assumed to be located at same position. Receptor locations restricted to 36 azimuths (Every 10°) and five user-specified radial distances. Arbitrary stack height for each source. Unique topographic elevation for each receptor: must be less than stack heights. Receptors must be at ground level. Precise downwind/crosswind distance for each source receptor pair.	Treatment: Single arbitrary value for each source. Monthly variation allowed.
Study Model: PTMAX	Study Model: PTMAX
Importance Rating: HIGH	Importance Rating: HIGH
Comparative Evaluation: COMPARABLE	Comparative Evaluation: COMPARABLE
Treatment: Single stack of arbitrary height. Determines downwind distance of maximum ground level concentration. Flat terrain assumed.	Treatment: Single arbitrary constant value.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Plume Behavior	Application Element: Horizontal Wind Field
Reference Model: Single Source (CRSTER)	Reference Model: Single Source (CRSTER)
Treatment: Briggs' (1971, 1972) final plume rise, not treated as a function of downwind distance. If plume height exceeds mixing height, concentrations further downwind assumed equal to zero. Does not treat either fumigation or downwash.	Treatment: Semiempirical/Sequential (Steady-State). Constant, uniform wind speed and direction assumed for each of a sequence of hours. Wind speeds (arbitrary) and directions (nearest 10°) input by user; directions randomized by addition of (n-4)° with n=random integer from zero to nine. Wind speed corrected for release height, correction using power law variation with exponents dependent on stability class.
Study Model: PTMAX Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Two step procedure using Briggs' (1971, 1972) final plume rise formulae. Does not treat fumigation or downwash.	Study Model: PTMAX Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Steady-State. Wind directions implicit along source-receptor direction. No variation in wind speed with height. Constant, uniform (steady-state) wind assumed. Uses fixed, internally defined set of wind speed values ranging from 0.5 to 20 m/sec.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Vertical Wind Field	Application Element: Horizontal Dispersion
Reference Model: Single Source (CRSTER) Treatment: Assumed equal to zero (implicit).	Reference Model: Single Source (CRSTER) Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into seven classes (Pasquill-Gifford); Class 7 - extremely stable - elevated plume assumed not to touch ground. Dispersion coefficients from Turner (1969). Surface roughness not treated explicitly. One-hour averaging time.
Study Model: PTMAX Importance Rating: LOW Comparative Evaluation: COMPARABLE Treatment: Assumed equal to zero (implicit).	Study Model: PTMAX Importance Rating: LOW Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Steady-State. Gaussian plume function assumed. Calculations for each of six Pasquill-Gifford stability classes. Dispersion coefficients from Turner (1969); no adjustments made for variations in surface roughness, averaging time or travel time. Averaging time unknown, approximately 10-60 minutes.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Vertical Dispersion	Application Element: Background, Boundary, Initial Conditions
Reference Model: Single Source (CRSTER)	Reference Model: Single Source (CRSTER)
Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into seven (Pasquill-Gifford) classes; Class 7 - extremely stable - elevated plume does not touch ground. Dispersion coefficients from Turner (1969). Surface roughness not treated explicitly.	Treatment: Background not treated explicitly. Lower boundary: perfect reflection in horizontal plane at receptor height. Upper boundary: Perfect reflection: method of multiple images treated by summation of series until vertical dispersion coefficient = 1.6× (mixing height); uniform vertical mixing thereafter. Mixing height for a given hour obtained by interpolation of radiosonde data.
Study Model: PTMAX Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Steady-State. Gaussian plume function assumed. Calculations done for six Pasquill-Gifford stability classes. Dispersion coefficients from Turner (1969). Surface roughness not treated explicitly.	Study Model: PTMAX Importance Rating: HIGH Comparative Evaluation: WORSE Treatment: Background not treated explicitly. Lower boundary: perfect reflection at ground level. Upper boundary: mixing height assumed high enough to have no effect.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Temporal Correlations	Application Element:
Reference Model: Single Source (CRSTER)	Reference Model:
Treatment: Sequential; correlations automatic for meteorological parameters. User supplies hourly values of wind speed, wind direction, mixing height, and other meteorological variables required for determining stability class and plume rise. Monthly emission variation allows limited emission-meteorology correlations.	Treatment: Three IRRELEVANT Elements: • Composition of emissions • Chemistry and Reaction Mechanism • Physical Removal
Study Model: PTMAX Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE Treatment: Correlations automatic - user supplies appropriate data for situation of interest.	Study Model: Importance Rating: Comparative Evaluation: Treatment:

EVALUATION FORM

Part D: Technical Comparison

Application Index: 1213 Reference Model: Single Source (CRSTER) Study Model PTMAX

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL	0	-	-	-	-
HIGH	7	0	6	1	WORSE
MEDIUM	1	0	1	0	WORSE
LOW[a]	1	0	1	0	
IRRELEVANT	3	XXX	XXX	XXX	
Total	12	(Should equal 12)			

TECHNICAL EVALUATION WORSE

[a]Used only in ambiguous cases.

C.5. EXAMPLE 5: PTMTP/1213

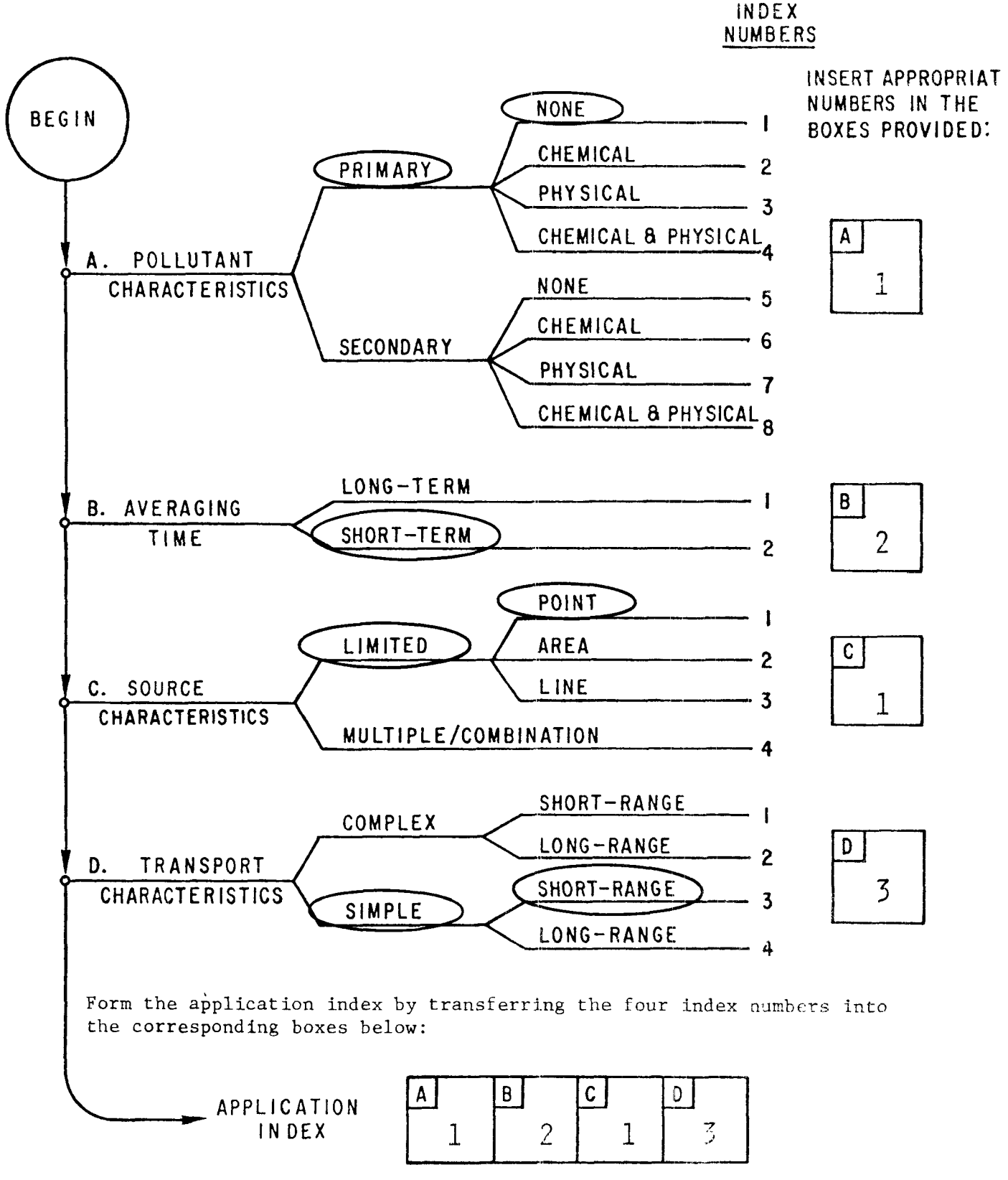
The application of interest involves the estimation of total one and 24-hour ground level sulfur dioxide concentrations from a few (less than 10-20) nearby power plants located in gently rolling rural terrain. The application index is 1213 and in this example the suggested reference model is RAM, since the application involves several sources at different locations. PTMTP is classified as a Semiempirical/Sequential (Steady-State) model and is determined to be applicable.

The importance ratings, shown on Part B of the Evaluation Form, incorporate the modification of composition of emissions, chemistry and reaction mechansim, and physical removal processes from LOW to IRRELEVANT. No other modifications are made.

