AIRSHED MANAGEMENT SYSTEM FOR THE ALBERTA OIL SANDS

VOLUME I

A GAUSSIAN FREQUENCY DISTRIBUTION MODEL

by

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ABSTRACT

A climatological air quality dispersion was developed which provides more powerful analyses capabilities than are available in traditional CDM-type models.

The model incorporates a time series approach to satisfy identified user needs. The three components of the model are: the time series file of meteorological variables, the program (GLCGEN) used to generate ground level concentrations, and the frequency analysis program (FRQDTN) which defines the analyses for a particular run.

The time series file contains the meteorological data necessary to define dispersion classes and also includes other meteorological parameters which can be used to further classify the ground level concentrations analyzed in the frequency distribution program.

Program GLCGEN incorporates the disperision formulations and computes ground level concentrations for each receptor source pair for each dispersion class utilizing user-defined source characteristics and an emission rate of unity. This array of ground level concentration values is stored on a random access file for access by FRQDTN. This precalculation of procedure permits considerable saving of computer costs when long time series of data are processed.

The model assumes a Gaussian plume framework with plume sigmas defined by a modification to statistical theory. Effective downwind distances are utilized to allow for source affects and to simplify the analytical downwind dependence of the plume sigmas. The standard deviation of the azimuth and elevation wind fluctuations are estimated from a planetary boundary layer parameterization involving similarity theory and empirical results.

The analysis program, FRQDTN, is designed for ease of user operation. Once GLCGEN has been used to generate the ground level concentration file, the user can proceed to consider various scenarios. Source emission rates are set in FRQDTN and so various sources can be turned off or on and various emission strengths can be assigned. Different chemical species can thus be readily examined. The ground level concentration values can also be weighted according to user-selected parameters from the meteorological time series. FRQDTN can be used to generate average ground level concentrations, frequency distributions of ground level concentrations, average dry and wet deposition, and time series of ground level concentration values.

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1. INTRODUCTION

1.1 DEVELOPMENT OF AN AIRSHED MANAGEMENT SYSTEM

The Alberta Oil Sands Environmental Research Program, now part of the Research Management Division of Alberta Environment, had instituted a multi-year program to develop and implement a series of air quality models. These models were designed to provide air quality assessments to be used in conjunction with studies in other disciplines to ensure that the development of the Athabasca Oil Sands could be accomplished without undue environmental degradation. The requirements for air quality models were defined by a previous study on users' needs and model characteristics (Davison and Lantz 1979). In response to the recommendations of that study, a model development program was instituted.

The first priority was the development of a frequency distribution model which more closely related to user needs than available models. In addition, there was the desire to utilize measurements and results of studies over the previous five years in the Athabasca Oil Sands area to improve upon existing models. Among the desired model features was a capability to differentiate between concentrations occurring when receptors were sensitive and when they were not. The model was to be able to weight the impact of ground level concentrations by means of biologically or sociologically important weighting parameters. For example, this meant discriminating between the effect of high ground level concentrations occurring when trees were dormant and when they were actively transpiring and susceptible to injury. The dispersion model was to be of a Gaussian type. However, some considerable effort was to be directed towards implementation of a plume sigma scheme which more realistically reflected the dispersion than the Pasquill-Gifford scheme. In addition, a data base was to be assembled from available data sources to provide the necessary input for both the weighting parameters and the dispersion specifications.

In the first year of the program, the development of a data base for winds and dispersion parameters was a primary concern. The original plan was to utilize data from the 152 m tower at the Lower Syncrude site in order to specify the wind speed and direction fluctuations needed for the dispersion estimates. However, comparisons of the wind roses from the tower with wind roses from other sources gave convincing evidence that the tower was affected by valley flow a considerable portion of the time. This meant that the tower data were probably not suitable to give representative wind statistics at typical plume heights. One consequence of the inapplicability of the tower winds was the need to embark upon an alternative analysis of 850 mb charts to generate winds. The other major consequence was the need to parameterize the wind direction fluctuations for the plume sigma estimates by means of boundary layer classifications specified by available parameters. Both of these changes required considerable additional work.

The External Quality Assurance Team for this project met in mid-February of 1980 to comment on the work-to-date. Their report emphasized the importance of the model development and the need to have further interaction with potential users. Additional tuning of and modifications to the frequency distribution model were anticipated to be a major effort in the second year of the program, fiscal year 1980-81.

The effort in the second year of the program has been largely directed towards sensitivity studies, improvement of model capabilities, including the addition of a wet and dry deposition formulation, improvement of the mixing height formulations, validation studies, and the development of more complete model documentation.

The present report is divided into four volumes. Volume 1 describes the frequency distribution model, the rationale for the various parts of the formulation, and provides a detailed model documentation. Volume 2 documents the data base developed for use by the model. Volume 3 describes the sensitivity and

validation studies for the model and data base. Finally, Volume 4 is a user's guide to the model.

1.2 STRUCTURE OF THE PROJECT TEAM

The work described in this report was done by INTERA Environmental Consultants Ltd. and Western Research and Development. In the first year, Western's major tasks were to develop the procedures and analyze the data for the wind speed and direction and the convective mixing height. INTERA's major tasks were to develop the plume sigma specifications and the model, and to administer the project. In the second year, model improvements and sensitivity studies were primarily done by INTERA. The validation studies and preparation of the final report were undertaken by both companies.

2. OVERVIEW OF THE FREQUENCY DISTRIBUTION MODEL

2.1 RATIONALE FOR MODEL DESIGN

2.1.1 Description of Possible Approaches

A review of user needs (Davison and Lantz 1979) identified specific features that many users felt were necessary for an effective model. Potential model users identified the problem that the susceptibility of the ecosystem and hence the importance of ground level concentrations depended upon ambient meteorological conditions. Thus, there ideally should be a mechanism to weight the importance of predicted ground level concentrations. A second concern of many of the potential model users was that the time between exposures to larger ground level concentrations was important. For the biologists, this time between exposures was related to a recovery concept. For land-use planners, the time between exposures and duration of exposures was important in assessing the nuisance value of the occasional higher concentrations.

The traditional frequency distribution model or climatological dispersion model (CDM) does not recognize these user-identified problems. In the traditional approach, the ground level concentrations are calculated for a given wind speed and direction and stability. Then, the frequency of occurrence of each of the possible dispersion classes is used to give an average ground level concentration. This approach is not designed to address either the susceptibility variations or the timing between events. The fundamental structure of the traditional frequency distribution model design can limit its usefulness as a management tool. The present model was designed to overcome these limitations in order to provide potential users with a more flexible and powerful research and management tool.

Two approaches were considered for the frequency distribution model design. Both are basically two-stage models. The first stage computes ground level concentrations (GLC) based

on wind and dispersion classes. The second stage generates and displays the desired statistics from the time series of meteorological parameters and the GLC computed in the first stage. It is in this latter stage that the two approaches differ.

The first approach had some features of a traditional frequency distribution climatological dispersion model with modifications for classification by biologically important meteorological parameters. This was called the "diagonal" method and is illustrated in Figure 1. Wind and dispersion classes are assigned to each record in the time series. A frequency distribution is then generated for each of these classes. By weighting the GLC computed in the first stage by the corresponding frequency of occurrence, appropriately averaged GLC values are calculated (along the diagonal element in Figure 1). In a traditional frequency distribution model, there would be no further analysis. However, it would be possible to modify the original frequency of occurrences by including in the frequency distribution only that part of the time series which satisfies the specified range of seasonal or biologically important meteorological parameters. Note that in the diagonal approach, information on the timing between GLC events is lost by the formation of a frequency distribution. The selection of the permitted range for the biological parameters is effectively a weighting of 1 or 0. A further modification would be to calculate a weighting parameter between 0 and 1 for each entry in the time series. This procedure would permit a more refined selection of susceptibility. A variety of weighting parameters could be chosen to test the sensitivity of the GLC values to realistic ranges of biological susceptibility. Clearly, the variations in susceptibility for different plant species, or the nuisance value to people, could be readily simulated.

The second approach, called the "time series" approach, retains the time series of meteorological parameters for simultaneous interactions of the biologically important weighting parameters and the ground level concentrations. This approach,

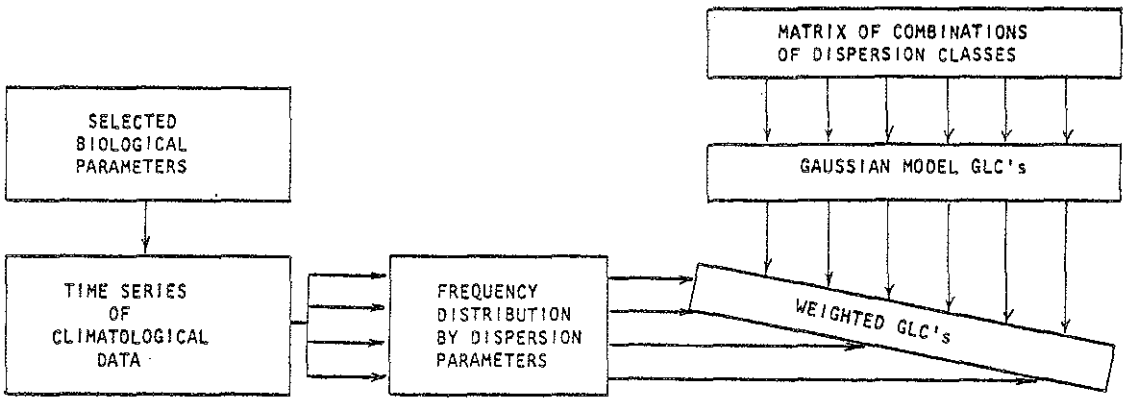

Figure 1. Traditional frequency distribution model -- diagonal approach.

illustrated in Figure 2, includes a weighting of the importance of the GLC depending upon the current values of the biologically important parameters. Thus, a weighted ground level concentration time series can be produced for each receptor point. Then time-domain statistical analyses become possible. Although the second approach initially appears to be rather complex, the generation of the computer files requires only a slight increase in the number of calculations and the amount of computer disc storage required. The weighted time series of GLC can then be applied in more powerful statistical analysis routines which can lead to much greater utility for environmental management. Average weighted GLC can be calculated; these correspond to the results from the first approach. The time series data can be analyzed to calculate the statistics of return periods for pollution episodes weighted by their biological importance; the biological recovery concept can then be applied. Changes in the averaging times become possible while still permitting temporal changes in dispersion classes and biological susceptibility within the averaging times. Another major feature is that the time series of GLC values produced can be used for model validation analysis through comparison with time series of observed concentrations.

2.1.2 Selection of Model Approach

The two approaches discussed in the preceding section were evaluated based upon the terms of reference for this contract, and the user needs identified in a previous study (Davison and Lantz 1979).

The diagonal approach is simple in concept and rapid in operation but lacks the ability to maintain time relationships between events. For new sets of biological parameters, the time series data bank must be read again, although it is not necessary to repeat the first stage in which values of ground level concentration are computed for various dispersion classes.

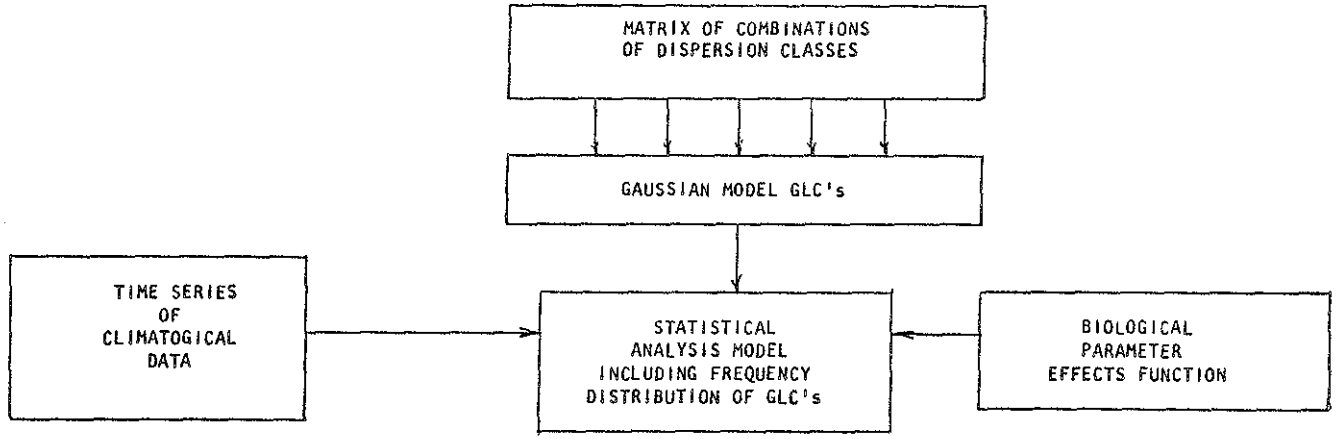

Figure 2. Time series approach.

The second approach clearly has technical advantages over the first approach in terms of flexibility and potential usefulness as an environmental management tool. However, it was important to assess whether the increased flexibility would itself cause operational problems and whether it required significantly increased computer support. Preliminary analyses were done of the generation and structure of the related computer files and the approximate amount of computer time involved in running the program. It became evident that the second approach could be designed to have a default operation that would be similar to the first approach. In this way, the increased flexibility of the second approach would only be available if specifically requested by the user. In this mode of operation, there was minimal increase in computer requirements. By proper design of the structure, generation, and use of the files, the increased potential of the second approach was not considered as significantly increasing the computer requirements. Of course, the runtime would be increased whenever the more elaborate analyses were desired, but the actual runtime involved for additional analyses proved to be quite small.

The second method, the time series approach, was selected primarily because it considers time relationships between events without significantly increased complexities. This method is also more flexible in terms of output capabilities and provides a superior tool for environmental management.

2.2 MODEL COMPONENTS

The model has three basic components. The typical user would access the frequency distribution model itself, called FRQDTN. This program calculates frequency distributions and performs other statistical analyses based upon input parameters including the susceptibility weighting descriptors. The program FRQDTN utilizes two pre-generated files which are the remaining two major components of the model system.

The first major file accessed by FRQDTN is the time series of the meteorological data. The meteorological data presently include wind speed and direction, temperature, relative humidity, mixing height, cloud cover, precipitation, and snow depth. The time series file is the result of a series of analysis programs for the various parameters. The final program which synthesizes the data sets and performs some additional analyses is called TIMSER. The typical user would not need to run TIMSER since the time series file would normally be available.

The second major file is the ground level concentration file generated by the program GLCGEN. The ground level concentrations are pre-calculated for all possible dispersion classes, for specified sources and receptors. This pre-calculation avoids the necessity of separately computing the ground level concentrations at each time series entry. Although there is an approximation involved in the discretization of the parameters controlling dispersion into dispersion classes, the pre-calculation reduces the model run-time by about an order of magnitude.

2.3 GENERATION OF THE GROUND LEVEL CONCENTRATION FILE

The ground level concentration file is created by the program GLCGEN. It is assumed that the plume spread has a Gaussian distribution in both horizontal and vertical planes with lateral and vertical standard deviations σ_y and σ_z, respectively. The following additional assumptions are made:

1. That air flow is parallel to the ground (flat terrain);
2. That perfect reflection occurs at the ground and at the bottom of any existing inversion layer;
3. That the source emission is constant in time; and
4. That a steady state exists over the entire distance of plume travel for each 1 h period.

Ground level concentrations are computed as functions of wind direction, wind speed, atmospheric stability, mixing height, and source. A suitable range of discrete values are assigned to each dispersion parameter in order to limit the number of computations. Assigning discrete classes of dispersion parameters introduces some error into the resulting ground level concentrations which will be used in the frequency distribution programs. However, the effect of this discretization approximation is small when a large number of realizations are analyzed. Furthermore, the values of each parameter in the time series are subject to error and the Gaussian formulation is only an approximation to the real situation. The discretization approximation is not considered to be the limiting error.

The number of parameters that must be input to GLCGEN at run- time is deliberately relatively small. They include only the discrete classes of wind direction, wind speed, heat flux, convective mixing height, receptor locations, source locations, and stack characteristics. All other parameters are set internally as part of the program code. This limitation was imposed to avoid complicated input procedures which can be confusing and are error prone, and also to prevent casual modification of model parameters by users of the frequency distribution model. GLCGEN is designed, however, to be readily understood so that experienced users can easily make modifications to test and tune the ground level concentration file.

During execution, the program GLCGEN first chooses wind speed and heat flux classes. If the heat flux is less than zero, the program ignores the mixing height; otherwise, a mixing height class is also selected.

The next program step is to compute the stability of the planetary boundary layer and set values of the standard deviations of lateral and vertical wind direction fluctuations, σ_A and σ_E, and also values of the Lagrangian length scales, using the parameterization scheme described in section 3. The boundary layer is classifed as stable or unstable depending on the value of

the sensible heat flux. If it is positive, the boundary layer is assumed to be unstable; if negative, the boundary layer is assumed to be stable.

After computing boundary layer stability, the program calculates plume rise and transition distances for each source. The transition distance is the downwind distance at which the environmental turbulence is assumed to dominate further dispersion. Plume rise and transition distance are functions of stability and wind speed as described in section 3.

The program then chooses a wind direction class and computes the ground-level concentrations for each receptor position for the specific sources. The Gaussian formulation makes allowance for reflections from the ground and from the top of the mixed layer, if appropriate.

The input wind directions are classified into discrete sectors. A sector averaging procedure is applied to the plume centerline position to prevent the occurrence of artificial peaks in the computed ground level concentrations. The criteria for the selection of an optimum sector angular width are discussed later in this report.

For a given wind direction at a particular source, only those receptors lying within the sector were considered to be influenced by the emissions from that source. This limitation was imposed to limit the required computations and does not introduce any significant error.

The sources are given an emission rate of unity and their effects are kept separate in GLCGEN. This procedure permits the specification by the model user in FRQDTN of the source strengths. Thus, several species of contaminants can be analyzed without the need for rerunning GLCGEN. The effects of different emissions from potential new sources can be studied by FRQDTN without needing to rerun GLCGEN. However, the size and location of the stacks and the flue gas rates must be specified for the plume rise computation in GLCGEN. This flexibility of source characterization may prove to be very useful for users who may want to assess various emission scenarios.

The receptors in GLCGEN can be either a grid system of arbitrary size (up to 400 receptors) or specified receptors.

Once the ground level concentrations are computed for all receptors for each source, the values are stored as a record on a random access file. This file is indexed according to the class of wind speed, wind direction, heat flux, and mixing height. The frequency distribution program can then access the ground level concentrations due to each source for all receptors at a given time by a simple computation of the appropriate index entry.

2.4 GENERATION OF THE TIME SERIES DATA FILE

The meteorological data base was processed to form a time series of relevant meteorological parameters for use by the frequency distribution program. In the first year of the program a limited data base was generated. It was considered appropriate to thoroughly test the model sensitivities to determine what parameters are necessary to what level of accuracy prior to embarking on a major data synthesis program. This initial limited data base generation was necessary since very little meteorological data are presently available in a computer-compatible form. The present base consists of four months (January, April, July, October) for three years (1976 to 1978). This analyzed data base has been adequate to test the model and to generate meaningful results. However, further efforts in data analysis, including assessments of other data sources, are clearly required.

The development of wind speed and direction data was based upon 850 mb weather charts. The minisonde data from both AOSERP- and Syncrude-sponsored studies provided a basis for the development of empirical power laws and turning angles used to estimate 400 m winds from the 850 mb maps. The wind data from the 152 m tower in the Athabasca River valley were shown by the minisonde data to be dominated by valley effects and to be very

poor predictors for winds at plume height. It was recognized that the 850 mb analyses had significant problems, but their adoption for the initial data base seemed reasonable.

The convective mixing heights were estimated from the minisonde data as a function of time of day and season (i.e., month for the presently analyzed data set). The height where the temperature profiles became less than adiabatic was defined as the convective mixing height. It was taken as zero when there was no surface mixed layer. The height of the convective mixing height was taken as the median height of the non-zero values for all minisonde ascents within a given season and hour.

The surface weather records from Fort McMurray Airport were used for the standard meteorological parameters and precipitation. The hourly parameters extracted were temperature, relative humidity, surface weather activity, and opaque cloud cover. The precipitation values were available as 6 h totals; daily snow depth was also abstracted.

The program TIMSER synthesizes the various data into an hourly time series with one record per hour. The times and dates for all data were converted to GMT and separate output files were produced for each month. A radiation routine was included in TIMSER to estimate hourly net radiation based upon solar altitude, cloud cover, and season. The radiation routine involved separate formulations for both solar and terrestrial radiation and used the AOSERP radiation data as processed by Kumar (1978) for evaluation of constants. GLCGEN requires surface heat flux estimates to classify the boundary layer dispersion. It was decided to keep this conversion from radiation to heat flux estimates within the program FRQDTN, since the adopted formulation was tentative. In this way, the time series file becomes a basic data file which would not normally need to be modified for use in models of varying complexities. Refinements of the parameters would then be carried out in the normal operating programs (in this case, FRQDTN) depending upon the level of refinement necessary for the particular model's use.

Details of the uncertainties in the data and of the programs used to generate the time series file are presented in Volume 2 of this report.

2.5 OVERVIEW OF THE FREQUENCY DISTRIBUTION PROGRAM

The program FRQDTN is the operational frequency distribution program that would be run by most users. It accesses the files of ground level concentration produced by GLCGEN and the hourly time series file of meteorological parameters produced by TIMSER.

FRQDTN accesses one record of the ground level concentration file to determine the source receptor layout and the dispersion classes used to generate ground level concentrations. The user provides FRQDTN with various additional parameters to determine what the model does on a particular run. The source strengths are specified in FRQDTN. In this way, various emission rates can be simulated separately for each source to permit multiple emission species to be examined. The contribution of each source to the overall concentrations can be distinguished; sources may be "turned off" in FRQDTN by specifying zero discharge rates.

Weighting parameters are specified by the user to determine the relative importance of ground level concentrations depending upon ambient meteorological conditions. This feature was specifically identified by many potential model users as being very desirable for a useful frequency distribution model.

The time series of weighted ground level concentrations is then analyzed. At the present time, three types of analysis are available. The first is a frequency distribution and an inverse cumulative frequency distribution of the concentrations at each receptor; this distribution analysis was identified in the project objectives as the primary purpose of the model. The second type of analysis available is the frequency distribution of the time between user-defined ground level concentration events. This second type of analysis is possible because of the time

series structure of the model. Although it is somewhat limited by the present discontinuous data time series, it can be used to statistically generate return periods for extreme events and can also be used to assess the likelihood of recovery between significant ground level concentration events. A third option is the calculation of average ground level concentration and dry and wet deposition estimates. All of the options can be utilized for either specified receptors or for a grid. Other options for time series analyses could be added to the model without difficulty.

3. FORMULATION OF THE DISPERSION SUBROUTINES

There are three basic components of the dispersion formulations. These are the the multiple source and receptor Gaussian formulation, plume rise, and the sigma specification. These three components are discussed in the following sections.

3.1 GAUSSIAN FORMULATION

3.1.1 Basic Formulation

The dispersion formulation in the model is of a Gaussian type. Thus, an effluent plume is assumed to have a Gaussian distribution in both horizontal and vertical planes with lateral and standard deviations σ_y and σ_z respectively. Reflections are permitted from the surface and an elevated inversion. Values of the standard deviations depend on wind speed, heat flux, and boundary layer height and are computed as functions of downwind distance X, as described in the following sections.

In convective conditions, the expression for ground level concentration, allowing for multiple reflections at the ground and at the mixing height, is (following Bierly and Hewson 1962):

$$GLC = \frac{Q}{2\pi\sigma_y\sigma_z U}\left[\exp\left\{-\frac{y^2}{2\sigma^2_y}\right\}\right]\left[2\exp-\left\{\frac{H^2}{2\sigma^2_z}\right\} + 2\sum_{j=1}^{N}\left(\exp-\left\{\frac{H-2jZ_i}{2\sigma^2_z}\right\}^2 + \exp-\left\{\frac{H+2jZ_i}{2\sigma^2_z}\right\}^2\right)\right] \quad (1)$$

where:

GLC = calculated ground level concentration

Q = stack emission

y = crosswind distance of a receptor from the plume centerline

H = height of the plume centerline above the ground

N = number of reflections

The summation term is repeated until the effect of additional reflections on the computed ground level concentration is less than 1%, usually after N = 2 or 3.

This multiple reflection procedure is used to compute ground level concentrations only if σ_z is less than 1.6 Z_i. If σ_z is larger than 1.6 Z_i, then uniform mixing between the ground and the inversion height is assumed and

$$GLC = \frac{Q}{(2\pi)^{\frac{1}{2}}\sigma_y Z_i U} \exp\left(\frac{y^2}{2\sigma_y^2}\right) \qquad (2)$$

In stable conditions where no boundary layer height is assumed, there is only one reflection off the ground, resulting in the following expression:

$$GLC = \frac{Q}{\pi\sigma_y\sigma_z U} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{H^2}{2\sigma_z^2}\right) \qquad (3)$$

3.1.2 Sector-Averaging

The wind direction looping within the program GLCGEN for the generation of ground level concentration required a discretization of the wind direction into a small number of directions (for example, 8 or 16). However, calculations along only discrete directions could give fictitious peaks for receptors along these directions compared to off-centerline receptors. This problem was avoided by assuming that the wind direction is actually uniformly distributed across a sector. Sector-averaging was accomplished within the model by combining the effects at a single receptor from plumes whose centerlines had the lateral displacements of 0, ± 1, ± 2 σ_y from the receptor. This value was then normalized by the number of such centerline displacements necessary to cover the sector width; that is, the lateral width of

the sector at the downwind distance of the receptor divided by σ_y. This procedure is equivalent to marching the plume centerline across the sector in sufficiently small angular steps to ensure that every point is significantly affected by at least four realizations. Since the sector-averaging in the model is computed after the ground level concentration below the centerline has been calculated, the actual calculations involved are few.

The angular width of the sectors, or equivalently the number of wind directions, is presently a variable in the program GLCGEN. There are at least three criteria a user should consider when choosing the number of wind directions. The first is the accuracy of the wind directions on the time series file; the second is the need to have a representative population of values for a frequency distribution analysis; and the third is the problem of implicit lateral dispersion.

The wind direction estimates in the time series file are based upon a statistical modification of wind directions estimates abstracted from the 850 mb analyses available every 12 h. Linear interpolation was used for intermediate hours. Errors in the wind direction data can be estimated based upon the analysis of the cumulative frequency distribution of the turning angles between the 850 mb winds and winds measured at plume height by minisonde. In addition, the amount of systematic error in wind directions can be estimated from a comparison of wind roses for the minisonde data, and for the corresponding derived winds from the 850 mb analysis. The wind direction uncertainties in the present data file are substantial, particularly in winter. Details are presented in Volumes 2 and 3 of this report.

The need for a representative population provides a further constraint on sector width. With a small data base, the use of small angular sectors may mean that some wind directions are not represented adequately, particularly when subsets of the time series are used. Thus, the angular width of sectors must be wide enough to ensure a reasonably representative distribution of wind directions.

The angular width of sectors is also constrained by the implicit lateral dispersion inherent in sector-averaging. If a map of integrated average values is the only desired output from the model, then lateral dispersion becomes of minor importance. However, if a time series or frequency distribution of concentrations at a particular receptor is desired, then it is important to discriminate an infrequent high concentration from a more frequent lower concentration. Sector- averaging can smear out the high concentrations into more frequent lower concentrations.

Sector-averaging may approximate some of the low frequency effects on plume dispersion. If there is a wind direction shift due to, for example, the advection of a meso-scale system, then the wind can move the centerline of a plume in a fashion analogous to sector- averaging. However, the turbulence responsible for mixing about the plume centerline may be unchanged by the wind direction change, if it is generated strictly from local mechanical effects. Thus, the σ_A value entering the plume sigma formulation, [or equivalently the Pasquill (1976) or Taylor statistical theory formulation from which the previous two are derived], is unchanged.