The reverse side of Part A of the Evaluation Form gives the equations used by PTMTP and Part C gives the treatments, importance ratings, and comparisons results. As can be seen, the treatments by PTMTP are all quite similar to those used by RAM and are rated COMPARABLE in all cases. The treatments by RAM of those aspects of source-receptor relationship, emission rate, and other elements that involve consideration of area sources are not given in Part D in this example, because area sources are not involved in this application. These treatments by RAM are irrelevant and are not considered in making the comparisons. A question may arise with regard to horizontal wind field, because PTMTP does not adjust the input wind speed for the source release heights in estimating the contribution of each as does RAM. However, PTMTP does not require that the wind speed near the surface be input, and the user is free to input values appropriate for an average release height for the sources involved. PTMTP does not distinguish between different heights and uses the input wind speed for all sources. This difference between RAM and PTMTP is not considered significant enough to rate PTMTP worse.

The results of the element-by-element comparisons are summarized in Part D of the Evaluation Form and clearly indicate that PTMTP should be rated COMPARABLE to RAM for this application.

APPLICATION CLASSIFICATION FORM



Form the application index by transferring the four index numbers into the corresponding boxes below:

APPLICATION INDEX

A	B	C	D
1	2	1	3

EVALUATION FORM

Part A: Abstract and References

Study Model: PTMTP

References: Environmental Protection Agency. *User's Network for Applied Modeling of Air Pollution (UNAMAP)*, NTIS PB 229771, National Technical Information Service, Springfield, Va. (1974).

Turner, D.B., *Workbook of Atmospheric Dispersion Estimates*, NTIS PB 191482, National Technical Information Service, Springfield, Va. (1969).

Abstract: PTMTP is a steady-state, Gaussian plume model that estimates for a number of arbitrarily located receptor points at or above ground-level, the concentration from a number of point sources. Plume rise is determined for each source. Downwind and crosswind distances are determined for each source-receptor pair. Concentrations at a receptor from various sources are assumed additive. Hour by hour calculations are made based on hourly meteorological data; both hourly concentrations and averages over any averaging time from one to 24 hours can be obtained.

Classification: Semiempirical/Sequential (Steady-State)

Application Index: 1213 Reference Model: RAM

Application Description: Short term (one and 24 hour) ground level concentrations of sulfur dioxide from several power plants, relatively flat terrain, short range, rural area.

Model Applicability: Applicable [X] Not Applicable [ ]

EVALUATION FORM

Part A(reverse): Equations

Study Model: PTMTP

Equations:

$$\chi(x,y,z) = \sum_{n=1}^{N} \chi_n(x,y,z;H_n)$$

with

$$\chi_n(x,y,z;H_n) = \frac{Q_n}{2\pi u \sigma_y \sigma_z} g_1 g_3$$

$$g_1 = \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]$$

$$g_3 = \sum_{k=-\infty}^{+\infty} \left\{ \exp\left[-\frac{1}{2}\left(\frac{z-H_n + 2kL}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z + H_n + 2kL}{\sigma_z}\right)^2\right] \right\}$$

$\chi_n = 0$ if $H_n > L$.

EVALUATION FORM

Part B: Importance Ratings

Application Index: 1213

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship	H	H
Emission Rate	H	H
Composition of Emissions	L	I ✓
Plume Behavior	H	H
Horizontal Wind Field	H	H
Vertical Wind Field	L	L
Horizontal Dispersion	H	H
Vertical Dispersion	H	H
Chemistry and Reaction Mechanism	L	I ✓
Physical Removal Processes	L	I ✓
Background, Boundary, Initial Conditions	M	M
Temporal Correlations	M	M

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Source-Receptor Relationship	Application Element: Emission Rate
Reference Model: RAM Treatment: Arbitrary location and release height for each point source. Flat terrain. Arbitrary receptor locations - all at the same height above (or at) ground. Precise downwind, crosswind distances for each source-receptor pair.	Reference Model: RAM Treatment: Arbitrary constant emission rate for each point source.
Study Model: PTMTP Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Point sources only. Arbitrary location and release height for each of up to 25 point sources. Flat terrain assumed. Arbitrary location and height for each of up to 30 receptors. Precise downwind, crosswind distances evaluated for each source, receptor pair.	Study Model: PTMTP Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Single constant emission rate for each point source.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Plume Behavior	Application Element: Horizontal Wind Field
Reference Model: RAM Treatment: Two step procedure. Uses Briggs' (1971, 1972) downwind distance dependent plume rise formulae for point sources. If plume height exceeds mixing height, ground level concentrations assumed zero. Fumigation, downwash not treated.	Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Constant, uniform wind speed and direction assumed for each of a sequence of hours. Arbitrary wind speeds and direction values to 10° input by user; directions randomized by addition of (n-4)° with n=random integer from zero to nine. Wind speed is modified to correspond to value at release height, modification dependent only on stability class.
Study Model: PTMTP Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Two step procedure. Uses Briggs' 2/3 (1971, 1972) downwind distance dependent plume rise formulae. Does not treat fumigation or downwash. If plume height exceeds mixing height, concentration further downwind assumed zero.	Study Model: PTMTP Importance Rating: HIGH Comparative Evaluation: COMPARABLE (WORSE) Treatment: Semiempirical/Sequential (Steady-State). Uses sequence of up to 24 user-supplied hourly values of wind speed (arbitrary) and direction (nearest degree). Constant, uniform wind speed and direction for each hour; no variation of wind speed, direction with height; no correction made for release height.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Vertical Wind Field	Application Element: Horizontal Dispersion
Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Assumed equal to zero (implicit).	Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes, determined hourly. Dispersion coefficients from Turner (1969) or McElroy and Pooler (1968) at user's option. Surface roughness not treated explicitly. One hour averaging time used.
Study Model: PTMTP Importance Rating: LOW Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Assumed equal to zero (implicit).	Study Model: PTMTP Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes, supplied hourly. Dispersion coefficients from Turner (1969). Surface roughness not treated explicitly. One hour averaging time.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Vertical Dispersion	Application Element: Background, Boundary, Initial Conditions
Reference Model: RAM	Reference Model: RAM
Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes, determined hourly. Dispersion coefficients from Turner (1969) or McElroy and Pooler (1968) at user's option. Surface roughness not treated explicitly.	Treatment: Background not treated explicitly. Both upper and lower boundaries - perfect reflection. 1) Neutral and unstable conditions: method of multiple images treated by summation of infinite series until σ_z = 1.6× (mixing height); uniform mixing assumed thereafter; 2) Stable conditions: mixing height assumed to have no effect. Mixing height for a given hour obtained by interpolation of radiosonde data.
Study Model: PTMTP Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmosperic stability divided into six (Pasquill-Gifford) classes, supplied hourly. Dispersion coefficients from Turner (1969). Surface roughness not treated explicitly. One hour averaging time.	Study Model: PTMTP Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE Treatment: Background not treated explicitly. Both upper and lower boundaries - perfect reflection assumed. Multiple reflections treated by summation of series. Uses user-supplied hourly mixing height.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1213

Application Element: Temporal Correlations	Application Element:
Reference Model: RAM Treatment: Sequential. User supplies hourly values of wind speed, wind direction, mixing height, and other meteorological variables required for determination of stability class and plume rise. (Correlations automatic.) Emission rates constant, not correlated with other parameters.	Reference Model: Treatment: Three IRRELEVANT elements: • Composition of Emissions • Chemistry and Reaction Mechanism • Physical Removal Processes
Study Model: PTMTP Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE Treatment: Sequential. User supplies hourly values of wind speed, wind direction, stability class, mixing height. Correlations among these parameters are automatically treated. Emission rates constant.	Study Model: Importance Rating: Comparative Evaluation: Treatment:

EVALUATION FORM

Part D: Technical Comparison

Application Index: 1213 Reference Model: RAM Study Model PTMTP

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL	0	-	-	-	-
HIGH	6	0	6(5)	0(1)	COMPARABLE
MEDIUM	2	0	2	0	COMPARABLE
LOW[a]	1	0	1	0	
IRRELEVANT	3	XXX	XXX	XXX	
	Total 12 (Should equal 12)				
			TECHNICAL EVALUATION		COMPARABLE

[a]Used only in ambiguous cases.

C.6 EXAMPLE 6: HANNA-GIFFORD/1243

In this example, the application of interest involves the estimation of one and twenty-four hour total suspended particulate concentrations from near ground-level area sources within an urban area located in relatively flat terrain. The application index is 1243 and the suggested reference model is RAM.

There are two forms of the Hanna-Gifford model which have been discussed in the modeling literature. One form is that used in this example, and the other form is used in Example 7, Appendix C.7. The user may examine the equations presented on the reverse side of Part A of the Evaluation Form in these two examples to see the differences between the two versions of the model.

The Hanna-Gifford model is not available as a computer program accompanied by a comprehensive user's manual. Rather, the model has been presented and discussed in a series of literature publications, three of which are cited on Part A of the Evaluation Form. Consequently, different users may implement the methods of Hanna and Gifford in different ways and the results obtained may not be strictly said to have arisen from the same algorithm. In this example it is assumed that the equations are applied separately to each of a sequence of twenty-four hours. The reference model, RAM, works in the same manner.

The Hanna-Gifford model is classified Semiempirical/Sequential (Steady-State) and is determined to be applicable to the situation to be modeled.

The importance ratings shown on Part B incorporate three modifications. Chemistry and reaction mechanism has been designated as IRRELEVANT. The importance of plume behavior has been changed from MEDIUM to LOW on the assumption that the particular area sources in question do not give rise to significant plume rise. Also, since the sources are near ground-level, there is no need to consider downwash and fumigation. Finally, the importance rating of horizontal dispersion has been changed from HIGH to MEDIUM due to the fact that only area sources are of interest in this case. The modified rating corresponds to the rating for horizontal dispersion in application number 1223, which involves area sources only.

Part C gives the treatments, importance ratings, and comparison results. It should be noted that the treatments by RAM, the reference model, of the various aspects of each element that deal with point sources have been omitted. These treatments are irrelevant in this particular application and are not considered in making the evaluation.

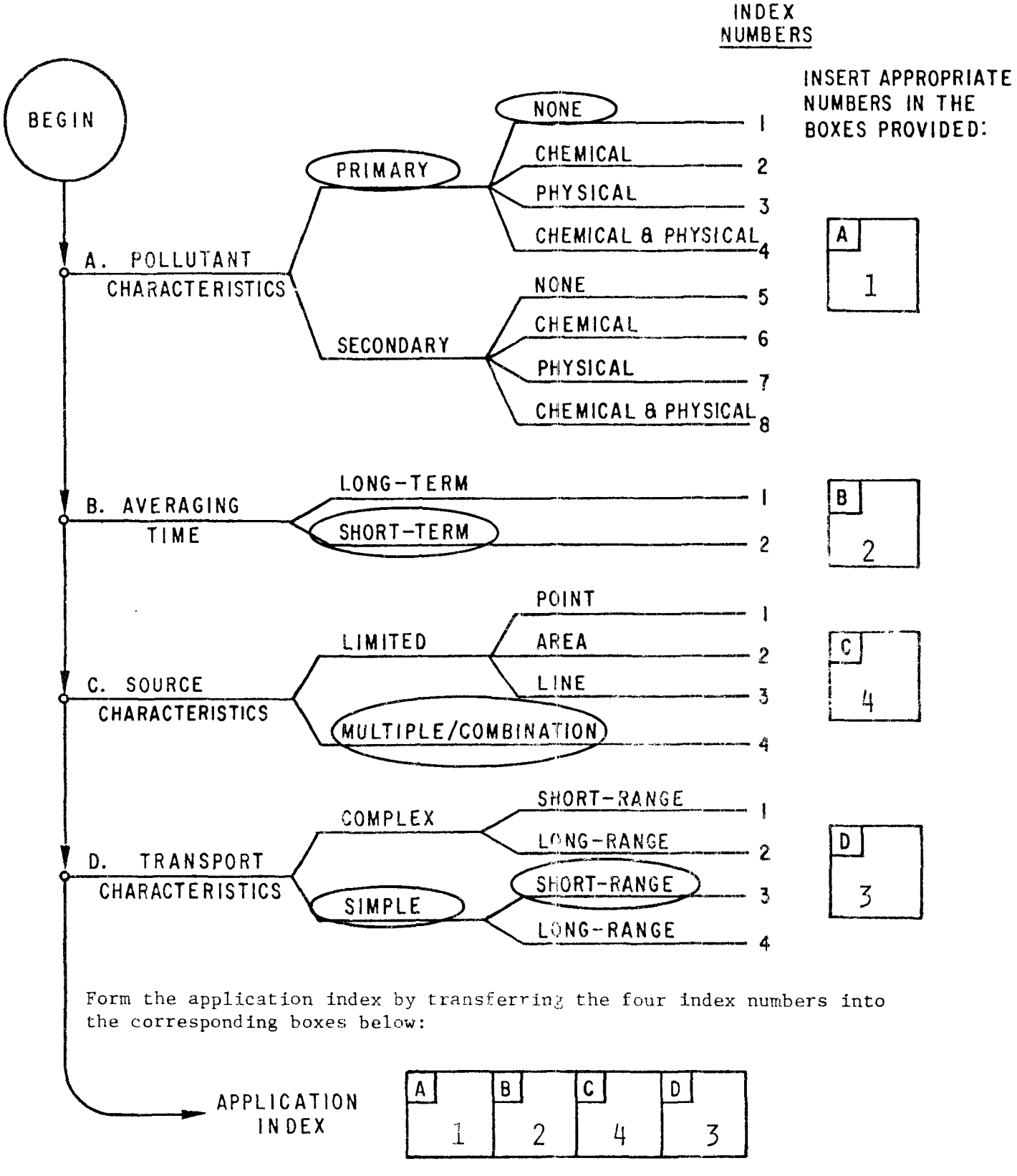
Both RAM and the Hanna-Gifford model make use of similar methods for estimating total area source contributions and this similarity is reflected in the treatments of many of the application elements. Significant differences in the two models occur, however, as a result of differences in the implementation of these similar methods. Nevertheless, the initial comparative evaluation of the Hanna-Gifford model is COMPARABLE, based on comparable treatments of the three HIGH-rated elements. It should be noted that for one of the high elements, source-receptor relationship, the Hanna-Gifford model was rated COMPARABLE even though it assumes ground level emissions while RAM allows the user to specify non-zero effective emission heights. In the application of interest this difference is unimportant, because the emissions are known to be released near the ground. In other applications, in which it is known that some or all such emissions effectively occur above ground level, this difference may be significant enough to justify a WORSE rating. This type of decision can only be made by a person familiar with the actual situation of interest.

The two MEDIUM-rated elements whose treatments by the Hanna-Gifford model are rated WORSE are horizontal wind field and background, boundary and initial conditions. The treatment of horizontal wind field by the Hanna-Gifford model is rated WORSE, because only sixteen possible wind directions are used whereas RAM accepts wind directions to the nearest 10° and randomizes these so that the wind direction may correspond to any of 360 different values. The treatment of background, boundary and initial conditions is rated WORSE, because the Hanna-Gifford model does not treat the effects of the upper boundary. A secondary comparison of COMPARABLE is indicated, because for ground level sources, the effects of the upper boundary may not be felt for a substantial distance downwind, depending on the depth of the mixed layer and the wind speed.

The substantial number of MEDIUM-rated elements that are treated WORSE by Hanna-Gifford together with the relatively small number of HIGH-rated elements and the absence of any HIGH or MEDIUM-rated elements that are treated

BETTER provides adequate justification for modifying the comparative evaluation from COMPARABLE to WORSE in this application. The treatments of the LOW-rated elements support this modification since little weight is attached to them. The appropriate technical evaluation of the Manna-Gifford model in application 1243 is therefore WORSE.

APPLICATION CLASSIFICATION FORM



Form the application index by transferring the four index numbers into the corresponding boxes below:

APPLICATION INDEX

A	B	C	D
1	2	4	3

EVALUATION FORM

Part A: Abstract and References

Study Model: Hanna-Gifford

References:

Hanna, S.R., "A Simple Method of Calculating Dispersion from Urban Area Sources." *J. Air Pollution Control Assn.*, Vol. 21, No. 12, pp. 774-777, December 1971.

Gifford, F.A., and S.R. Hanna, "Modeling Urban Air Pollution." *Atmospheric Environment*, Vol. 7, pp. 131-136, 1973.

Gifford, F.A. and S.R. Hanna, "Urban Air Pollution Modeling." Paper No. ME-320, Proc. 2nd International Clean Air Congress, Washington, D.C., pp. 1146-1151 (December 1970).

Abstract: The Hanna-Gifford model is an area source model based upon the assumption of a Gaussian pollutant distribution in the vertical and using the narrow-plume approximation (homogeneous emissions in the crosswind direction) in the horizontal direction.

Classification: Semiempirical/Sequential (Steady-State)

Application Index: 1243 Reference Model: RAM

Application Description: One and twenty-four hour concentrations of total suspended particulate matter from area sources in an urban area for a given period, flat terrain.

Model Applicability: Applicable [X] Not Applicable [ ]

EVALUATION FORM

Part A(reverse): Equations

Study Model: Hanna-Gifford

Equations:

$$\chi = \sqrt{\frac{2}{\pi}} \frac{1}{u} \int_0^{\infty} \frac{q(x)}{\sigma_z} dx$$

Narrow plume approximation, ground level sources.

$$\chi = \sqrt{\frac{2}{\pi}} \frac{1}{u} \frac{(\Delta x/2)^{1-b}}{a(1-b)} \left[Q_o + \sum_{i=1}^{N} Q_i \left[(2i+1)^{1-b} - (2i-1)^{1-b} \right] \right]$$

$$\sigma_z(x) = ax^b$$

N = number of upwind grid squares.

Δx = width of a grid square.

EVALUATION FORM

Part B: Importance Ratings

Application Index: 1243

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship	M	M
Emission Rate	M	M
Conversion of Emissions	L	L
Plume Behavior	H	L ✓
Horizontal Wind Field	M	M
Vertical Wind Field	L	L
Horizontal Dispersion	H	M ✓
Vertical Dispersion	H	H
Chemistry and Reaction Mechanism	L	I ✓
Physical Removal Processes	L	L
Background, Boundary, Initial Conditions	M	M
Temporal Correlations	M	M

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element: Source-Receptor Relationship	Application Element: Emission Rate
Reference Model: RAM	Reference Model: RAM
Treatment:	Treatment:
Area sources defined as square cells (or multiples) in a rectangular array; up to three effective release heights (for u = 5m/sec) user-specified; sides lie along grid boundary directions.	Arbitrary constant emission rate for each area source.
Arbitrary receptor locations - all at the same height above (or at) ground.	Area source contributions obtained by numerical integration along upwind distance of narrow-plume approximation formulae for area source with given effective release height.
Flat terrain assumed.	Includes only those areas intersected by the upwind ray.
Downwind distance calculated for points along rays which intersect area sources.	
Study Model: Hanna-Gifford	Study Model: Hanna-Gifford
Importance Rating: MEDIUM	Importance Rating: MEDIUM
Comparative Evaluation: COMPARABLE	Comparative Evaluation: COMPARABLE
Treatment:	Treatment:
Area sources only, square cells in a rectangular array.	Arbitrary constant emission rate for each area source.
Receptors and sources both at ground level.	Area source contributions obtained by analytic integration along upwind distance of narrow-plume approximation formulae for area source at ground level oriented perpendicular to upwind direction.
Each receptor assumed located at center of a grid square.	Includes only grid squares directly upwind of receptor.
Flat terrain assumed.	