Low frequency wind direction changes can have effects quite dissimilar to these of sector-averaging. Consider a sinusoidal wind direction change of the form:

$$\theta = \theta_o + A \sin \omega t \qquad (4)$$

where A and ω are the amplitude and frequency of the change and θ_o is the centerline about which the oscillation is occurring. If the frequency of the motion is sufficiently slow, then the oscillation will be completely decoupled from the higher frequency turbulence causing mixing about the plume centerline. The concentrations at a particular receptor may then appear as two peaks within the period of oscillation as shown in Figure 3. If the receptor is on the mean centerline, then the peaks may be

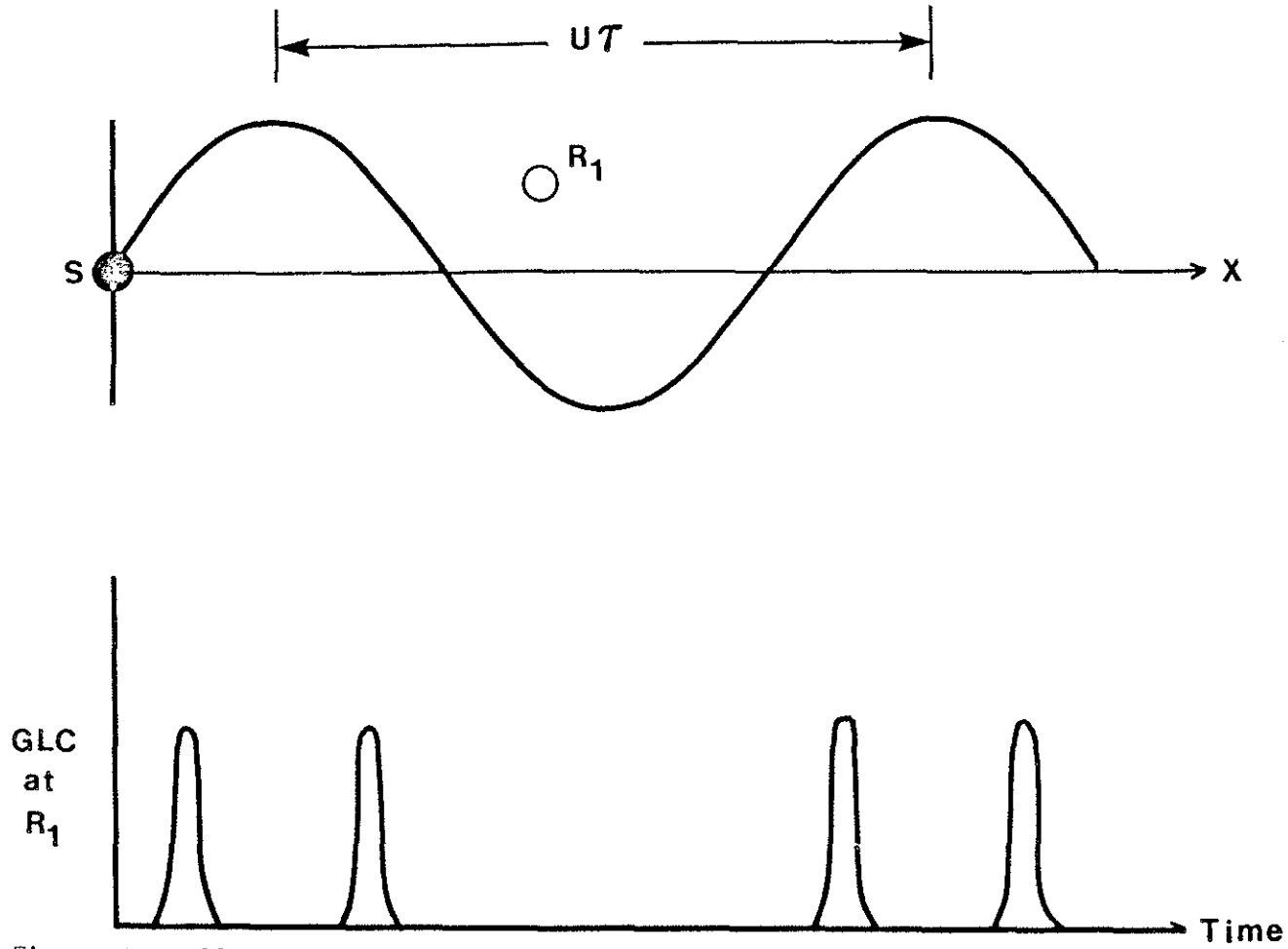

Figure 3. Effect of a low frequency wind direction oscillation on ground level concentrations. The average GLC values will be the same for any receptor within the crosswind amplitude of the low frequency wave and there will be no decrease with increasing downwind distance.

equi-spaced; whereas, towards the edges of the range covered by the centerline oscillations, the two peaks will occur closer together. There are two significant features about such a scenario:

1. The total exposure for any receptor within range of the centerline variations is the same for any given downwind distance.
2. If the plume is mixed in the vertical, there is limited change in the concentrations with downwind distance until dispersion about the centerline exceeds the magnitude of the wind direction fluctuations.

The impact of a linear or sinusoidal wind direction change will depend upon the time scale of the changes compared to the time scale of the σ_A specification. If the changes are very slow, then a value of σ_A estimated from local turbulence parameters may be fully adequate for estimating a 1 h GLC. Sector-averaging in this case would tend to smooth out real local GLC maxima across a sector. However, if the time scales of the wind direction changes are equivalent to the σ_A calculational period, (presently 1 h), then the sector-averaged GLC may give a best estimate of the 1 h observed GLC.

The correct measurement of σ_A is also dependent upon the separation of turbulence from decoupled low frequency wind direction changes. If a large measured value of σ_A due to low frequency effects is inadvertently used in a turbulent dispersion formulation, then an incorrect power law dependence for GLC with distance will result. The standard deviations of wind direction should be calculated from a de-trended data set. The trend information is part of a different dispersion process which may or may not be important.

In the present frequency distribution model, sector-averaged GLC values are used exclusively. With the limited data base presently on the time series file, this 16-direction discretization appears to be a reasonable compromise for the

constraints discussed above. However, the sector-averaging over 22.5° does produce an implicit lateral dispersion. Note that for the worst case scenarios, there should be no sector-averaging. Although the ground level concentrations under the centerline can be printed out as an intermediate step in GLCGEN, the present version of the model is not designed for effective use in a worst case mode.

3.2 PLUME RISE

The plume rise formulations used in the present model are based on the recommendations of Briggs (1975) with some minor modifications. For neutral and unstable conditions, a final plume rise has been adopted of the form:

$$\Delta h = C_I \, F^{1/3} \, (x_f)^{2/3} \, U_s^{-1} \qquad (5)$$

where: F = $gVs\,(0.5d)^2\,(T_s-T_a)/T_s$ is the buoyancy flux parameter and has units of (m^4/s^3)

U_s = mean wind speed from stack top to plume top (m/s)

V_s = stack exit velocity (m/s)

d = stack diameter (m)

T_s = stack gas exit temperature (°K)

T_a = ambient temperature (°K)

X_f = a downwind distance chosen to produce a useful effective stack height and

C_I = $\left[3/(2\beta^2)\right]^{1/3}$

C_I has a value of about 1.4 based on AOSERP data (Davison and Leavitt 1979). Briggs (1975) recommends a value of 1.6. The parameter β is an entrainment constant used to close the conservation equations for plume rise.

All of the above parameters are standard except for X_f. Briggs

(1975) points out that plume rise may continue during neutral conditions. There has been some recent work that suggests that a more detailed theoretical analysis of the problem leads to a final plume rise (Djurfors and Netterville 1980). However, for the purposes of obtaining a reasonable effective stack height in a climatological dispersion model using a Gaussian formulation, the plume rise needs to be limited to the downwind distance at which significant ground level concentrations are likely. An arbitrary value of 2000 m was adopted for all sources. Briggs (1969) applied a similar line of reasoning and recommended an explicit formulation

$$X_f = 3.5\ X^* \qquad (6)$$

where: $X^* = 34\ F^{2/5}$

for values of F greater than 55 m^4/s^3. For the Suncor plume, Briggs' formulation would lead to an X_f value of about 1750 m. Considering the approximate nature of the specification, a standard value of X_f = 2000 m seemed reasonable for neutral and unstable conditions.

In stable conditions, the plume rise formulation adopted was that recommended by Briggs (1975):

$$h = C_2 \left(\frac{F}{US}\right)^{1/3} \qquad (7)$$

where: $s = \frac{g}{T_a} \frac{\partial \theta}{\partial z}$

The constant C_2 was taken as 2.6 following Briggs (1975).

The choice of plume rise formulation depended upon whether the transition from source-dominated to environmentally dominated dispersion was controlled by the mechanical or thermal stability constraints. This transition is discussed in the following section. The criterion adopted was that if mechanical turbulence was dominant in the specification of turbulent dissipation, then, for consistency, rise should also be calculated according to the neutral formulation of Equation 5. The value of

X_f in such cases was taken to be the transition distance. The rationale for this choice was that the plume rise could not cease until the plume dissipation values, which are due to the plume's thermally generated turbulence, were equal to environmental dissipation values.

The specification of $\partial\theta/\partial Z$ for the stable plume rise formulation was based upon empirical measurements. Values of 0.1, 0.5 and 1.2 C°/100 m were considered appropriate for slightly, moderately, and very stable conditions. The latter two values are the average of TVA classes B and C and classes D and E, respectively. In addition, they correspond to the average temperature gradients for the moderately and very stable groupings of Suncor plume rise data collected by Fanaki et al. (1979 a, b, c) as analyzed by Davison and Leavitt (1979). The stability parameter for stable conditions according to the similarity theory discussed below is μ_*. Slightly, moderately, and very stable conditions were taken to correspond to values of 5, 15, and 40. Then, $\partial\theta/\partial Z$ was made a continuous variable based on values at those three points. The advantage of making $\partial\theta/\partial Z$ a continuous variable was to minimize any unnecessary effects of discretization on a parameter as important for dispersion estimates as the plume rise.

The plume rise formulations adopted are recognized as being approximate values. However, the formulations are considered adequate in the light of their application in a frequency distribution model where ranges of meteorological parameters are grouped together.

3.3 SIGMA SPECIFICATION

The third major aspect of dispersion formulation is the choosing of a procedure to specify the plume sigma values.

3.3.1 Characteristics of the Three Regions of Sigma Specification

In defining the plume sigmas for an industrial source,

it is well known (e.g., Pasquill 1974) that there are up to three distinctive regions as the downwind distance from the source increases. These regions are determined by the dominant dispersive mechanism acting at a given downwind distance. These regions are:

1. The source-dominated region;
2. The environmentally dominated region; and
3. The lateral shear-dominated region.

The characteristics of these regions have been discussed by many authors and were summarized in a previous report (Davison and Leavitt 1979). In the paragraphs below, the procedures used in the model are briefly outlined, with more details following in subsequent sections.

In the source-dominated region, the plume itself has greater energy in the higher frequencies of motion responsible for initial plume spread than the ambient environmental turbulent eddies. Thus, the spread of the plume is governed by the source characteristics. How long this situation lasts, or equivalently at what downwind distance the source turbulence becomes equal to the ambient, depends upon source characteristics and the magnitude of the ambient turbulence. The present understanding of this concept of source-dominated dispersion has been well reviewed by Briggs (1975); however, some practical problems remain. There are some uncertainties in the specification of the transition distance, given routine meteorological data. For the present study involving a frequency distribution model, some simple assumptions are probably adequate. These are discussed in a subsequent section.

The case of unstable conditions brings out a more fundamental limitation. The assumption of a source-dominated region implies a spectral gap in energies between the low frequency eddies which cause the plume direction to meander and the higher frequency mixing eddies. For a source-dominated region to be a useful concept, the relative dispersion about the plume centerline must be dominated by source-generated turbulence. In

unstable conditions, however, the dominant ambient mixing eddies tend to have lower frequencies (larger size scales) and may markedly influence the dispersion very near the source. The plume material in a looping plume segment may have more energy than the ambient in the higher frequencies, but this frequency of energy may not be too important for mixing. Source region transition formulas based upon dissipation values as proposed by Briggs (1975) are probably questionable for moderately or strongly convective situations. Adoption of a small ad hoc transition distance of the order of a few hundred metres is probably more appropriate for convective situations as discussed below.

The environmentally dominated region of dispersion is the downwind range of distances within which the dispersion is largely governed by the standard deviations of the wind elevation and azimuthal angles (σ_E and σ_A , respectively). Taylor's formulation as presented by Pasquill (1976) has found wide acceptance for lateral dispersion (Hanna et al. 1977). A similar formulation for vertical dispersion has problems in that the turbulence structure changes significantly with height. However, in a Gaussian model, the vertical variations of wind speed and plume geometry are neglected. The σ_E value does characterize the amount of vertical mixing. The major problem in adopting a Taylor theory expression involving σ_E for vertical mixing from a tall stack appears to be the observations that in stable conditions, the plume σ_z values do not scale as $X^{1/2}$. This problem appears to be overcome by adopting an effective downwind distance, X_{eff}, based upon the matching of σ_z at the transition to environmentally dominated dispersion. The values scaling according to $X_{eff}{}^{1/2}$ appear to generate very reasonable σ_Z curves as a function of X. In the model, σ_Z values in the environmentally dominated region are calculated using a Taylor theory expression involving σ_E and X_{eff}. Details are presented in a later section.

The matching of the source and environmentally dominated regions of dispersion has not been widely discussed. If there is a significant source-dominated region (as there usually is for the

typically hot plumes from a synthetic oil sands plant), then this matching needs attention. As outlined below, the requirement is to define an effective downwind distance for the environmentally dominated region that is different from the actual downwind distance based upon sigma matching at the transition distance. This distinction has been included in the present model.

For cases of significant vertical wind direction shear, combined with non-negligible environmental vertical mixing, lateral dispersion can become dominated by a mechanism of shear-enhanced dispersion. The theory was presented by Pasquill (1974) for simple linear shears. Pasquill suggests that these effects may dominate under ideal conditions at downwind distances of the order of 10 km. The σ_y values would then increase at a rate of $X^{3/2}$ compared to the long-range Taylor theory limit of $X^{1/2}$.

Slawson et al. (1978) found shear effects much closer to the source than 10 km and proposed an empirical formulation to account for shear effects. As part of the present study, Leavitt and Davison (1980) re-examined some of the Slawson et al. data and proposed an alternative interpretation. The basic idea was that within the source-dominated region the environmental directional shear can interact with the source-induced vertical mixing to generate an $X^{5/3}$ region of lateral plume spread. The size of the effect can amount to 100% of the normal spread within 1 or 2 km of the source and can account for the enhanced near-source dispersion found by Slawson et al. Beyond the transition to environmental turbulence, Leavitt and Davison concluded that the Slawson et al. plume sigma data were consistent with an $X^{1/2}$ spread of Taylor's theory, although lack of σ_θ data precluded a more definitive conclusion.

The effects of shear-induced dispersion were not included in the present version of the model. The shear-induced dispersion can greatly increase the lateral dispersion of a plume and so reduce the maximum ground level concentrations. However, in a frequency distribution model, the sector-averaging dominates

the effects of lateral dispersion. In addition, there were major problems in determining a reliable mean wind direction at plume height; so that generating a direction shear data base would be much more difficult. The analysis of the shear effects in the Slawson et al. data did permit the resolution of the apparent discrepancies between that data base and the data base used in the previous sigma study (Davison and Leavitt 1979). In addition, the procedures for inclusion of directional shear effects have been defined. The present model was designed so that inclusion of directional shear effects on the plume sigmas could be readily accomplished in the future when an adequate data base has been derived.

3.3.2 Source-Dominated Region of Dispersion

3.3.2.1 Plume sigma specification. The plume sigma formulations appropriate for the source-dominated region of dispersion were reviewed by Davison and Leavitt (1979). Basically, the recommended formulations followed the outline presented by Briggs (1975), with modifications of the empirical constants based upon an analysis of the AOSERP data base, especially the data collected by Fanaki (1979 a, b, c). Within the source-dominated region, the plume sigmas scale with the plume rise. The formulations used for plume sigmas were:

$$r = \beta \Delta H$$
$$\sigma_z = 0.42\ r \qquad (8)$$
$$\sigma_y = 1.4\ \sigma_z$$

where ΔH is the plume rise in neutral or stable conditions and r is the radius of the plume. The factor 0.42 arises from the assumption that the "radius" of the visual plume corresponds to the 10% concentration in a normal distribution. The ratio of 1.4 between the lateral and vertical sigmas was recommended by Davison and Leavitt (1979) based upon an analysis of preliminary LIDAR data of the Suncor plume presented by Hoff and Froude (1979).