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element: Composition of Emissions	Application Element: Plume Behavior
Reference Model: RAM	Reference Model: RAM
Treatment:	Treatment:
Single representative pollutant only; no treatment of size distribution.	No plume rise calculated for area sources; assumed to be included in release height. Fumigation, downwash not treated.
Study Model: Hanna-Gifford	Study Model: Hanna-Gifford
Importance Rating: LOW	Importance Rating: LOW
Comparative Evaluation: COMPARABLE	Comparative Evaluation: WORSE
Treatment:	Treatment:
Single representative pollutant only. No treatment of size distribution.	Not treated explicitly; effective release height assumed zero. Fumigation, downwash not treated.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element: Horizontal Wind Field	Application Element: Vertical Wind Field
Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Constant, uniform wind speed and direction assumed for each of a sequence of hours. Arbitrary wind speeds and direction values to 10° input by user; directions randomized by addition of (n - 4)° with n = random integer from zero to nine. Wind speed is modified to correspond to value at release height, modification dependent only on stability class.	Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State) Assumed equal to zero (implicit).
Study Model: Hanna-Gifford Importance Rating: MEDIUM Comparative Evaluation: WORSE Treatment: Semiempirical/Sequential (Steady-State). Constant, uniform wind speed, direction assumed for each of a sequence of hours. Wind speed arbitrary; wind direction restricted to one of 16 equally spaced directions.	Study Model: Hanna-Gifford Importance Rating: LOW Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Assumed equal to zero (implicit).

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element: Horizontal Dispersion	Application Element: Vertical Dispersion
Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Narrow plume approximation for area sources; horizontal dispersion not treated explicitly.	Reference Model: RAM Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into six (Pasquill-Gifford) classes, determined hourly. Dispersion coefficients from Turner (1969) or McElroy and Pooler (1968) at user's option. Surface roughness not treated explicitly.
Study Model: Hanna-Gifford Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Narrow plume approximation; horizontal dispersion not treated explicitly.	Study Model: Hanna-Gifford Importance Rating: HIGH Comparative Evaluation: COMPARABLE Treatment: Semiempirical/Sequential (Steady-State). Gaussian plume function assumed. Atmospheric stability divided into classes (Smith 1968). Dispersion coefficient $\sigma_z = ax^b$ with a,b from Smith (1968) or Briggs (1973). Surface roughness not treated explicitly.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Application Element: Physical Removal		Application Element: Background, Boundary, Initial Conditions	
Reference Model: RAM		Reference Model: RAM	
Treatment:		Treatment: Background not treated explicitly.	
Exponential decay - first order (linear) processes.		Both upper and lower boundaries perfect reflection.	
Single, constant user - specified decay constant.		1) Neutral and unstable conditions: method of multiple images treated by summation of infinite series until σ_z = 1.6×(mixing height); uniform mixing assumed thereafter;	
		2) Stable conditions: mixing height assumed to have no effect.	
		Mixing height for given hour obtained by interpolation of radiosonde data.	
Study Model:	Hanna-Gifford	Study Model:	Hanna-Gifford
Importance Rating:	LOW	Importance Rating:	MEDIUM
Comparative Evaluation:	WORSE	Comparative Evaluation:	WORSE (COMPARABLE)
Treatment:		Treatment:	
Not treated explicitly.		Background: single additive constant.	
		Lower boundary: perfect reflection.	
		Upper boundary: assumed high enough to have no effect; atmospheric stability assumed constant to above the the plume height.	

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1243

Study Element: Temporal Correlations	Application Element:
Reference Model: RAM	Reference Model:
Treatment: Sequential.	Treatment:
User supplies hourly values of wind speed, wind direction, mixing height, and other meteorological variables required for determination of stability class and plume rise. (Correlations automatic.)	One IRRELEVANT element: • Chemistry and Reaction Mechanism
Emission rates constant, not correlated with other parameters.	
Study Model: Hanna-Gifford	Study Model:
Importance Rating: MEDIUM	Importance Rating:
Comparative Evaluation: COMPARABLE	Comparative Evaluation:
Treatment: Sequential.	Treatment:
Hourly values of wind speed, direction, stability supplied by user. (Correlations automatic.)	
Emission rates constant; not correlated with other parameters.	

EVALUATION FORM

Part D: Technical Comparison

Application Index: 1243 Reference Model: RAM Study Model Hanna-Gifford

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL	0	-	-	-	-
HIGH	1	0	1	0	COMPARABLE
MEDIUM	6	0	4 (5)	2 (1)	WORSE
LOW	4	0	2	2	
IRRELEVANT	1	XXX	XXX	XXX	

Total 12 (Should equal 12)

TECHNICAL EVALUATION WORSE

C.7 EXAMPLE 7: HANNA-GIFFORD/1143

The application of interest involves the estimation of long-term ground-level total suspended particulate concentrations arising from near ground-level area sources in an urban area located in relatively flat terrain. The application index is 1143 and the suggested reference model is CDM.

As explained in Example 6, Appendix C.6, two forms of the Hanna-Gifford model have been discussed in the references given on Part A of the Evaluation Form. One was used in Example 6 and the other is used in this example. Also, as pointed out in Example 6, the Hanna-Gifford model has been presented in a series of literature publications rather than in a user's manual accompanied by a computer code. As a result, the implementation of the Hanna-Gifford model in a specific application may depend to some extent on the user. In this example the procedure used by Hanna (1971) is considered.

The Hanna-Gifford model is classified Semiempirical/Climatological (Steady-State). The climatological classification seems most appropriate, since a climatological average wind speed is used in the equation, even though this form of the model does not appear to exactly correspond to the definition of a climatological model used in this workbook. In fact however, the equation used in this example may be derived from a climatological version of the other form of the model given certain assumptions regarding the nature of the stability-wind rose used. The Hanna-Gifford model is determined to be applicable to the situation to be modeled.

Two modifications have been made in the importance ratings. Chemistry and reaction mechanism has been rated IRRELEVANT, and the importance rating of plume behavior has been changed from MEDIUM to LOW due to the assumed nature of the area sources in question, as in the previous example.

The working equations are given on the reverse side of Part A and the treatments, importance ratings, and comparisons are given on Part C of the Evaluation Form. The treatments by the reference model (CDM) [illegible] related aspects of each element have been omitted as they [illegible] this application.

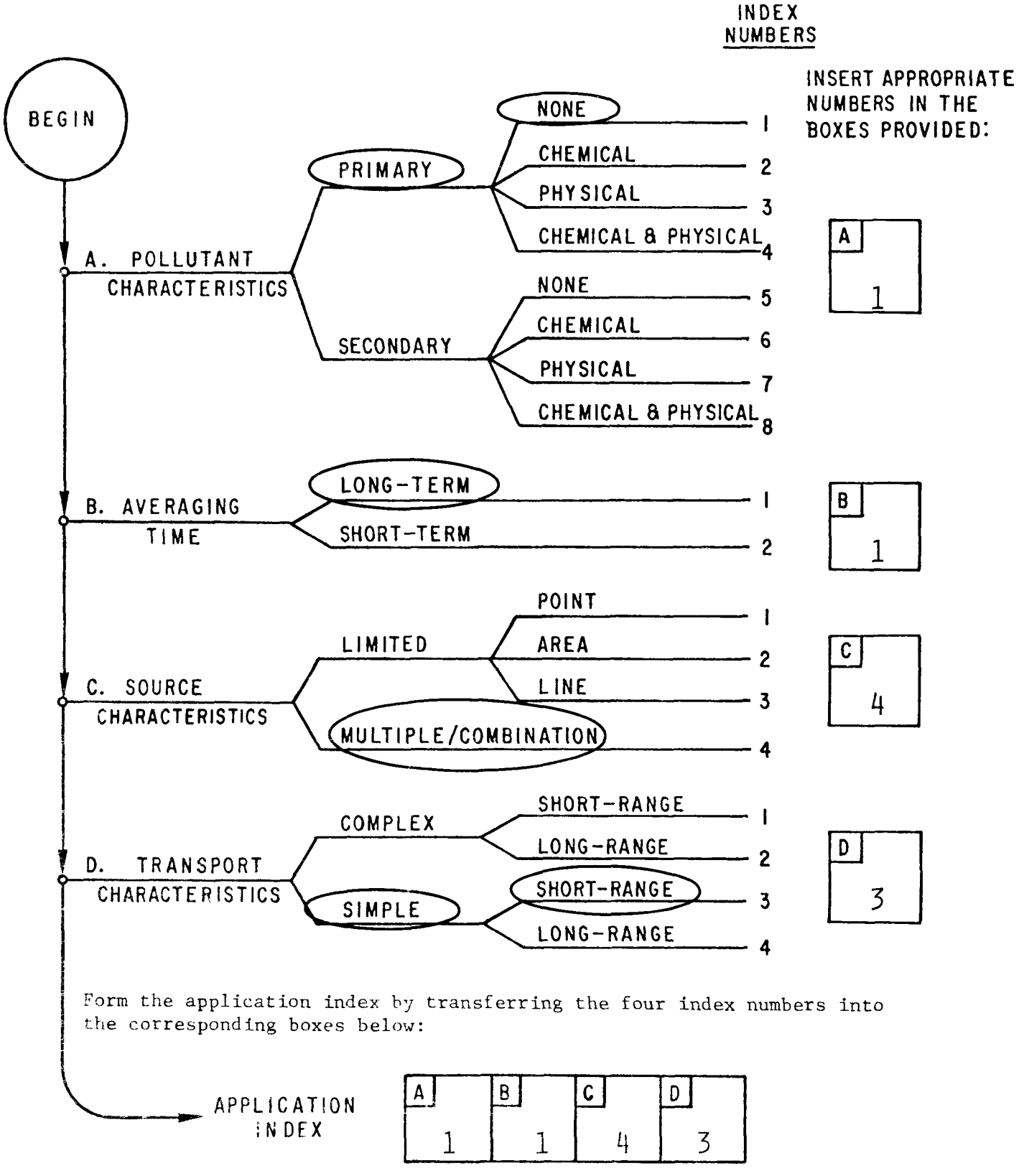
Only one element, vertical dispersion, is rated as being [illegible] portance in this application and the treatment by [illegible]

Gifford model is considered WORSE than that used by CDM, because only one stability class (neutral) is considered. Had the model been implemented in a slightly different way, this particular aspect of the treatment could have easily been modified. A secondary comparison of COMPARABLE is indicated, because neutral stability is indeed expected to occur more frequently than any other in an urban area. A user familiar with the specific area to be modeled is in the best position to judge the adequacy of this treatment in that area. Other aspects of the two treatments of vertical dispersion are comparable.

The treatments of the MEDIUM-rated elements show a definite bias toward a WORSE rating. The treatments of emission rate and horizontal dispersion are rated definitely COMPARABLE, and the treatment of source-receptor relationship is rated COMPARABLE although with a secondary rating of WORSE due to the treatment of only the one grid square containing the receptor. The validity of this procedure is related to the spatial variability of the emission rates for nearby grid squares, which in turn depends in part on the size of the grid square used. The treatment of horizontal wind field is rated WORSE, as is the treatment of background, boundary and initial conditions although for this element on a secondary rating of COMPARABLE is indicated. The uncertainty in the comparison for background, boundary and initial conditions arises because, although the Hanna-Gifford model does not treat effects due to the upper boundary, these effects may not be important for ground level sources at short to moderate range, depending on the depth of the mixing layer. Of the two uncertain ratings, the one for background, boundary and initial conditions is considered the greater, and the distributions of treatments for MEDIUM-rated elements which deserve the most consideration are 0,3,2 and 0,2,3.

The results for the MEDIUM-rated elements clearly support the initial rating of WORSE and the LOW-rated elements also support this rating. The appropriate technical evaluation for this form of the Hanna-Gifford model is therefore WORSE in this application.

APPLICATION CLASSIFICATION FORM



Form the application index by transferring the four index numbers into the corresponding boxes below:

APPLICATION INDEX

A	B	C	D
1	1	4	3

EVALUATION FORM

Part A: Abstract and References

Study Model: Hanna-Gifford

References:

Hanna, S.R., "A Simple Method of Calculating Dispersion from Urban Area Sources." *J. Air Pollution Control Assn.*, Vol. 21, No. 12, pp. 774-777, December 1971.

Gifford, F.A., and S.R. Hanna, "Modeling Urban Air Pollution." *Atmospheric Environment*, Vol. 7, pp. 131-136, 1973.

Gifford, F.A., and S.R. Hanna, "Urban Air Pollution Modeling." Paper No. ME-320, Proc. 2nd International Clean Air Congress, Washington, D.C., pp. 1146-1151 (December, 1970).

Abstract:

The Hanna-Gifford model is an area source model based upon the assumption of a Gaussian pollutant distribution in the vertical and using the narrow-plume approximation (homogeneous emissions in the crosswind direction) in the horizontal direction.

Classification: Semiempirical/Climatological (Steady-State)

Application Index: 1143 Reference Model: CDM

Application Description: Long-term ground-level total suspended particulate concentrations from near ground-level area sources in an urban area.

Model Applicability: Applicable [X] Not Applicable [ ]

EVALUATION FORM

Part A(reverse): Equations

Study Model: Hanna-Gifford

Equations:

$$\chi = C \frac{Q_o}{u}$$

with

χ = ground level concentration in a given grid square.

Q_o = emission rate per unit area in the same square.

u = average wind speed over the period of interest.

$$C = \sqrt{\frac{2}{\pi}} \left(\frac{2N+1}{2} \Delta x \right)^{1-b} \frac{1}{a(1-b)}$$

with

N = 4

Δx = grid spacing (meters)

a = 0.15 meters^{1-b}

b = 0.75

(a and b correspond to parameters in the representation of the vertical dispersion coefficient:

$$\sigma_z = ax^b.$$

The values are those recommended by M.E. Smith (1968) for neutral stability.)

EVALUATION FORM

Part B: Importance Ratings

Application Index: 1143

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship	M	M
Emission Rate	M	M
Composition of Emissions	L	L
Plume Behavior	M	L ✓
Horizontal Wind Field	M	M
Vertical Wind Field	L	L
Horizontal Dispersion	M	M
Vertical Dispersion	H	H
Chemistry and Reaction Mechanism	L	I ✓
Physical Removal Processes	L	L
Background, Boundary, Initial Conditions	M	M
Temporal Correlations	L	L

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Source-Receptor Relationship	Application Element: Emission Rate
Reference Model: CDM	Reference Model: CDM
Treatment: Area sources integral multiples of basic grid square. Receptor location arbitrary. Arbitrary release heights for area sources. Precise separation for each source-receptor pair. Receptors are at ground level. No terrain differences between source/receptor. Sides of area sources lie along grid boundary directions.	Treatment: Arbitrary emission rate for each area source. Area integrations are done numerically one 22.5° sector at a time; sampling at discrete points defined by specific radial and angular intervals on a polar grid centered on the receptor. Day/night variations in emissions, same variation assumed for all sources; no other temporal variation.
Study Model: *Hanna-Gifford* Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE (WORSE) Treatment: Single square, ground-level area source over which emissions are approximately uniform, considered for each receptor. Arbitrary grid size, user-specified. Ground-level receptors, located arbitrarily within source area. Flat terrain assumed. Area sources square cells in user-specified grid.	Study Model: Hanna-Gifford Importance Rating: MEDIUM Comparative Evaluation: COMPARABLE Treatment: *Single constant emission rate for the source area.* Area source contribution obtained by analytic integration along upwind direction of narrow-plume approximation formulae for ground-level source.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Composition of Emissions	Application Element: Plume Behavior
Reference Model: CDM	Reference Model: CDM
Treatment:	Treatment:
Treats up to two independent pollutants.	No plume rise calculated for area sources. Does not treat fumigation or downwash.
Study Model: Hanna-Gifford	Study Model: Hanna-Gifford
Importance Rating: LOW	Importance Rating: LOW
Comparative Evaluation: COMPARABLE	Comparative Evaluation: COMPARABLE
Treatment:	Treatment:
Independent pollutants, treated one at a time.	Not treated explicitly; effective release height assumed zero.
	Does not treat downwash or fumigation.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Horizontal Wind Field	Application Element: Vertical Wind Field
Reference Model: CDM	Reference Model: CDM
Treatment: Climatological. 16 wind directions. 6 wind speed classes. Wind speed corrected for release height based on power law variation; exponents from DeMarrais (1959), Stability class dependent. Constant, uniform (steady-state) wind assumed.	Treatment: Assumed equal to zero (implicit).
Study Model: Hanna-Gifford Importance Rating: MEDIUM Comparative Evaluation: WORSE Treatment: Climatological Only average wind speed in area of interest is considered. No variation of wind speed with height.	Study Model: Hanna-Gifford Importance Rating: LOW Comparative Evaluation: COMPARABLE Treatment: Assumed equal to zero (implicit).

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Horizontal Dispersion	Application Element: Vertical Dispersion
Reference Model: CDM	Reference Model: CDM
Treatment: Semiempirical/Climatological (Steady-State),	Treatment: Semiempirical/Climatological (Steady-State).
Uniform distribution within each of 16 sectors (sector averaging).	Gaussian plume function assumed.
Averaging time = one month to one year.	Five stability classes as defined by Turner (1964), neutral stability split into day/night cases.
Atmospheric stability and surface roughness not treated explicitly.	Dispersion coefficients taken from Turner (1970).
	Area sources - stability class is decreased by one category from input values to account for urban effects.
	Neutral dispersion coefficients are used for all neutral and stable classes.
	Surface roughness not treated explicitly.
Study Model: Hanna-Gifford	Study Model: Hanna-Gifford
Importance Rating: MEDIUM	Importance Rating: HIGH
Comparative Evaluation: COMPARABLE	Comparative Evaluation: WORSE (COMPARABLE)
Treatment: Semiempirical/Climatological (Steady-State),	Treatment: Semiempirical/Climatological (Steady-State)
Narrow-plume approximation; horizontal dispersion not treated explicitly.	Gaussian plume function assumed.
	Single atmospheric stability (neutral) considered.
	Dispersion coefficient $\sigma_z = ax^b$; a, b from Smith (1968).
	Surface roughness not treated explicitly.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Physical Removal	Application Element: Background, Boundary, Initial Conditions
Reference Model: CDM Treatment: Treats only first-order (linear) processes. Single, constant user-supplied halflife used - exponential decay.	Reference Model: CDM Treatment: Input single constant background value for each pollutant. Lower boundary (ground): Perfect reflection. Upper boundary (mixing height): Perfect reflection. No effect until vertical dispersion coefficient equals 0.8 of mixing height, uniform vertical mixing assumed beyond this point.
Study Model: Hanna-Gifford Importance Rating: LOW Comparative Evaluation: WORSE Treatment: Not treated explicitly.	Study Model: Hanna-Gifford Importance Rating: MEDIUM Comparative Evaluation: WORSE (COMPARABLE) Treatment: Background: single additive constant. Lower boundary: perfect reflection. Upper boundary: Assumed high enough to have no effect; atmospheric stability assumed constant to above the plume height.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 1143