The parameter β is an entrainment constant first used as a closure hypothesis for the plume rise conservation equations by Morton et al. (1956), as discussed below Equation 3. Values of β are normally determined from observations of plume rise and plume thickness. A value of $\beta = 0.5$ gives good agreement with observations of the ratio of plume rise and plume radius (Briggs 1969), but leads to a value of $C_1 = 1.8$ in Equation 5 for plume rise. Briggs (1975) has proposed a concept of modified volume flux to define an effective value of β, with a recommended value of 0.6 [see Davison and Leavitt (1979) for a more complete discussion].

In neutral conditions, the values of β, and hence σ_z and σ_y depend upon $C_1\beta$ and thus have only a 1/3 power dependence on β, as shown in Table 1. Because of the uncertainty in the 0.42 factor relating σ_z to r, a value of $C_1\beta = 1.0$ is considered to be sufficiently accurate and was adopted in the model.

In stable conditions, the plume geometry defined by Equation 8 was assumed. However, the maximum plume rise, HR, given by

$$HR = 0.79\ HR_f \tag{9}$$

where HR_f is the final plume rise, was used to compute the value of σ_z at the transition distance.

Note that the size of the sigmas is such that the plume rises faster than the plume spreads downward. Thus, the ground level concentrations for flat terrain are minimal at downwind distances within the source-dominated region. A reasonably accurate estimate of the plume sigmas is required, however, to permit a proper matching of the sigma formulations at the transition to the environmentally dominated region of dispersion. The determination of the transition distance and the matching at that transition are outlined in the next two sections.

Table 1. Typical values for the neutral plume rise coefficients (C_1) and the corresponding values for the entrainment constant.

C_1	β	$C_1\beta$
1.40	0.74	1.03
1.60	0.61	0.97
1.80	0.51	0.91

3.3.2.2 Formulation of the transition distance. For neutral and unstable conditions, the transition distance from source-dominated to environmentally dominated dispersion regimes was defined by the criterion of dissipation matching as suggested by Briggs (1975). As discussed in Davison and Leavitt (1979), the dissipation can be affected by both thermal and mechanical turbulent energy, or can be dominated by one or the other. The significance for the present study is that the dissipation, and hence the transition distance, has a different dependence on the wind speed (U), depending upon whether the thermal or mechanical effects dominate. From Briggs (1975) and Davison and Leavitt (1979),

$$\varepsilon_p = 0.8 \frac{T_s}{T_a} F^{2/3} UX^{-5/3} \tag{10}$$

where ε_p represents the dissipation rate inside the plume. The transition distance defined by dissipation matching becomes

$$X_t = \left\{ 0.8 \frac{T_o}{T_a} F^{2/3} \frac{U}{\varepsilon} \right\}^{3/5} \tag{11}$$

where ε is the environmental dissipation. The problem now reduces to specifying the environmental dissipation.

For a mechanically dominated planetary boundary layer (PBL), the environmental dissipation is

$$\varepsilon = \frac{u_*}{kz} \tag{12}$$

where u_* is the friction velocity evaluated in the surface layer, Z is height, and k is von Karman's constant. Using a logarithmic wind profile, the dissipation matching criterion for mechanically dominated conditions becomes

$$X_t = \left\{ 0.8 \frac{T_o}{T_a} F^{2/3} \frac{Z}{k^2 U^2} \left[\log \left(\frac{Z_1}{Z_o} \right) \right]^3 \right\}^{3/5} \tag{13}$$

where Z_1 is the height in the surface layer where the friction velocity is evaluated (typically 10 m), and Z_o is the roughness

length. This value can be used as a limit for the approach to mechanically dominated conditions.

For a convectively dominated PBL, the environmental dissipation, (ε), was made a function of $\overline{w\theta}$. According to similarity theory, the dissipation, when non-dimensionalized by the relevant velocity and length scales, should be a function of the stability scaling parameter Z_i/L. The details of the selection of the relevant scales and of the scaling parameter are discussed in a section below on PBL parameterization. The expression for dissipation in convective conditions reduces to

$$\varepsilon = \frac{g}{T_a} \overline{w\theta} \quad f\left(\frac{Z_i}{L}\right) \tag{14}$$

where $\overline{w\theta}$ is the surface heat flux and $f(Z_i/L)$ is a function to be specified. Based upon measurements of dissipation in the AOSERP study area (Davison and Grandia), the expression for dissipation adopted in the model was

$$\varepsilon = 1.4 \frac{g}{T_a} \overline{w\theta} \quad \approx \quad 0.05 \ \overline{w\theta} \tag{15}$$

where a mean value of T_a was adopted. The values for the dissipation generated by the above expression are about a factor of 2.8 larger than those adopted by Venkatram, 1980. However, the values are typical of observed values. The 1.4 factor is consistent with turbulent energy conservation because of the effects of heat flux at the top of the PBL and of the effects of water vapour flux, and also mechanical energy generation at the surface.

The transition distance in the model was taken to be the minimum of the mechanically dominated and convectively dominated estimates. This minimum criterion ensures that the mechanical limit is used for a mechanically mixed PBL in strong winds and the convective limit is used for weak winds when convective effects should dominate. Examples of the estimated transition distances as function of wind speed for the Suncor plume based upon the

above formulations are presented in Table 2. It is seen that for higher wind speeds, the mechanically dominated estimate is the controlling limit.

The transition distances for strongly convective cases may be questionable due to the importance of larger scale environmental eddies. In very unstable conditions, the looping of plumes and the plume break-up close to the source imply that the adoption of a source-dominated region may be inappropriate even when the dissipation levels inside the plume (or plume segments) are large. The transition distances for the very unstable case in Table 2 are less than 1 km only for lighter winds. However, highly organized convective structures are known to exist in the presence of strong surface heating even in moderate winds. Thus, it seems appropriate to restrict the transition distance in the highest positive heat flux class to a maximum value of 800 m.

There are considerable uncertainties in the constants involved in the plume dissipation expressions needed for transition estimates in neutral and convective situations. A discrepancy of 50% was noted by Davison and Leavitt (1979) between alternative formulations of the mechanically dominated plume dissipation discussed by Briggs (1975). The uncertainties in the convective case may even be larger. Fortunately, these large uncertainties do not have a major effect upon the final ground level concentration values. The dissipation values enter the formulation only in the calculation of the transition distance, and even there, only to the power of 0.6. Thus, a 50% uncertainty in dissipation becomes about a 25% uncertainty in transition distance. The resultant uncertainty in the ground level concentration will be a function of many parameters and cannot be simply expressed, but will consist of both a slightly changed magnitude and location of the maximum ground level concentration. Results of sensitivity tests are presented in Volume 3 of this report. The relevant conclusion is that the dissipation formulation uncertainties are far from being the controlling uncertainties and often have minimal effect upon the ground level concentrations.

Table 2. Examples of values for the transition distance based upon mechanical and convectively dominated values of the ambient dissipation. The estimates are for the Suncor plume.

WIND SPEED	TRANSITION DISTANCES X_T (km)[a]			
m/s	Mechanical	Slightly Stable (0.001)	Moderately Stable (0.005)	Very Stable (0.010)
2	18.6	1.9	0.7	0.5
5	6.2	3.3	1.3	0.8
10	2.7	5.0	1.9	1.3
15	1.2	6.4	2.4	1.6

[a] The examples for the convective PBL correspond to dissipation rates as shown: 0.001, 0.005, 0.010 m^3/s. These dissipation rates correspond to heat flux values of 0.02, 0.10 and 0.20, respectively. In the model, the minimum of the mechanical and convective estimates was adopted.

For stable boundary layers, the transition distance was taken to be the distance to maximum plume rise. Following Briggs (1975), the maximum plume rise for a buoyant plume will occur when

$$\omega' t = \pi/2 \tag{16}$$

where ω' is the Brunt-Vaissala frequency modified for the effective momentum flux. The transition distance is then defined as

$$X_t = \frac{\pi}{2} U \left\{ \frac{g}{\theta} \frac{\partial \theta}{\partial Z} \frac{M}{M_e} \right\}^{-1/2} \tag{17}$$

where M and M_e are the actual and effective momentum fluxes as defined by Briggs. Briggs (1975) suggests a value,

$$\frac{M}{M_e} \simeq 2.3 \tag{18}$$

The values of $\partial\theta/\partial Z$ for stable conditions are those presented earlier in the discussion of plume rise. In the present model, the expression for transition distance then becomes

$$X_t = 12.7\ U \left\{ \frac{\partial \theta}{\partial Z} \right\}^{-1/2} \tag{19}$$

where an ambient temperature of 5°C has been adopted. The values of X_t for a range of typical wind speeds are shown in Table 3 along with the corresponding transition distance for a mechanically dominated mixing layer based upon the dissipation criterion discussed above. In the present model, the minimum of the mechanical and stable transition values are adopted.

Table 3. Examples of values for the transition distance for stable conditions, taking the distance of maximum plume rise as the transition distance. The values for a mechanically mixed boundary layer based on the dissipation criteria are also calculated in the model, and the smaller value of X_T is adopted in each case.

WIND SPEED	TRANSITION DISTANCES X_T (km)[a]			
m/s	Mechanical	Slightly Stable (0.001)	Moderately Stable (0.005)	Very Stable (0.012)
2	18.6	0.8	0.4	0.2
5	6.2	2.0	0.9	0.6
10	2.7	4.0	1.8	1.2
15	1.2	6.0	2.7	1.7

[a] The bracketed values are the typical values of the dissipation rate in m^3/s.

The formulation for the transition distance indicates that the transition distance is typically of the order of 1 km. However, it can be greater than 3 km for wind speeds of about 7 m/s for near neutral conditions. This limit is in agreement with the case study of 22 June 1977 presented by Davison and Grandia (1979). In that case study, the transition distance was observed to be greater than 3 km just after sunset with a wind speed of 7.5 m/s. The transition distance was less than 3 km for all other case studies in that field study and in the March 1976 AOSERP field study (Davison et al. 1976).

3.3.2.3 Sigma matching at the transition distance. The presence of a source-dominated region means that a matching of the sigmas at the transition point is required. The matching results in the definition of an effective downwind distance coordinate for use in the environmentally dominated region. The matching of sigmas at the transition point leads to

$$\sigma_s(X_{ts}) = \sigma_e(X_{te}) \tag{20}$$

where subscripts s and e refer to the source region and environmental regions, respectively, and where the subscript t on the X - coordinate refers to the transition point. If the environmental sigmas are functions of X,

$$\sigma_e = f(X) \tag{21}$$

then the value of X which corresponds to a value of σ_e equal to σ_s at the transition distance can be called X_{te}. The value of X_{te} corresponds to the downwind distance at which would be equal to $\sigma_s(X_{ts})$ in the absence of any source region effects. In general,

$$X_{te} \neq X_{ts} \tag{22}$$

For example, a tracer emitted into a stable elevated layer might take a long distance to disperse to a size scale equal to that obtained by the source-dominated dispersion. In such a case, the effective source location for the environmentally dominated dispersion formulations would be significantly upwind of the actual source, as is sketched in Figure 4. The appropriate downwind distance coordinate for use in environmental formulations is changed by $(X_{te} - X_{ts})$ from the actual downwind distance coordinate. This effective downwind distance correction can clearly be different for the vertical and lateral spreads. Allowance for effective downwind distance coordinates has been included in the present model for sigma calculations in the environmentally dominated region.

A further constraint was imposed upon the values of the plume sigmas in the source-dominated region. The value of the sigmas had to be at least as large as the values predicted by the formulation presented by Pasquill (1976). The formulation was changed to a power law of the form $F(X) = 0.6\ X^{0.2}$ and was extended to σ_z/σ_e, where σ_e is the standard deviation of the wind elevation angle fluctuations. This constraint ensured that an error in the transition distance, due to such uncertainties as the dissipation specification inside the plume, could not lead to unrealistic values. The results of sensitivity tests on this constraint are discussed in Volume 3 of this report.

The use of effective downwind distances had a very significant effect upon the apparent power law for σ_z in stable conditions. By having a significant positive offset on X, then adopting a constant power law of $\sigma_z \propto X_e^{1/2}$ lead to much lower power laws based upon true downwind distance X. The result was that a stability and downwind distance dependence of the power law exponent on X was implicity contained. One of the major theoretical advantages of such an approach is that the same environmental dispersion formulation is applicable regardless of downwind distance and the degree of stability. The changing of

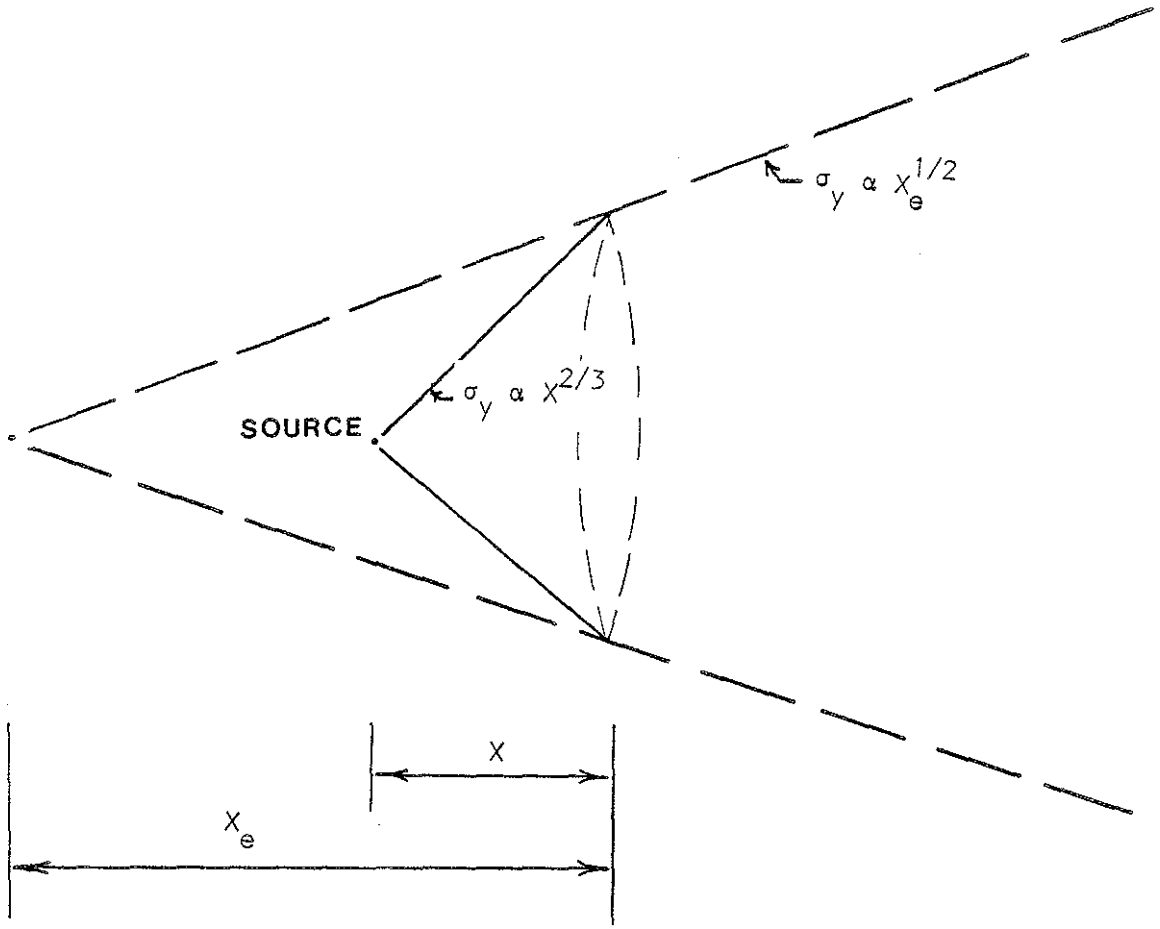

Figure 4. Illustration of the difference between the actual downwind distance (X) and the effective downwind distance (X_e).

empirical power laws with stability and downwind distance common to most sigma specification schemes can be avoided. Results of a limited comparison to observations are shown in Volume 3 of this report.