Application Element: Temporal Correlations	Application Element:
Reference Model: CDM	Reference Model:
Treatment: Wind speed, direction, stability correlated via wind rose; mixing height is adjusted according to stability class: Class A - 1.5 x afternoon climatological value; Class D (night) - average of morning and afternoon climatological values; Class E - morning climatological value.	Treatment: One IRRELEVANT element: ● Chemistry and reaction mechanism.
Emission rates: day-night variation allowed; all sources assumed to vary by same factor.	
Non-sequential (climatological) limited correlation.	
Study Model: Hanna-Gifford	Study Model:
Importance Rating: LOW	Importance Rating:
Comparative Evaluation: WORSE	Comparative Evaluation:
Treatment: Correlations not treated explicitly.	Treatment:

EVALUATION FORM

Part D: Technical Comparison

Application Index: 1143 Reference Model: CDM Study Model: Hanna-Gifford

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL	0	-	-	-	-
HIGH	1	0	0 (1)	1 (0)	WORSE
MEDIUM	5	0	3 (4-2)	2 (1-3)	WORSE
LOW	5	0	3	2	
IRRELEVANT	1	XXX	XXX	XXX	
	Total 12 (Should equal 12)				

TECHNICAL EVALUATION: WORSE

C.8. EXAMPLE 8: APPENDIX J/6243

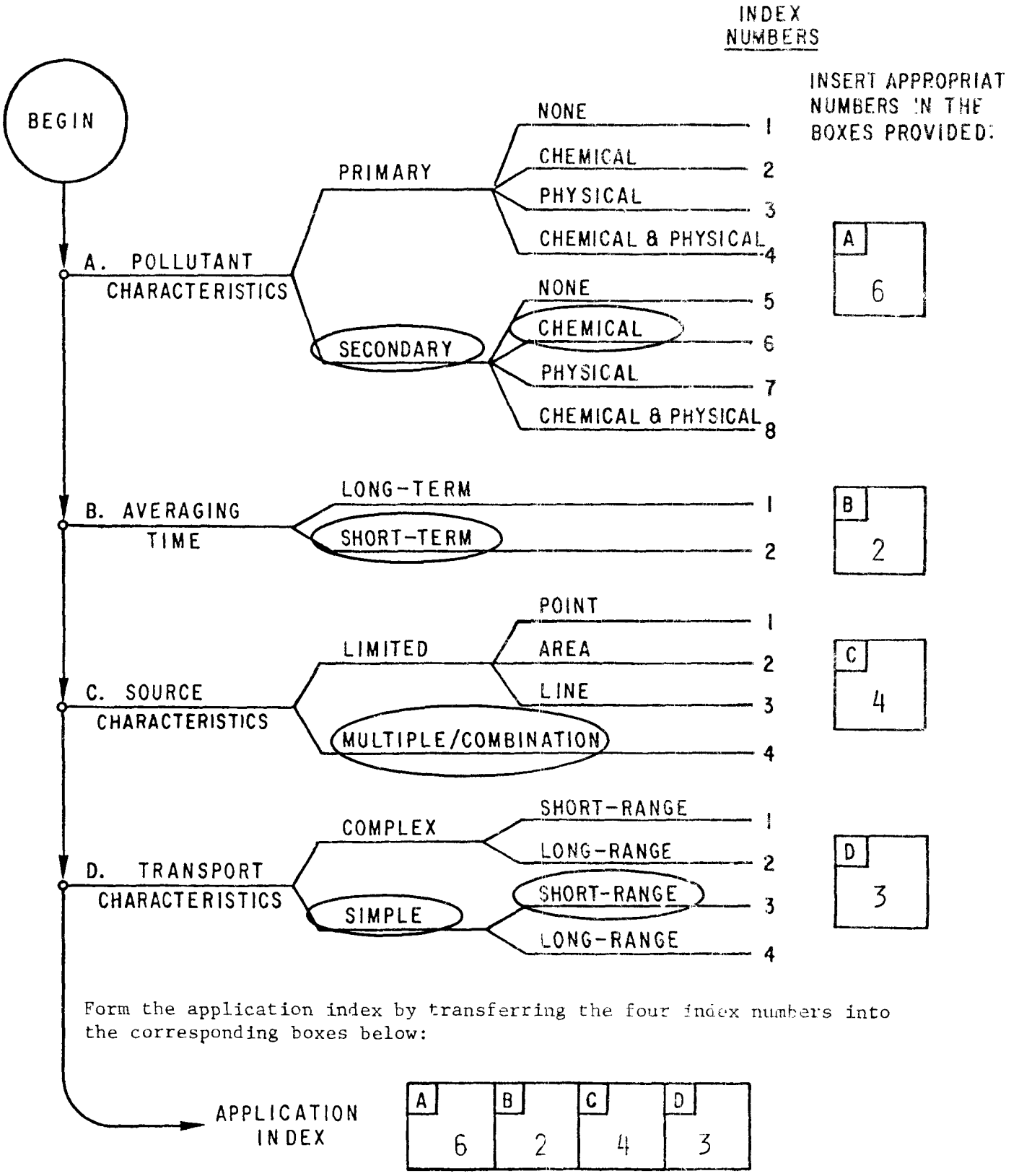
In this example, the application involves the estimation of the percent reduction of hydrocarbon emissions required in order to achieve the National Ambient Air Quality Standard for photochemical oxidant in Sample City, a moderately sized urban area located in gently rolling terrain. The appropriate Application Index is 6743 and the suggested reference model is the SAI urban photochemical model.

The study model in this example is Appendix J. Appendix J consists of a single graph of percent hydrocarbon reduction against maximum measured one-hour photochemical oxidant concentration. Given the appropriate oxidant measurement from Sample City, the required percent reduction may be read directly from the graph. The curve is based on a simple rollback model in combination with an empirical "upper limit curve," which represents the upper envelope of a plot of maximum daily one-hour oxidant levels against 6-9 AM non-methane hydrocarbon levels, the data being accumulated from several U.S. cities. The upper limit curve provides an approximate relationship between oxidant levels and precursor (hydrocarbon) levels under worst case conditions. The appropriate classification of Appendix J is therefore Rollback/Statistical.

The equations are documented and Appendix J is determined to be applicable and the "applicable" box of Part A of the Evaluation Form is checked. Then, in accordance with the instructions in Section 2, the guidelines in Section 7 are consulted immediately following Step 4 of the procedure, the classification of the study model as a Rollback/Statistical model. It is assumed that an element-by-element examination of the approximations inherent in Appendix J compared to the SAI model is desired. Therefore, Parts B, C, and D of the Evaluation Form are filled out in the same manner as if two simulation models were being compared.

With only one exception, the element-by-element comparisons of Appendix J with the SAI model indicate that Appendix J is WORSE. The single element in which they are rated COMPARABLE is physical removal, which is not treated by the version of the SAI model used as a reference model in this workbook. The technical evaluation of Appendix J is clearly WORSE. This should be interpreted as meaning that the approximations that must be made to reduce the SAI working equations to the Appendix J curve are determined to be not justified in this application.

APPLICATION CLASSIFICATION FORM



Form the application index by transferring the four index numbers into the corresponding boxes below:

APPLICATION INDEX

A	B	C	D
6	2	4	3

EVALUATION FORM

Part A: Abstract and References

Study Model: Appendix J

References: Federal Register 36 No. 158, August 14, 1971.

Air Quality Criteria for Nitrogen Oxides, AP-84, Environmental Protection Agency, Washington, (January 1971).

Abstract: Appendix J is a method for estimating the percent reduction of hydrocarbon emissions within an urban area required in order to achieve the National Ambient Air Quality Standard for photochemical oxidant in that area. The method is based on the use of simple rollback together with an empirical relationship between the maximum observed oxidant concentration and measured non-methane hydrocarbon concentractions.

Classification: Rollback/Statistical

Application Index: 6243 Reference Model: SAI

Application Description: Estimate percent reduction in hydrocarbon emissions in given urban area required to meet photochemical oxidant standard.

Model Applicability: Applicable [X] Not Applicable [ ]

EVALUATION FORM

Part A (reverse): Equations

Study Model: Appendix J

Equations:

$$\text{Percent hydrocarbon emission reduction} = \frac{\chi_{max} - \chi_{std}}{\chi_{max}} \times 100$$

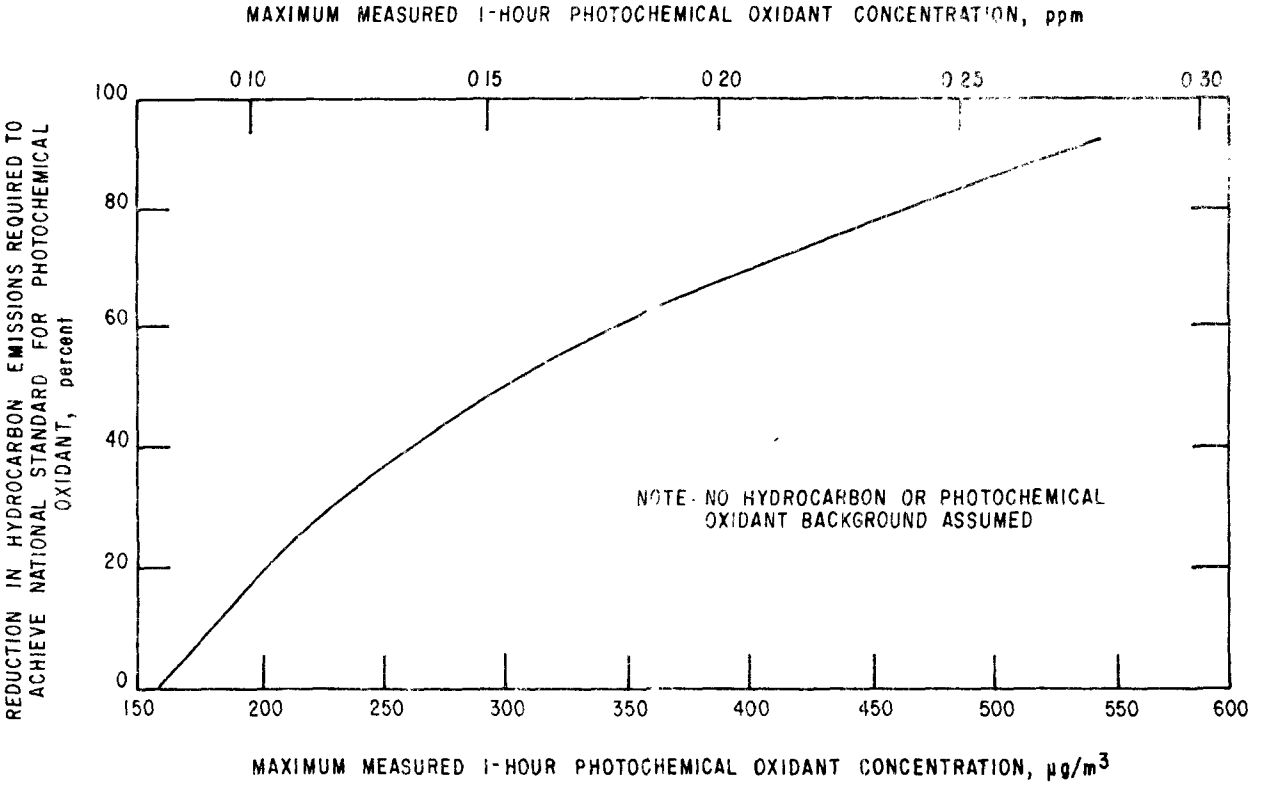
(Assumes zero background hydrocarbon concentration).

χ_{max} = nonmethane hydrocarbon concentration associated with the observed maximum oxidant level.

χ_{std} = nonmethane hydrocarbon concentration (0.24 ppmC) associated with the photochemical oxidant national ambient air quality standard (0.08 ppm over a 1-hour period).

The hydrocarbon concentration for a given oxidant concentration is determined using the empirical "upper limit curve," the upper envelope curve of a plot of maximum daily oxidant level against observed 6-9 AM hydrocarbon level, the data being accumulated from several U.S. cities.

The result is the Appendix J curve:



EVALUATION FORM

Part B: Importance Ratings

Application Index: 6243

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship	H	H
Emission Rate	H	H
Composition of Emissions	H	H
Plume Behavior	H	M ✓
Horizontal Wind Field	H	H
Vertical Wind Field	L	L
Horizontal Dispersion	H	H
Vertical Dispersion	H	H
Chemistry and Reaction Mechanism	H	H
Physical Removal Processes	L	L
Background, Boundary, Initial Conditions	H	H
Temporal Correlations	H	H

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 6243

Application Element: Source-Receptor Relationship	Application Element: Emission Rate
Reference Model: SAI	Reference Model: SAI
Treatment: All sources except power plants aggregated to square grid cells in 25 X 25 array; location of power plant specified only by grid cell; grid cell size arbitrary.	Treatment: Point source (power plant) emissions distributed homogeneously throughout entire vertical column above grid square containing the source; emission rates supplied by user.
Arbitrary release height for power plant; other emissions treated as upward fluxes at ground level; topographic elevation arbitrary.	Other emissions treated as upward pollutant fluxes at ground surface.
Receptors at ground level and in each of up to five vertical cells; horizontal location arbitrary.	Sequence of hourly average rates for mobile sources.
Areas oriented by fixed grid boundaries.	Stationary source rates assumed constant.
	Rates for mobile sources determined from user-supplied emission factors and traffic data.
	Rates for stationary sources input by user.
Study Model: Appendix J	Study Model: Appendix J
Importance Rating: HIGH	Importance Rating: HIGH
Comparative Evaluation: WORSE	Comparative Evaluation: WORSE
Treatment:	Treatment:
Receptors at ground level.	Does not treat variations within study area explicitly.
Other aspects not treated explicitly.	Accounts for change in total emissions in region of interest between baseline and prediction periods.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 6243

Application Element: Composition of Emissions

Reference Model: SAI

Treatment: Treats emissions of reactive hydrocarbons, unreactive hydrocarbons, NO, NO_2, and CO.

User inputs mobile source emissions of hydrocarbons, NO_x, and CO.

Mobile source NO_x emissions assumed to be 99% NO_2; converted internally to NO.

Mobile source hydrocarbon emissions split internally into 67.4% (mole fraction) reactive fraction and 32.6% unreactive fraction.

Study Model: Appendix J

Importance Rating: HIGH

Comparative Evaluation: WORSE

Treatment:

Non-methane hydrocarbon emissions only.

Application Element: Composition of Emissions - (Contd.)

Reference Model: SAI

Treatment:

User inputs stationary source (both point and area) emissions of reactive hydrocarbons, unreactive hydrocarbons, NO, NO_2, and CO.

Study Model:

Importance Rating:

Comparative Evaluation:

Treatment:

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 6243

Application Element: Plume Behavior	Application Element: Horizontal Wind Field
Reference Model: SAI Treatment: Uses Briggs' formulae (1971) for point sources only to determine if plume from a power plant penetrates inversion. If plume height exceeds mixing height, emissions from source are not treated. Does not treat either fumigation or downwash. Plume rise not treated explicitly for sources other than power plants.	Reference Model: SAI Treatment: Numerical/Dynamic. Fixed grid model. Wind speed and direction specified for each of a sequence of hours at points on a horizontal grid, interpolated from surface measurements. Arbitrary wind speed, direction values allowed. Wind speed, direction independent of height.
Study Model: Appendix J Importance Rating: MEDIUM Comparative Evaluation: WORSE Treatment: Not treated explicitly.	Study Model: Appendix J Importance Rating: HIGH Comparative Evaluation: WORSE Treatment: Rollback/Statistical. Not treated explicitly.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 6243

Application Element: Vertical Wind Field	Application Element: Horizontal Dispersion
Reference Model: SAI	Reference Model: SAI
Treatment: Numerical/Dynamic.	Treatment: Numerical/Dynamic.
Vertical wind speed specified for each of a sequence of hours at points on a three-dimensional grid.	Numerical solution of advection-diffusion equation in three dimensions.
Values assumed linearly increasing functions of height, values near surface determined from horizontal wind speed, directions using mass consistency requirement.	Horizontal eddy diffusivity value assumed uniform and constant and is fixed in the computer code.
Study Model: Appendix J	Study Model: Appendix J
Importance Rating: LOW	Importance Rating: HIGH
Comparative Evaluation: WORSE	Comparative Evaluation: WORSE
Treatment: Rollback/Statistical.	Treatment: Rollback/Statistical.
Not treated explicitly.	Not treated explicitly.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 6243

Application Element: Vertical Dispersion	Application Element: Chemistry and Reaction
Reference Model: SAI	Reference Model: SAI Mechanism
Treatment: Numerical/Dynamic.	Treatment: Photochemical Smog System.
Numerical solution of advection-diffusion equation in three dimensions.	Fifteen reactions involving 10 species (NO, NO_2, O_3, Hc, O, OH, HO_2, RO_2, NO_3, HNO_2).
Vertical eddy diffusivity an empirical function of wind speed and height above ground.	Lumping approximation for 2 species (Hc, RO_2).
	Steady-state approximation for 6 species (NO_3, O, RO_2, OH, HO_2, HNO_2).
	NO_2 photolysis rate calculated internally as a function of time.
	No adjustments made for the effects of incomplete turbulent mixing below the resolution of the grid.
Study Model: Appendix J	Study Model: Appendix J
Importance Rating: HIGH	Importance Rating: HIGH
Comparative Evaluation: WORSE	Comparative Evaluation: WORSE
Treatment: Rollback/Statistical.	Treatment: Photochemical oxidant estimation only.
Not treated explicitly.	Two species only: non-methane hydrocarbon and photochemical oxidant.
	Empirical relation (the "upper limit curve") used to describe relation between hydrocarbon concentrations under worst case conditions.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 6243

Application Element: Physical Removal	Application Element: Background, Boundary, Initial Conditions
Reference Model: SAI	Reference Model: SAI
Treatment: Not treated explicitly.	Treatment: Numerical/Dynamic. Background (see treatment of fluxes at vertical sides). Upper: Perfect reflection for pollutants within region of interest (turbulent diffusive flux = 0). Allows for entrainment of pollutants from above mixing layer. Lower: Implicit perfect reflection; no adjustment made to emission fluxes to account for removal.
Study Model: Appendix J	Study Model: Appendix J
Importance Rating: LOW	Importance Rating: HIGH
Comparative Evaluation: COMPARABLE	Comparative Evaluation: WORSE
Treatment: Not treated explicitly.	Treatment: Rollback/Statistical. Background levels of non-methane hydrocarbon and photochemical oxidant both assumed zero. Boundary, initial conditions not treated explicitly.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: 6243

Application Element: Background, Boundary, Initial Conditions (Contd.)

Reference Model: SAI

Treatment: Numerical/Dynamic.

Vertical: Treated as a function of position and elevation; total flux normal to side of region required to be continuous across boundary.

Initial: Mean initial concentrations of six species (reactive HC, NO, O_3, NO_2, CO, unreactive HC) specified for each grid cell.

Study Model:

Importance Rating:

Comparative Evaluation:

Treatment:

XXX

Application Element: Temporal Correlations

Reference Model: SAI

Treatment: Sequential up to 24 hours.

Correlations automatic.

Parameters updated every hour: mobile source emission for each ground-level grid square, point source (power plant) emissions, wind speed and direction, mixing height at every vertical column of grids, vertical eddy diffusivity at every vertical interface of grid cells, incoming fluxes at boundaries, NO_2 photolysis rate constant.