3.3.3 Environmentally Dominated Region of Dispersion

3.3.3.1 Rationale for boundary layer parameterization. As mentioned above, the environmentally dominated region is the downwind range within which dispersion is governed by the standard deviations of wind azimuth and elevation angles. Davison and Leavitt (1979) report that the lateral plume spread is reasonably well predicted by variations of Taylor's statistical theory. Such an approach is currently widely accepted (e.g., Hanna et al. 1977).

In the present version of the model, the vertical spread for all stability has been specified using an approach equivalent to that adopted for lateral dispersion. The sigma specification subroutine does include, however, a calculation of the parameters necessary to implement a simplified TVA scheme as recommended by Davison and Leavitt for predicting σ_z in stable conditions. A comparison of the present scheme based on an amalgam of results from the literature on boundary layer parameterization with the simplified version of the TVA scheme of Carpenter et al. (1971) is recommended during future tuning of the model. Because the procedure used to calculate either sigma value is similar, it is outlined below for σ_y only.

As mentioned above, the procedure used to calculate σ_y is a variant of the statistical theory first derived by G.I. Taylor in the 1920's . For long dispersion times (or equivalently, large downwind distances),

$$\sigma_y = \sigma_v \, (2t_{ve})^{1/2} \, T^{1/2} \qquad (23)$$

where σ_v is the standard deviation of lateral wind fluctuations, t_{ve} is the Lagrangian integral time scale and T is the pollutant travel time from release. Details of the derivation of this equation and specifications for appropriate sampling of σ_v are given in Pasquill (1974).

Assuming $\sigma_A = \sigma_v/U$, where U is the mean wind speed, this formula can be rewritten as

$$\sigma_y = \sigma_A (2\ell_v)^{1/2} X^{1/2} \quad (24)$$

where, $\ell_v = t_{ve} U$ is the Lagrangian length scale. Because it is difficult to measure the Lagrangian length scales, various approximations have been derived. A useful abbreviation to Equation 24 is

$$\sigma_y = \sigma_A X f(X) \quad (25)$$

Estimates of f(X) are available from Pasquill (1976). At large downwind distances, Pasquill suggests

$$f(X) = 0.33 (10/X)^{1/2} \quad (26)$$

where X is the downwind distance in km. Comparison of these two equations suggests that

$$\ell_v \simeq 540 \text{ m} \quad (27)$$

The equivalent expression for σ_z is

$$\sigma_z = \sigma_E X f_w(X) \quad (28)$$

where $f_w(X)$ is not necessarily equal to f(X).

As discussed above, the plume dispersion formulas for the environmentally dominated phase should be modified to account

for the enhanced spread during the source-dominated phase where the sigma values are proportional to $X^{2/3}$. The simplest procedure is to use the concept of an effective downwind distance X_E.

The correction factor is found by matching sigma predictions at the transition distance X_t. In the environmentally dominant region, the equivalent downwind distance for lateral dispersion, X_{ety}, at the transition point is given by Equation 24 as

$$X_{ety} = \left(\frac{\sigma_{yt}}{\sigma_A}\right)^2 \frac{1}{2\ell_v} \tag{29}$$

where σ_{yt} is the value of σ_y at the transition distance. Then the correction factor for effective downwind distance is

$$\Delta X_y = X_{ety} - X_t \tag{30}$$

The expression for σ_y in the environmentally dominated region becomes

$$\sigma_y(X) = \sigma_A(2\ell_v)^{1/2} \left\{X + \frac{\sigma_{yt}^2}{\sigma_A^2(2\ell_v)} - X_t\right\}^{1/2} \tag{31}$$

The equivalent expression for σ_z can be derived in a similar fashion:

$$\sigma_z(X) = \sigma_E(2\ell_w)^{1/2} \left\{X + \frac{\sigma_{zt}^2}{\sigma_E^2(2\ell_w)} - X_t\right\}^{1/2} \tag{32}$$

Note that the correction factors are different for lateral and vertical dispersion.

Values of σ_y, σ_z can be calculated if estimates of σ_A, σ_E, or σ_v and σ_w are available. For this first version of the model, Pasquill's (1976) suggested value for f(X) at large X is used to generate a value of the Lagrangian integral length scale of about 500 m. This value is used for both

vertical and lateral dispersion. It is consistent with the results of estimated values of the Eulerian integral length scales based on integrals of the auto-correlation functions as measured in the AOSERP study area by Davison and Grandia (1979).

Values for σ_A and σ_E were estimated from a PBL parameterization scheme. Any parameterization scheme is inferior to use of measured values, and is resorted to here because of the absence of reliable, direct measurements of σ_A and σ_E. Although there were wind fluctuation data at the 152 m height of the tall tower, there was a serious question as to their representativeness for plume dispersion calculations. The minisonde winds at typical plume height had been found to have wind roses very different from the tall tower wind roses. The major differences in the shapes of the wind roses (as presented in Volume 2 of this report) suggested that the wind fluctuation statistics at the 152 m height on the tall tower may have been inappropriate for use as dispersion parameters for significant periods of time. Because of this uncertainty, it was decided to utilize a boundary layer parameterization scheme to estimate σ_A and σ_E.

The parameterization scheme outlined below has been drawn both from the literature and the results of previous AOSERP studies. The scheme as developed requires some estimates of certain physical parameters such as roughness length. Presently, other data sources exist in the oil sands region that could be analyzed to give better parameter estimates, and to validate or improve certain simplification adopted in the formulation as necessary.

3.3.3.2 Scaling parameters in boundary layer similarity theory. The basis of the adopted parameterization scheme is Monin-Obukhov similarity theory (Obukhov 1971). Obukhov proposed that over a horizontally homogeneous surface, the turbulence structure is a function of surface stress τ_a, the buoyancy parameter g/T, the surface heat flux $H_o = c_p \overline{w\theta} \rho_a$, and the height Z above the surface.

Here, ρ_a is the density of air, c_p is the specific heat of air at constant pressure, $\overline{w\theta}$ is the vertical flux of potential temperature, g is the acceleration due to gravity, and T is the mean air temperature. From these variables, velocity, temperature, and length scales can be formed:

$$u_* = (\tau_a/\rho_a)^{1/2} \qquad \text{velocity scale}$$

$$\theta_* = -\overline{w\theta}\,/u_* \qquad \text{temperature scale} \qquad (33)$$

$$Z \qquad \text{height scale}$$

A given turbulence property should then depend only on these parameters. For example, the mean vertical gradients of horizontal wind speed can be written as:

$$\frac{kZ}{u_*}\,\frac{\partial Z}{\partial U} = \phi_u\left(\frac{Z}{L}\right) \qquad (34)$$

This expression leads to the familiar logarithmic wind profile:

$$U = \frac{u_*}{k}\,\log\left(\frac{Z}{Z_o}\right) - \Psi_u\left(\frac{Z}{L}\right) \qquad (35)$$

where:

$$L = u_*^2 \Big/ \left(\frac{g}{T}\,k\,\theta_*\right) \qquad (36)$$

Here, L is the Monin-Obukhov length, U is the mean wind speed at height Z, Z_o is the roughness length, and k is von Karman's constant. ϕ_u, a function of Z/L that must be determined empirically, is defined so that ϕ_u (0.0) = 1.0. There is still disagreement in the literature, but an approximate value for von Karman's constant is 0.4 (Hicks 1976). The form of the Ψ_u function is determined during integration of Equation 34, as in Paulson (1970). Similar equations can be derived for the mean vertical potential temperature gradient:

$$\frac{kZ}{\theta_*}\frac{\partial\theta}{\partial Z} = \phi_\theta\left(\frac{Z}{L}\right) \tag{37}$$

Integrating this equation gives an expression for the mean potential temperature as a function of height:

$$\Delta\theta = \theta(Z) - \theta(Z_o) = \frac{\theta_*}{k}\left\{\log\frac{Z}{Z_o} - \Psi_\theta\left(\frac{Z}{L}\right)\right\} \tag{38}$$

Here, ϕ_θ and Ψ_θ are analogues to ϕ_u and Ψ_u.

The above equations for parameterizing the surface fluxes have been extensively verified by experimental study (e.g., Kaimal et al. 1976; Businger et al. 1971).

For parameterization of dispersion of elevated plumes, it is necessary to parameterize the turbulent properties of the whole boundary layer rather than just those in the surface layer. Arya (1977) and Arya and Sundarajan (1976) reviewed similarity theories which have been proposed for the PBL. The required addition to the surface layer parameterization theory is to include the boundary layer height Z_i as an additional length scale.

Turbulence properties in the outer boundary layer, that is, for heights Z greater than about 0.1 Z_i, should then depend on the ratio of this height to the M-O length L. In convective situations, (L <0), it is generally accepted that the most appropriate boundary layer height scale is the height of the lowest temperature inversion. This was suggested by Deardorff (1979) on the basis of both experimental and model results. He also suggested a new velocity scale for the convective boundary layer above the surface layer:

$$w_* = \left\{\frac{g}{T_a}\,\overline{w\theta}\,Z_i\right\}^{1/3} \tag{39}$$

Kazanski and Monin (1960) proposed that the PBL could be parameterized if the earth's rotation was included in the similarity theory. Their theory, which is also known as Rossby number similarity theory, assumes that the boundary layer height is proportional to u_*/f:

$$h \propto u_*/f \tag{40}$$

Here f is the coriolis parameter (0.00012). An appropriate non-dimensional stability scale for the boundary layer is then

$$\mu_* = \frac{u_*}{fL} \tag{41}$$

Results from several theoretical model studies have suggested that the stable boundary layer height h can be expressed as a function of μ_*:

$$\frac{h}{L} = \beta_2 \, \mu_*^{1/2} \tag{42}$$

Estimates of β_2 range from approximately 0.2 to 1.0 (Arya 1977). The predicted value of β_2 is strongly dependent on the particular theoretical assumptions. Because of the uncertainty in determining h in stable conditions, the stability parameter will be used to classify stability in the stable PBL and the ratio Z_i/L will be used for the convective PBL. The non-dimensional boundary layer height h/L is computed and is available on intermediate GLCGEN output if desired.

It is important to point out the limitations of this boundary layer parameterization. The development as outlined above assumed stationary and horizontally homogeneous conditions which at best are only a rough approximation to the real atmosphere.

There is evidence that characteristics of the outer boundary layer depend on large scale factors such as horizontal temperature advection (e.g., Nieuwstadt and Driedonks 1979). The use of a measured boundary layer height in convective cases would

permit some influence of the large scale effects in this parameterization. At present, the use of seasonal climatological values of convective mixing height ignores any shorter period large scale effects. The large scale influences are not included in the parameterization of the stable boundary layer.

In spite of the above limitations, it is hoped that this parameterization should lead to σ_A and σ_E estimates which are less likely to contain major systematic errors than might occur by the adoption of a questionable time series from the tall tower. It is desirable, however, to compare the parameterization scheme with all available data sets to ensure that it has been optimized for the AOSERP study area.

3.3.3.3 Estimated value of surface roughness. The value of surface roughness affects the amount of mechanical turbulence, as specified by the friction velocity u_* , that will be generated by a given wind speed. Thus to estimate the mechanical mixing effects on the plume dispersion, a value for the roughness length in the AOSERP study area must be adopted. No direct estimates of Z_o are apparently available for the AOSERP region. It may be possible to analyze the extensive set of pibal profiles to provide some estimates of the value of Z_o. However, this apparently has not been attempted to date.

Weber et al. (1975) reported an analysis of measurements collected from a 366 m television tower in South Carolina. Their program included measurements of wind and temperature profiles and standard deviations of wind elevation (σ_E) and azimuth (σ_A). The estimate of Z_o for rolling terrain, with patches of trees and pasture land, was 0.36 m. Slade (1969) found Z_o values of 0.2 to 0.5 m for flow over irregular terrain, including a river valley. Garratt (1978) reported a value of 0.4 $\pm$ 0.2 m for a heterogeneous surface comprising 8 m high trees, grass, and dry soil. Based on this admittedly small amount of data, the Z_o value adopted was 0.3 m. This value of Z_o was used to estimate source-environment region transition distances in a previous

section and was found to give relatively satisfactory results.

Sensitivity and validation tests involving various values of Z_o were undertaken in Phase 2 of this program. These tests are discussed in detail in Volume 3 of this report.

3.3.3.4 Computation of boundary layer parameters. The first step in the parameterization scheme is to compute values of u_* and L to use in estimating other boundary layer parameters. These parameters can be evaluated in the surface layer typically at a height of 10 m. Although evaluated at 10 m, the parameters can have major scaling effects throughout the boundary layer.

The value of u_* can be found from the mean wind speed in the surface layer as

$$u_* = C_D U \tag{43}$$

where:

$$C_D = k \left\{ \log \left(\frac{Z}{Z_o} \right) - \Psi_u \left(\frac{Z}{L} \right) \right\} \tag{44}$$

Note that this definition of C_D is the square root of the usual definition. If the appropriate profile expressions are substituted for u_* and $\overline{w\theta}$, the Monin-Obukhov length can be written in terms of u and Z_o as

$$\frac{Z}{L} = \frac{g}{T_a} (Z) \frac{\Delta\theta}{U^2} \frac{\left\{ \log (Z/Z_o) - \Psi_u \right\}^2}{\left\{ \log (Z/Z_o) - \Psi_\theta \right\}} \tag{45}$$

Empirical forms for Ψ_u (Z/L) and Ψ_θ (Z/L) based on observations are given in Paulson (1970) and Carson and Richards (1978). Note that by definition Ψ_u (0) = Ψ_θ(0) = 0.0.

For unstable conditions (Z/L <0), the Ψ functions are complicated and have a relatively small effect on the computation of Z/L or U . Given the uncertainty in the value of Z_o, it is therefore reasonable to compute U*, assuming that C_D = k/log (Z/Z_o).