Update based on user input values.

Study Model: Appendix J

Importance Rating: HIGH

Comparative Evaluation: WORSE

Treatment:

Not treated explicitly.

Total emissions allowed to change between baseline and forecast periods.

EVALUATION FORM

Part D: Technical Comparison

Application Index: 6243 Reference Model: SAI Study Model Appendix J

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL	0	-	-	-	-
HIGH	9	0	0	9	WORSE
MEDIUM	1	0	0	1	WORSE
LOW	2	0	1	1	
IRRELEVANT	0	XXX	XXX	XXX	

Total 12 (Should equal 12)

TECHNICAL EVALUATION WORSE

APPENDIX D
APPLICATION CLASSIFICATION AND MODEL EVALUATION FORMS

APPENDIX D. APPLICATION CLASSIFICATION AND MODEL EVALUATION FORMS

Included in this appendix is an outline of the steps in the model evaluation methodology presented in this workbook together with a copy of each form required by the procedure.

The following page, entitled, WORKBOOK SECTION AND FORM FOR EACH STEP IN COMPARISON, lists the nine steps in the comparison procedure. It refers the reader to the workbook section containing instructions for each step and identifies which form to use for documenting the results.

The first step classifies the application and the results are recorded on the APPLICATION CLASSIFICATION FORM. Some basic information about the study model is also recorded on the EVALUATION FORM - Part A.

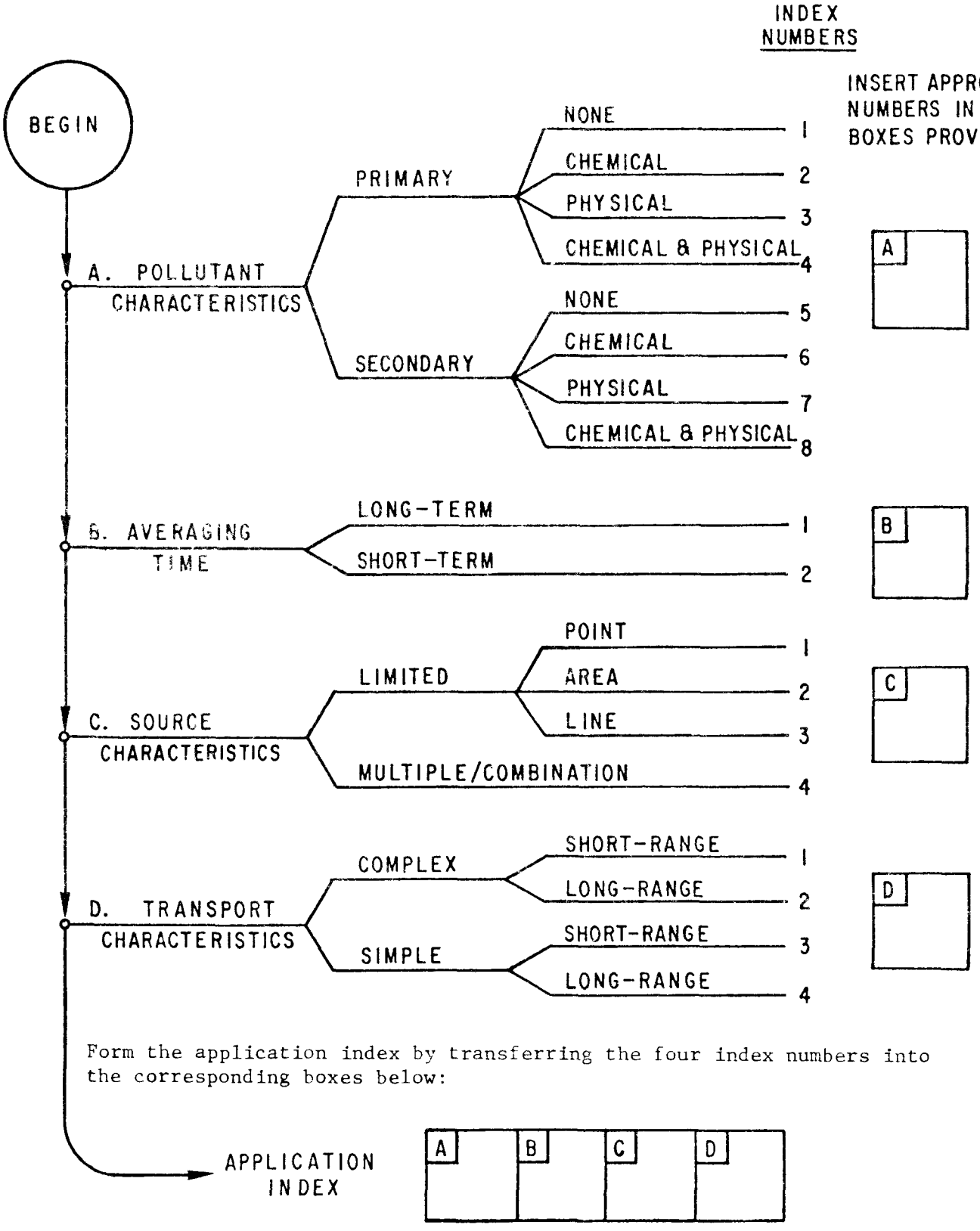
The results of steps 2 - 5 are also documented on the EVALUATION FORM - Part A. These steps involve documenting the study model equations (reverse side of form), checking the study model compatibility, classifying the study model, and identifying the reference model.

In step 6, the importance rating of the application elements are reviewed and modified if necessary. The EVALUATION FORM - Part B is used to record both the initial and modified importance ratings.

The treatment of the application elements by both models are described on the EVALUATION FORM - Part C and then compared. Results of the element-by-element comparisons are recorded on the form to complete steps 7 and 8.

In the last step of the procedure, the comparisons of individual elements are combined with the importance ratings to arrive at a technical evaluation of the study model. EVALUATION FORM - Part D provides a convenient framework for making this overall comparison.

APPLICATION CLASSIFICATION FORM



WORKBOOK SECTION AND FORM FOR EACH STEP IN COMPARISON

Step Number	Action	Workbook Sections	Form in Appendix D
1	Classify application	3	Application Classification Form
	Record study model information	2.3	Evaluation Form A
2	Document study model equations	2.3	Reverse side of Evaluation Form A
3	Check study model compatibility	4.2	Evaluation Form A
4	Classify study model type[a]	4.3	Evaluation Form A
5	Identify reference model	4.4	Evaluation Form A
6	Review importance ratings	4.5	Evaluation Form B
7	Determine treatments of elements	5	Evaluation Form C
8	Compare treatments on element-by-element basis	6.2.1	Evaluation Form C
9	Synthesize individual comparisons into overall comparison	6.2.2	Evaluation Form D

[a]If the study model has been classified as a rollback/statistical model, the user should proceed directly to Section 7 wherein such models are discussed.

EVALUATION FORM

Part A: Abstract and References

Study Model:

References:

Abstract:

Classification:

Application Index:

Reference Model:

Application Description:

Model Applicability: Applicable ☐ Not Applicable ☐

EVALUATION FORM

Part A (reverse): Equations

Study Model:

Equations:

EVALUATION FORM

Part B: Importance Ratings

Application Index:

Application Element	Importance Rating	
	Initial	Modified[a]
Source-Receptor Relationship		
Emission Rate		
Composition of Emissions		
Plume Behavior		
Horizontal Wind Field		
Vertical Wind Field		
Horizontal Dispersion		
Vertical Dispersion		
Chemistry and Reaction Mechanism		
Physical Removal Processes		
Background, Boundary, Initial Conditions		
Temporal Correlations		

[a]With the exception of the designation of IRRELEVANT elements, it is expected that at most one CRITICAL designation and possibly one other modification may be made.

EVALUATION FORM

Part C: Treatment of Elements

Application Index: _____

Application Element:	Application Element:
Reference Model:	Reference Model:
Treatment:	Treatment:
Study Model:	Study Model:
Importance Rating:	Importance Rating:
Comparative Evaluation:	Comparative Evaluation:
Treatment:	Treatment:

EVALUATION FORM

Part D: Technical Comparison

Application Index:_____ Reference Model:_____ Study Model:_____

Importance Rating of Application Elements	Number of Treatments				Comparative Rating of Study Model
	Total	BETTER	COMPARABLE	WORSE	
CRITICAL					
HIGH					
MEDIUM					
LOW					
IRRELEVANT	_____	XXX	XXX	XXX	
	Total	(Should equal 12)			

TECHNICAL EVALUATION _____

D17

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D-1

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1 REPORT NO	2	3 RECIPIENT'S ACCESSION NO
EPA-450/2-78-028b	OAQPS No. 1.2-097A	

4 TITLE AND SUBTITLE	5 REPORT DATE
Workbook for the Comparison of Air Quality Models - Appendices	May 1978
	6 PERFORMING ORGANIZATION CODE
7 AUTHOR(S)	8 PERFORMING ORGANIZATION REPORT NO
	OAQPS No. 1.2-097A
9 PERFORMING ORGANIZATION NAME AND ADDRESS U.S. Environmental Protection Agency Office of Air and Waste Management Office of Air Quality Planning and Standards Research Triangle Park, NC 27711	10 PROGRAM ELEMENT NO
	11 CONTRACT/GRANT NO
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15 SUPPLEMENTARY NOTES

16 ABSTRACT

The document consists of appendices to the Workbook for the Comparison of Air Quality Models. Appendix A presents guidance on emissions, plume dispersion, chemistry and reaction mechanisms, and physical removal processes. Appendix B provides background information on some suggested reference models. Examples of the application of the workbook methodology are presented in Appendix C.

17 KEY WORDS AND DOCUMENT ANALYSIS

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