In stable conditions, the Ψ functions can be approximated as (e.g., Carson and Richards 1978)

$$\Psi_\theta = \Psi_u = -\alpha \left(\frac{Z}{L}\right) \tag{46}$$

This is the familiar log-linear formulation; the value of α is assumed equal to 4.5, following Leavitt et al. (1977) and Businger et al. (1971). Recall that this relationship is being used only in the surface layer to calculate the parameters defined at the surface which govern the PBL characteristics. Using the log-linear formulation, the equation Z/L can be rewritten as

$$\frac{Z}{L}\left\{\log\left(\frac{Z}{Z_o}\right) + \frac{\alpha Z}{L}\right\}^{-1} = \frac{g}{T} Z \frac{\Delta\theta}{U^2} \tag{47}$$

Note that the left-hand side (LHS) of this equation depends on Z, Z_o, L, and α and that the RHS depends only on measurable quantities or quantities fairly easily estimated from available measurements. It is necessary to include the correction represented by the second term in the bracket in Equation 47 in stable conditions because it makes a significant difference in the computed values of L and u_*. This equation can be solved numerically for the value of L which can then be used to compute u_*. The computed values of u_* and L are in turn used to compute μ_* or the ratio of Z_i/L, depending on the sign of $\Delta\theta$.

Thus, if there are representative estimates of $\Delta\theta$ and U, and if the estimates of Z_o and α are reasonable, then similarity theory scaling parameters for the plantetary boundary layer can be estimated. The applicability of the procedure clearly requires that the plumes remain in a region of the atmosphere coupled to the surface. If the plumes penetrate on elevated inversion, then this boundary layer parameterization scheme is not appropriate and is not applied in the model.

In the present time series data file, values of the temperature gradient are not available. A modification to the above formulation using heat flux estimates had to be adopted.

The procedure to calculate u_* and L described above can be modified to use the estimated heat flux rather than $\Delta\theta$. Given the value of $\overline{w\theta}$, the expression for L can be rewritten as:

$$L \left\{ \log\left(\frac{Z}{Z_o}\right) - \Psi_u\left(\frac{Z}{L}\right) \right\}^3 = k^2 U^3 \Big/ \left(\frac{g}{T}\,\overline{w\theta}\right) \qquad (48)$$

In unstable conditions, this is not difficult to implement since Ψ_u is set equal to zero.

However, in stable conditions, for a given value of the RHS of Equation (48), there are either two solutions for L or no value of L for which a solution exists. The value of L for which the LHS of the equation has a minimum value is calculated using Equation 46 and differentiating the LHS of Equation 48 with respect to L. This gives:

$$L_{min} = 2\alpha Z \,/\, \log\left(\frac{Z}{Z_o}\right) \qquad (49)$$

This value of L corresponds to a maximum permitted heat flux for a given U in stable conditions (Carson and Richards 1978),

$$\overline{w\theta}_{max} = k^2 U^3 \left\{ \frac{g}{T}\, 2\alpha Z \log\left(\frac{Z}{Z_o}\right) \right\}^{-1} \qquad (50)$$

The physical occurrence is one of the atmosphere becoming more and more stable, turbulence being suppressed and the heat flux becoming smaller. Thus, the negative heat flux is small for both near neutral and very stable conditions. The negative heat flux reaches a maximum at an intermediate level of stability.

maximum at an intermediate level of stability. The formulation of Equation 47 involving $\Delta\theta$,implicitly includes this maximum negative heat flux effect.

Equation 48 was solved in the present model by creating a table of values of the LHS versus L. Measured parameters define the RHS, and hence, the appropriate value of L can then be chosen by equating the values of the left - and right-hand sides of the equation. If the value of the heat flux causes the RHS to be less than the minimum allowed value, the Monin-Obukhov length is set equal to L_{min}. Computed values of L are then limited to values equal or larger than this value to remove the problem of dual solutions. This means that the value of L in very stable situations with very low wind speed may be overestimated. Because of the relatively large Z_o value in the AOSERP study area, this minimum limit for L is seldom reached. The selection of parameters for stable boundary layers has been adjusted to prevent this problem from seriously impacting on the dispersion modelling.

3.3.3.5 Estimates of σ_A and σ_E in convective conditions. Panofsky et al. (1977) summarized field measurements of the standard deviation of horizontal velocity and showed that there was good agreement between the data and the following prediction:

$$\frac{\sigma_v}{u_*} = \left\{12 + 0.5\,\frac{Z_i}{-L}\right\}^{1/3} \qquad (51)$$

over a range of $Z_i/-L$ from 0.0 to 350. Most of the measurements, however, were made in the surface layer. In the limit of large $Z_i/-L$, this expression reduces to

$$\frac{\sigma_v}{w_*} = 0.6 \qquad (52)$$

This agrees with data from Caughey and Palmer (1979) who measured σ_v over the entire depth of the unstable PBL.

While the horizontal velocity fluctuations are relatively constant with height in the unstable boundary layer, the vertical velocity fluctuations increase with height in the lower boundary layer to a maximum value at $Z/Z_i \simeq 0.5$. Above that height, σ_w decreases with height to some small minimum value above the inversion height, possibly associated with internal waves (Caughey and Palmer 1979). In the surface layer, $Z < 0.1\ Z_i$, Panofsky et al. (1977) suggest that

$$\frac{\sigma_w}{u_*} = 1.3 \left\{ 1 + 3 \frac{Z}{L} \right\}^{1/3} \tag{53}$$

McBean (1976) compared several different methods of scaling σ_w in the boundary layer and suggested the empirical formula:

$$\frac{\sigma_w}{w_*} = 0.4 + 1.1 \left(\frac{Z}{Z_i}\right) - 1.1 \left(\frac{Z}{Z_i}\right)^2 \tag{54}$$

According to McBean's equation, σ_w has a maximum value of $\sigma_w = 0.68\ w_*$ at $Z/Z_i = 0.5$. Caughey and Palmer (1979) found that the maximum value of σ_w occurred near $Z = 0.5\ Z_i$ but the observed maximum was only $\sigma_w/w_* \simeq 0.4$. Davison and Grandia's (1979) measurements of vertical and horizontal turbulence fluctuations can be used to partially verify these predictions. In unstable conditions in June 1977, it was generally found that $\sigma_w \simeq \sigma_v$ at plume level.

It is useful to compare calculations of σ_w and σ_v from the above formulas. Assuming $U = 5$ m/s, $Z_i = 1000$ m, $\overline{w\theta} = 0.2$°K m/s and $L = 22$ m, then substitution into the appropriate equations gives values of $w_* = 1.93$ m/s, $u_* = 0.5$ m/s, and $\sigma_v = 1.43$ m/s. According to Caughey and Palmer's formula, $\sigma_w = 0.8$ m/s or about one-half of σ_v. According to McBean, the maximum value of σ_w would be about 1.30 which is approximately equal to the estimated value of σ_v, in better

agreement with the observations of Davison and Grandia (1979) for unstable conditions. However, the scatter in Davison and Grandia's data precludes verification of any variation of σ_w/w_* with height. In fact, their data suggests that any variation is not as systematic as either Caughey and Palmer or McBean detected. Because of these uncertainties, and the application of the results in a Gaussian dispersion formulation, it seems best to set σ_w/w_* to a constant value (of 0.6) rather than to allow it to vary with height. The sensitivity of calculated GLC values to this assumption was examined in the sensitivity studies presented in Volume 3 of this report.

In the model, the value of σ_w was also computed from Equation 53 for mechanically mixed conditions by setting Z/L to zero:

$$\sigma_w = 1.3\ u_* \tag{55}$$

The program then selects the maximum of the convective and mechanical σ_w values computed by the two procedures for plume sigma computations. Assuming that $\sigma_A = \sigma_v \cdot u$ and that $\sigma_E = \sigma_w \cdot U$, then

$$\sigma_E = \text{MAX}\ \left(0.6\ w_*/U,\ 1.3\ u_*/U\right) \tag{56}$$

and

$$\sigma_A = \frac{u_*}{U}\ \left\{12 + 0.5\ \frac{Z_i}{-L}\right\}^{1/3}$$

Here, the wind speed U should be the mean wind speed at plume height. In the present data set, the available wind speed is estimated for a constant 400 m height. The model adopts the wind speed value from the time series file without any modifications.

3.3.3.6 Estimates of σ_A and σ_E in stable conditions. There are as yet, no expressions for σ_A and σ_E in stable conditions equivalent to the equations given in the preceeding section. Deardorff (1978) suggested that σ_v and σ_w have the following form:

$$\sigma_v^2 \propto u_*^2 \ (1 - Z/h) \qquad (57)$$

$$\sigma_w^2 \propto u_*^2 \ (1 - Z/h)$$

where h is the height of the stable boundary layer. However, available data suggest that it is unlikely that σ_v and σ_w would decrease to zero at the top of the boundary layer because of the effects of the variability of the large-scale flow on the boundary layer.

Because of the lack of a firmly established parameterization in stable conditions, estimates for the values of σ_A and σ_E are based upon measurements reported by Weber et al. (1975) and Luna and Church (1972) from tall towers located in non-homogeneous terrain.

The stable boundary layer was initially classified by the calculated value μ_* into three classes as shown in Table 4. Recall μ_* is the non-dimensional parameter formed from the boundary layer height according to Rossby number similarity theory and the M-O length (refer to Equation 41). It should be emphasized that these are only rough estimates and are a fairly poor substitute for hourly observations. The classes are based on Deardorff's (1978) recommendations for classifying the stable boundary layer and on results from Leavitt et al. (1978). The limit of $\mu_* = 30$ was adopted so that the setting of a minimum value for L does not cause very stable cases to be classified as moderately stable cases.

To minimize the effects of discretization, the above values of σ_A and σ_E were used to construct continuous values as functions of u_*. A constraint was imposed for small values (approaching neutral conditions), such that

$$\sigma_E \leq 1.0 \frac{u_*}{U} \tag{58}$$

$$\sigma_A \leq 1.8 \frac{u_*}{U}$$

The numerical values are consistent with the observations of Weber et al. (1975). A further constraint was that σ_E and σ_A must not drop below the values for very stable conditions in Table 4.

Table 4. Typical values of σ_A and σ_E as functions of μ_*.

μ_*	Stability	σ_A (deg.)	σ_E (deg.)
5	Slightly stable	8	4
20	Moderately stable	4	2
40	Very stable	2.5	1

4. FREQUENCY DISTRIBUTION PROGRAM

4.1 FEATURES OF FRQDTN

The program FRQDTN computes average ground level concentrations, frequency distributions of ground level concentration, and first-order estimates of wet and dry deposition. As input, it requires the ground level concentration file produced by GLCGEN and the hourly time series file produced by the program TIMSER. For many users, FRQDTN may be the only program run. Many options have been incorporated into this program to make it as useful as possible to a wide range of potential users. The program features include:

1. The GLC frequency distributions and deposition can be determined at specific locations or for the grid of receptors set up in GLCGEN, or for specific receptors set up in GLCGEN;
2. Three frequency distributions may be calculated. These are the frequency distribution of ground level concentration, an inverse cumulative frequency distribution of ground level concentrations, and the frequency distributions of time between successive extreme events;
3. The time series of GLC values are available for direct comparison with observations;
4. The GLC calculations can be limited to specific times of day and can be averaged over specified periods of up to 24 h;
5. The GLC calculations may be limited to specified months or may be done for the total of all time series files attached;
6. A weighting based on standard meteorological parameters can be applied to the ground level concentrations to simulate changes in receptor susceptibility. That is, the GLC calculations can be based on the normal hourly time series or they can be included, excluded, or

or included in part by the weighting option for a number of different meteorological conditions;

7. GLC calculations can be undertaken for any source emission values for any combination of sources without re-running the program GLCGEN; and
8. The deposition calculation can be undertaken using default deposition parameters or the parameters may be specified by the user.

The program FRQDTN first reads the user-supplied input which includes selection of options, specification of source strengths, and the limits of the frequency distribution classes. The program then reads the dispersion class boundaries from the first record of the ground level concentration file.

The time series file is then read and appropriate hourly records are selected. For each selected hour, the ground level concentration file index is computed. Determination of the file index involves the conversion of a radiation estimate to a heat flux estimate. The ground level concentrations for the desired index are then read from the random access file which was created previously by GLCGEN. The weighting function is applied, an hourly value of wet deposition is calculated based on precipitation rate in the time series, and the proper frequency distribution class is incremented. After each time series file is read, dry deposition is calculated and specified results are displayed. After all time series file are read, results for the total period are displayed in a pre-determined format.

4.2 WEIGHTING FUNCTION

The weighting scheme was developed to enable the user to simulate the susceptibility of a receptor according to meteorological conditions as described by any of the parameters on the time series file. The weighting can be applied for a single parameter or for several parameters, in which case, the effect is

multipicative. For weighting according to N parameters, the expression is

$$C_m = C \cdot (w_1 \cdot w_2 \cdot \ldots \cdot w_n) \qquad (59)$$

where C and C_m are the calculated and weighted ground level concentrations, respectively, and W_1, W_2, are the respective parameter weights.

The parameter weightings are specified by user-defined upper and lower threshold values denoted by p_u and p_l, where p is the time series parameter that controls the weight. There are two possible situations to consider: Case I, where the weight increases as the parameter increases in value; and Case II, where the weight decreases. In Case I, the weighting is zero for parameter values less than p_l, meaning that ground level concentrations occurring when p is less than p_l are treated as zero for this particular model run. When p is larger than p_u, then the weighting is unity and the modified concentrations are unaffected by parameter p. For values of p between p_l and p_u, a linear weighting is used:

Case I

$$W = \begin{cases} 0 & p \leq p_\ell \\ (p - p_\ell)/(p_u - p_\ell) & p_\ell < p < p_u \\ 1 & p \geq p_u \end{cases} \qquad (60)$$

The equivalent weighting definitions for Case II are:

Case II

$$W = \begin{cases} 1 & p \leq p \\ (p_u - p)/(p_u - p_\ell) & p_\ell < p < p_u \\ 0 & p \geq p_u \end{cases} \qquad (61)$$

An example may make the use of the weighting functions clearer. Suppose that for a particular type of receptor, the susceptibility to damage is temperature dependent, such that the receptor is insensitive to concentrations of SO_2 when the temperature is less than about -5°C, and is fully susceptible when the temperature is at or above 20°C. The susceptibility of this receptor would then be simulated by generating modified ground level concentrations using values of -5 and +20 for p_l and p_u, respectively, in a Case I mode for the parameter temperature.

Another example may make the interpretation of the weighting functions clearer. Suppose that FRQDTN has already been run and that unweighted annual average ground level concentrations have been calculated for a grid of receptors. The resulting map will have regions of high and low values. Suppose now that FRQDTN is run again, this time with the temperature-dependent weighting examined in the previous paragraph. The map from this computer run will, in general, have a different concentration pattern. The differences will be due to the lack of contribution of GLC values occurring when the temperature is below -5°C, and a reduced contribution when the temperature is between -5°C and 20°C. The weighted GLC values should be thought of as effective GLC values, not true GLC values.

The weighting parameters can be used to approximate meteorologically dependent receptor sensitivities. The concept was originally designed to allow for biological susceptibilities. However, the same procedure can be used for other applications, including deposition efficiency, and the nuisance factor of air pollutants to local residents. The full advantages of the concept of weighting parameters will only be realized when typical users have become familiar enough with the model to use it as an effective receptor sensitivity tool.

4.3 GENERATION OF THE HEAT FLUX ESTIMATES

In order to specify the dispersion class, the radiation estimates on the time series file need to be used to generate

surface heat flux estimates. The heat flux is defined as a function of net radiation and an allowance is made for dew/hoar-frost formation in negative heat flux situations in order to more closely approximate the surface energy budget.

The values for heat flux levels in GLCGEN can be set by the user, but some typical values may prove to be of general use. For positive heat fluxes, the levels 0.2, 0.1 and 0.02, (°C m/s) appear reasonable to represent strong, moderate, and slight net radiation. These values are consistant with Pasquill (1974) and Davison (1973). For clear-sky conditions in mid-July, Davison (1973) measured values for $\overline{w\theta}$ at 3.5 m, averaging about 0.26 °C at Suffield, Alberta. The latitude difference between Suffield and Fort McMurray represents a 7% effect. However, an albedo difference between short grass prairie and northern forest probably compensates. An estimate can now be made of the dimensional coefficient (which involves specific heat and air density) which relates the heat flux and net radiation. If

$$\overline{w\theta} = \alpha R \tag{62}$$

where R is the net radiation, then

$$\alpha = 5 \times 10^{-4} \quad \frac{m/s}{Wm^{-2}} \, ^{o}C \tag{63}$$

The above value of α is based upon the maximum net radiation at Fort McMurray of about 470 ($W \cdot m^{-2}$) calculated from the radiation subroutine. The corresponding levels of radiation and $\overline{w\theta}$ are shown in Table 5. It is recognized that these preliminary values do not account for changes in latent heat flux and ground heat flux.

For negative radiation conditions, the analysis of the surface energy budget becomes more difficult. Although in strong radiation most of the net radiation appears as sensible heat flux

Table 5. The adopted relationship between net radiation and heat flux for convective conditions.

DESCRIPTOR	NET RADIATION ($W\ m^{-2}$)	(°C m/s)
Strong	400	0.20
Moderate	200	0.10
Slight	40	0.02

(for land surfaces), for negative radiation a significant fraction of the net radiation is balanced by condensation processes. A further problem is that negative radiation generates a stable thermal regime which inhibits turbulent mixing and so permits a decoupling of the surface and upper parts of the boundary layer. Time and budgetary constraints did not permit a comprehensive analysis of the relationship between negative radiation and negative heat flux and the role that the mechanical mixing might play. However, review of typical observed negative heat flux values (e.g., Pasquill 1974, Leavitt et al. 1978), compared with corresponding radiation values, suggested that a relationship similar to that for convective conditions would lead to physically reasonable values of heat flux and of the stability parameter for stable conditions, u_* /fL. The effect of condensation on the surface energy budget for negative radiation conditions was allowed for in an approximate ad hoc way. The final formulation for heat flux in stable conditions is

$$HF = (5 \times 10^{-4})\ RAD\ (1 - 0.6\ DLOSS) \qquad (64)$$

where: $DLOSS = \frac{T + 20}{40}$

and

HF	=	heat flux
RAD	=	net radiation
DLOSS	=	condensation allowance
T	=	ambient temperature in °C

The above formulation for condensation is only applied if the relative humidity on the surface weather record is greater than 60%. The condensation allowance is in a preliminary ad hoc form. However, it is consistent with values reported by Hicks (1976) and has a temperature dependence that is reasonable for the present purposes.

4.4 DEPOSITION

A first-order estimate of deposition was required as part of the airshed management model. A deposition estimate is important in determining potential pollutant effects on vegetation, water, soils, and other materials within the AOSERP study area. The results of this estimate may be useful as input to more sophisticated deposition models.

4.4.1 Dry Deposition

A deposition velocity approach was used to estimate dry deposition of gases. With this approach, the deposition flux L_d is defined to be

$$L_d = V_d \chi \tag{65}$$

where V_d is the deposition velocity and χ is an airborne concentration. The units of L_d are mass per unit area per unit time. In practice L_d and χ are measured at a height of about 1 m. In the absence of a large vertical concentration gradient, χ is synonymous with the ground level concentration, or with the concentration at the top of a vegetative canopy.

Sehmel (1980) reviewed experimentally derived values of the SO_2 deposition velocity and found that they ranged over two orders of magnitude. He attributed this spread to the complexities of the actual deposition process and to the simplification of the deposition velocity concept for a complex process. He suggested that scatter in experimental V_d data is inescapable.

Sehmel (1980) identified many of the factors that complicate the actual deposition process. He grouped them into three classes: meteorological variables, pollutant properties, and surface characteristics. Although by no means definitive, the classification is useful in illustrating the multidisciplinary complexities of deposition.

Among meteorological variables that determine the transport of pollutants to the surface are stability, wind speed, and roughness length. The effect of changes of the magnitude of these variable on deposition rates is most pronounced above the surface layer but is also evident at relatively low levels (Wesely and Hicks 1977). In the lowest levels, the influence of surface characteristics becomes more important. Above a vegetative surface, the deposition process seems limited by the resistance of the surface to sorption. However, above a water or snow surface, deposition appears limited by wind speed and stability. Thus, immediately above vegetation, there is little dependence of deposition rate upon wind speed, but above snow and water surfaces, deposition rates are proportional to friction velocity (and so wind speed) and are substantially less in stable conditions than in neutral conditions (Shepherd 1974; Dovland and Eliassen 1976; Wesely and Hicks 1977).

Possibly the most important pollutant factors influencing gas deposition are gas water solubility, reactions occurring in water, and gas concentration increases in the water from prior deposition (Bird et al. 1960). Slinn et al. (1978) considered some of these factors. If the gas reacts in water, there is lessened resistance to additional surface mass transfer. However, if the gas dissolves with reversible chemical reactions, deposition may reach an equilibrium at lower rates than with irreversible reactions (Sehmel 1980).

The nature of the surface can have a significant effect upon rates of deposition. The effects of differences between vegetation and non-vegetative surfaces were briefly mentioned above. Differences also arise within vegetative surfaces due to differences in canopy height and density and amount of water on exposed areas. During dry days, stomata are an important pollutant sink (Fowler and Unsworth 1979). Wesely and Hicks (1977) state that the quantitative effects of stomata on the deposition rate are probably among the most difficult of all variables to estimate.

The rationale for using a first-order approach now becomes clearer. There is no existing firmly based theoretical or empirical specification of many of these properties. Even with the meteorological variables adequately specified, the estimate would still be limited by inaccuracies in the specification of surface properties. To minimize the uncertainties in the estimate, the deposition velocities in the model were averaged over a one-month period. Day-to-day estimates of dry deposition may thus be unreliable; however, an estimate based on many realizations should be more dependable.

The actual magnitudes of the deposition velocity were empirically estimated from the range of experimental values in Sehmel (1980), Dennison (1979), and Western Research Development (1978) based on seasonal variations of meteorology and surface characteristics in the AOSERP study area. The resulting deposition velocities are shown in Table 6.

The program FRQDTN allows the user several dry deposition options. The first is the option to calculate and display loading due to dry deposition. In addition, if this option is chosen, the user may use the default values of the deposition velocities shown in Table 6, or may specify alternate values at runtime.

4.4.2 Wet Deposition

Wet deposition is calculated in the program FRQDTN based on an irreversible capture mechanism. The calculation based on irreversible capture will result in an upper bound to the wet deposition estimate. The equilibrium scavenging mechanism was also investigated in some detail and is considered to produce more realistic wet deposition estimates (Hales 1978). The inclusion of the latter mechanism into the existing model, if though to be appropriate, could be accomplished simply and quickly. Because of this ease of modification, both wet deposition mechanisms will be discussed.

Table 6. Empirical estimates of deposition velocity V_d by season.

Season	V_d(cm/s)
Winter	0.2
Spring	0.5
Summer	1.0
Autumn	0.5

4.4.2.1 Irreversible capture. The assumption of irreversible capture results in irreversible wet loading (L_{iw}) given by (Dennison 1979):

$$L_{iw} = \Lambda \chi H \tag{66}$$

where χ is the average concentration throughout a depth H and Λ is a scavenging coefficient in units of s^{-1} accounting for the effects of all washout processes. The product χH can be thought of as a vertically integrated concentration and depends solely on the source strength. Thus, Equation 66 can be rewritten as

$$L_{iw} = \Lambda \frac{Q}{UL} \tag{67}$$

where Q is the source strength, U is the mean wind speed, and L is the plume width. In the present model, L was identified as the width of a sector at the location of a receptor. Because L rather than σ_y is used, wet deposition can be decoupled from the diffusion process.

The scavenging coefficient, Λ, will be a function of precipitation rate. In a recent review, Dennison (1979) quotes only four theoretical values of Λ. The following equation is representative of those given:

$$\Lambda = 1.4 \times 10^{-4} P^{0.57} \tag{68}$$

where P is precipitation rate in millimetres per hour. A factor of 2 scatter was evident in the data presented.

The assumption of irreversible capture places limitations on the physical and chemical processes of wet deposition. Hales (1972) identified some of these limitations as high solubility of the pollutant gases in water, large drop sizes, vertically thin plumes near the surface, and irreversible chemical

reactions. Although stable conditions resulting in vertically thin plumes occur frequently in the oil sands area, Hales (1978) characterizes SO_2 as only moderately soluble and the appropriate reactions involving SO_2 as readily reversible. Thus, at least two of the requirements for irreversible scavenging are not usually met. Therefore, the concept of irreversible scavenging is probably limited to calculating an upper limit to wet deposition.

4.4.2.2 Equilibrium scavenging. The basic precept of equilibrium scavenging is that gas molecules may absorb or desorb from individual raindrops (Hales 1978). The governing equations were given in Barrie (1981):

$$\left[SO_2\right]_{air} + \left[H_2O\right] \overset{K_H}{\rightleftharpoons} \left[SO_2 \cdot H_2O\right] \tag{69}$$

$$\left[H_2O\right] + \left[SO_2 \cdot H_2O\right] \overset{K_1}{\rightleftharpoons} \left[HSO_3^-\right] + \left[H_3O^+\right] \tag{70}$$

$$\left[H_2O\right] + \left[HSO_3^-\right] \overset{K_2}{\rightleftharpoons} \left[SO_3^{2-}\right] + \left[H_3O^+\right] \tag{71}$$

where K_H, K_1, and K_2 are equilibrium constants and the square brackets indicate concentration in moles per litre. Hales (1978) expressed the solution as

$$\left[SO_2\right]_{rain} = K_H\left[SO_2\right]_{air} - \tfrac{1}{2}\left[H_3O^+\right]_{ex} + \tfrac{1}{2}\left\{\left[H_3O^+\right]_{ex}^2 + 4\,K_1K_H\left[SO_2\right]_{air}\right\}^{\frac{1}{2}} \tag{72}$$

where $[H_3O^+]_{ex}$ denotes the concentration of hydrogen ion donated by sources other than sulphur dioxide. Generally, the

assumption is made that the concentration $[H_3O^+]_{ex}$ is equal to the free ion concentration, that is:

$$\left[H_3O^+\right]_{ex} \approx 10^{-pH} \tag{73}$$

The solution of Equation 72 thus requires estimates of airborne SO_2 concentrations and the pH of rain upwind of SO_2 sources.

Barrie (1981) derived an alternate solution to the governing equations by assuming that the reaction in Equation 71 occurred rapidly. In the range of precipitation pH values of 3 to 6, he assumed $[SO_2]_{rain} = [HSO_3]_{rain}$:

$$\left[SO_2\right]_{rain} = \frac{K_1 K_H \left[SO_2\right]_{air}}{\left[H_3O^+\right]_{rain}} \tag{74}$$

Note that the hydrogen ion concentration in this equation denotes the total from all sources. Thus, Equation 72 and Equation 74 are not directly comparable.

The equilibrium constants K_1 and K_H are temperature dependent. Barrie (1981) gave the following empirical relation valid over the temperature range 0°C to 30°C:

$$K_1 K_H = 6.22 \times 10^8 \exp(4755.5/T) \tag{75}$$

where T is temperature in °K. Wet loading due to reversible washout L_{rw} is then given by (Barrie 1981)

$$L_{rw} = W_{SO_2} P \chi \tag{76}$$

where W_{SO_2} is a washout ratio, P is precipitation rate, and χ is an airborne concentration. The washout ratio is given by

$$W_{SO_2} = \frac{\left[SO_2\right]_{rain}}{\left[SO_2\right]_{air}} \qquad (77)$$

and is a function of concentration, temperature, and acidity. In the model, the airborne concentration of SO_2, defined by χ , is replaced by a ground level concentration. This replacement assumes either a negligible vertical concentration gradient, or reaction rates sufficiently fast for a droplet to remain in equilibrium with the local concentrations. Hales (1978) stated that the governing reaction rates are very rapid, so that the replacement of χ by ground level concentration is perhaps justified.

The choice of a solution to the governing equations depended on the intended application of the results and on the pH of the air in the AOSERP study area. It was felt that the model should have the ability to estimate sulphur loading due to wet deposition in a pristine environment; that is, based on background pH measurements before the establishment of industry. Equation 72 gives this ability. In addition, there are indications (J.W. Bottenheim, AES, private communication, 1980) that the pH values in summertime precipitation in the AOSERP study area are near a value of pH = 7. This is somewhat outside the range of applicability of Barrie's (1981) solution. Thus, for this application, the use of Equation 72 was considered more appropriate.

The assumption of equilibrium scavenging places some limitations on the physical and chemical processes of wet deposition. Hales (1978) identified some of these limitations as small drop sizes, small changes in gas-phase concentration with height, and low solubilities. It should be borne in mind that these are limiting conditions; in practice, Hales (1978) suggested that equilibrium conditions should prevail beyond about 20 stack

heights downwind of tall stacks. That distance is about 4 km for a Syncrude-type source.

4.4.2.3 Model options. The program FRQDTN allows the model user several wet depositon options. The first option is whether or not to print the results of wet deposition calculations. If this option is specified, the user has the option to use the default form of the irreversible scavenging coefficient, or to specify alternate values. The default values are 1.4×10^{-4} for the constant and 0.57 for the exponent, as given in Equation 68.

The model does not recognize the difference between rain and snow in calculating wet deposition. If the precipitation is in the form of snow, the precipitation rate (P) in the time series will be in melted water equivalents. Thus, the effective surface area available for absorption by irreversible capture in the model will be larger than in reality. This effect will tend to counter the relatively large deposition rates produced by the assumption of irreversible chemical reactions. Had equilibrium scavenging been employed in the model, the temperature dependence of the equilibrium constants would have been a concern, since these constants are specified only to 0°C. It is likely that both reversible and irreversible wet deposition formulations would tend to overestimate wintertime sulphur deposition: the irreversible capture technique because of the assumption of irreversible chemical reactions, and the equilibrium scavenging technique because of its overestimation of the reaction rates below 0°C.

4.5 PROGRAM OUTPUT OPTIONS

The program FRQDTN can provide the user with a large variety of information in several formats, depending on the options requested by the user and on the data in the GLC file produced by GLCGEN. The display options are:

1. Average ground level concentrations;
2. Frequency distributions of ground level concentrations;

3. Inverse cumulative frequency distributions of ground level concentrations;
4. Frequency distributions of time between occurrence of extreme episodes of ground level concentrations;
5. Dry gaseous deposition;
6. Wet gaseous deposition;
7. Total gaseous deposition; and
8. Time series of GLC values.

The options above may be displayed for each month of the time series file, or for the total period of all the time series files. The values displayed may be averaged over a specified averaging period or may be weighted by meteorological variables on the time series file.

The options may be displayed at specific locations or over an entire grid of receptors, depending on the receptor mode run in GLCGEN. If GLCGEN was run at specific receptors only, then the specified receptor option must also be used by FRQDTN. In this case, ground level concentrations and depositions are listed for each receptor, and histograms and tables of frequency distributions are presented. If GLCGEN was run for a grid of receptors, then either the specified receptor or grid option may be used by FRQDTN. If specified receptors are chosen, the value at the receptor is defined as the value at the nearest grid point and options are displayed in the above format. If the receptor grid is chosen, two-dimensional maps of each option are produced. Ground level concentrations and depositions provide one map of mean values. Frequency distributions provide one map for each specified ground level concentration class. The mapping routine uses a second-order procedure to interpolate between grid points.

Examples of user-defined input data and output displays are presented in Volume 4 which is the User's Guide.

5. SUMMARY

The documentation for the frequency distribution model, and for the data base synthesized in order to test and run it, are presented in four volumes. Volume I has presented the description of the model itself and the rationale for the various formulations adopted. Volume 2 describes the synthesis of the data base. Volume 3 outlines the sensitivity and validation tests conducted on the data base and the model. Finally, Volume 4 is a Users' Guide to the model. The changes in authorship of the various volumes reflects the amount of effort given to the various aspects of the program by the individuals and by the two groups developing the system: INTERA Environmental Consultants Ltd., and Western Research and Development. The following paragraphs provide a summary of the model itself. Recommendations for further model testing and improvements are provided in Volume 3.

The model developed in this program is primarily designed to provide long-term averaged output of ground level concentrations (GLC). It was developed to provide a more flexible airshed management tool than other existing models such as the Climatological Dispersion Model (CDM). In addition, the development included a more realistic dispersion formulation based upon present understandings of dispersion of plume effluents in the planetary boundary layer (PBL) of the atmosphere.

There are several major features of the present model that permit a very flexible usage. The contributions of GLC values occurring at particular times of the day or under particular meteorological conditions can be included, excluded, or included with a fractional weighting when averages are calculated. Thus, for example, the GLC values occurring under reduced receptor sensitivity can be omitted or de-emphasized. The model is designed to be able to vary source strengths or "turn off" particular sources without having to rerun the whole model. Thus, the incremental effects of existing or proposed sources and the dispersion of different effluent species can be undertaken without a major model rerun. The model produces a time series of

predicted GLC values corresponding to the meteorological time series being used to drive the model. Thus model predictions can be used to evaluate whether particular mixing situations are being properly simulated, by comparison to observations. This is vitally important if the model is to be used as a management tool to examine the effects of alternative developmental scenarios. The time series of GLC values can be processed further as desired. Several statistical analyses have been included in the model and others can be added very easily.

The additional model capabilities are due to the way that the dispersion calculations are stored and utilized. The present model first calculates the ground level concentrations for each source-receptor pair for each dispersion class and stores this information on a random access file. A second program, FRQDTN, is then used to calculate a time series of GLC values corresponding to a time series of meteorological data. It is in this second program that source strengths are selected, and GLC contributions occurring under selected meteorological conditions can be included, excluded, or fractionally included depending upon receptor sensitivity. Thus, the typical variations needed for airshed management and impact studies can be undertaken using FRQDTN without the need to re-run the dispersion calculations.

The plume sigmas in the present model are related to the wind azimuth and elevation angle fluctuations through the statistical dispersion theory. The model contains the concept of a source dominated region and a sigma matching to environmental conditions by means of an effective downwind distance. The environmental σ_A and σ_E values are calculable from a PBL parameterization. The stability parameters used to establish the values of σ_A and σ_E are those defined by present day understanding of PBL similarity theory. These parameters are defined as continuous variables of the main input parameters of wind speed, surface heat flux, and convective mixing height. The discretization of the stability parameters, and hence of the plume sigma curves, is defined by the product of the number of levels of

the main input parameters chosen by the user, and typically, may be 80 levels for positive heat flux conditions and 18 for negative heat flux conditions.

Validation and model sensitivity studies are presented in Volume 3 of this report.

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7. APPENDIX

7.1 GLCGEN DESCRIPTION

7.1.1 Overview of GLCGEN Structure

Program GLCGEN calculates ground level concentrations at receptors due to multiple sources for a large number of dispersion classes. It creates a random access file onto which the GLC values are written. This GLC file is used as input to the frequency distribution program FRQDTN.

A brief summary of the program structure follows. User defined input data are read. Source-receptor geometry is calculated. Various dispersion parameters are computed and classified. Based on these dispersion parameters, the stability of the boundary layer is calculated. Plume parameters are then computed. Centerline and sector-averaged ground level concentration are determined for each source-receptor pair, for each dispersion class. Finally, the sector-averaged GLCs are written to the random access GLC file. Figure 5 illustrates the calling structure of the program and Figure 6 illustrates the loop structure within the program.

7.1.2 Subroutine Descriptions

This section gives a brief description of each subroutine, and lists all common blocks used in that subroutine. An "input" common block is defined as one that brings a value to a variable in the subroutine, while an "output" common block is one that is being written onto by the subroutine. Thus, if a common block appears in both the input and the output lists, it means that the variables that it carries are modified inside that subroutine. Table 7 summarizes the flow of all the common blocks through the different program units.

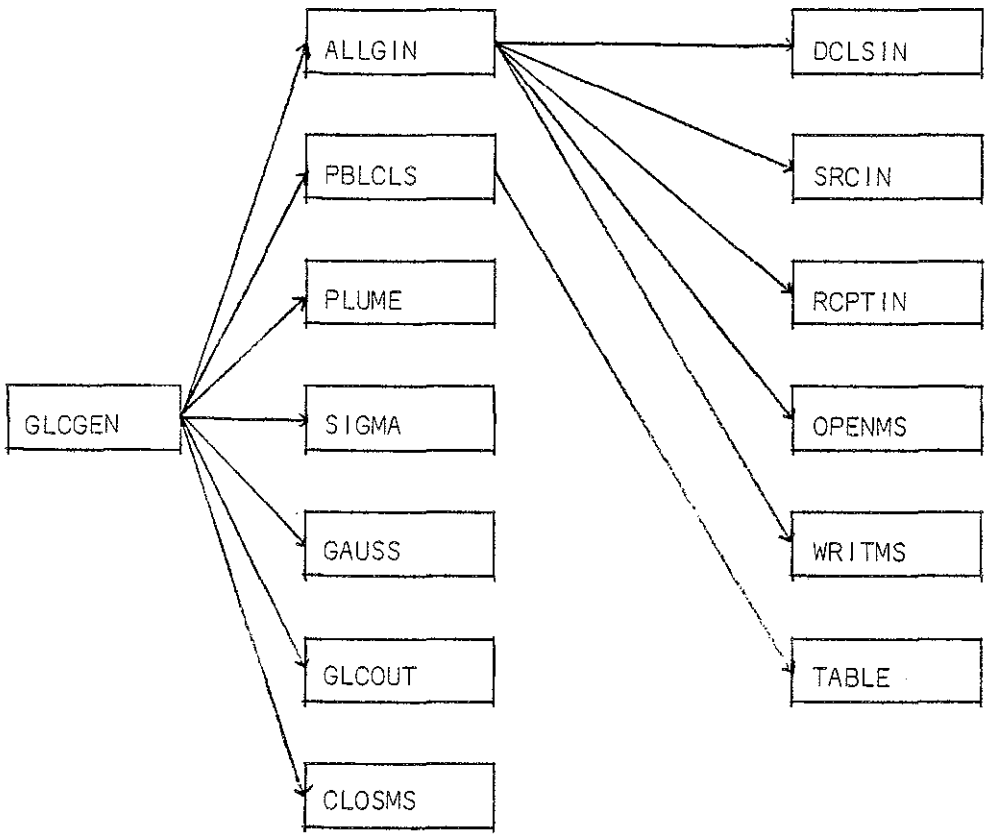

Figure 5. Subroutine call structure in GLCGEN.

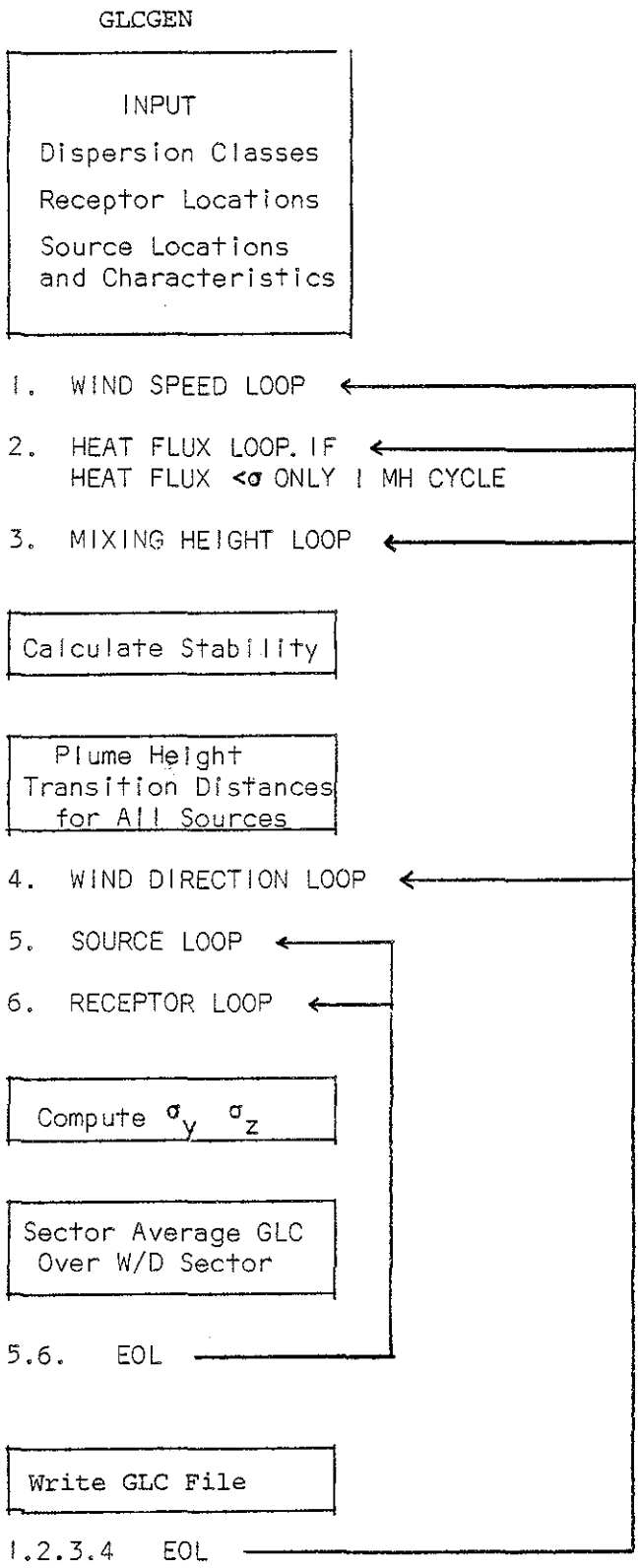

Figure 6. GLCGEN block flowchart.

Table 7. Subroutine-block common and subroutine-parameter list relationships in the program GLCGEN[a].

Common Block	Subroutine										
	GLCGEN	ALLGIN	DCLSIN	SRCIN	RCPTIN	PBLCLS	TABLE	PLUME	SIGMA	GAUSS	GLCOUT
CLASS	I	I	O								I
FILE	O	I	I	I	I						I
SOURCE	I	I		O							
STACK	O							I		I	
RECPT	I	I			O						
ENVR	O					IO		I		I	
PLMCH	IO							O		I	
SIGMA	IO							O	IO	I	
CONC	O	O								O	I
RSCIDX		I	O	O	O						
WIND	IO		IO								
SIGMA1	I					O		I	I		
SIGMA3						O	I				
Parameter List							IO				I

[a] I: Common block inputs a value or values to the subroutine

O: Common block is written to by the subroutine.

GLCGEN

PURPOSE: This program computes Gaussian ground level concentrations for all combinations of specified dispersion classes and source-receptor pairs. These GLC values are written to a GLC file which is accessed by the frequency distribution program FRQDTN.

INPUT:
```
COMMON/CLASS/NWD,NST,NWS,NMH,WDIR(16),WSPD(6),HMIX(6),
STAB(6)
COMMON/SOURCE/NSC,XS(10),YS(10),DS(10),VS(10),TS(10),
HS(10),QS(10)
COMMON/RECPT/NR,XR(400),YR(400)
COMMON/PLMCH/HP
COMMON/SIGMA/XSIG,SIGMY,SIGMZ,DXY,DXZ,XT
COMMON/WIND/DWD,PI
COMMON/SIGMA1/SIGT,SIGE,LAGV,LAGW,ZIL,UST
```

OUTPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,IIOF,IOF
COMMON/STACK/DSTK,VSTK,TSTK,HSTK,QSTK
COMMON/PLMCH/HP
COMMON/SIGMA/XSIG,SIGMY,SIGMZ,DXY,DXZ,XT
COMMON/CONC/GLCGS,NGLCF,GLC(4000)
COMMON/WIND/DWD,PI
```

PROCEDURE: The program first calls ALLGIN which reads all input data. Next source-receptor distances and angles are calculated. Entry point SETUP is called which creates a table of values of Monin-Obukhov length L. At this point, the program enters a series of nested loops, one for each dispersion class parameter. With values of wind speed, heat flux, and mixing height specified in these loops, subroutine PBLCLS is called to determine the stability of the boundary layer. For each source,

subroutine PLUME is called to determine plume heights, transition distances, and distance corrections. For each wind direction and each source receptor pair, plume height and wind angles are checked. If plume height is more than 100 m above the mixing height or if the wind direction is not within a specified angle from the source-receptor angle, ground level concentrations are set to zero for this particular source-receptor-dispersion class combination. If plume height and wind direction are within acceptable bounds, subroutine SIGMA is called to calculate plume spread. Then subroutine GAUSS is called which calculates a ground level centerline concentration. The program then calculates a sector-averaged GLC. For each dispersion class, ground level concentrations are written to the random access GLC file. The program ends with the closing of the random access file.

ALLGIN

PURPOSE: This subroutine controls reading and echoing of all input parameters for the run, and records receptor, source, and dispersion class information in the random access GLC file.

INPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,IIDF,IOF,IDATAC
COMMON/CLASS/NWD,NST,NWS,NMH,WDIR(16),WSPD(6),HMIX(6),
STAB(6)
COMMON/SOURCE/NSC,XS(10),YS(10),DS(10),VS(10),TS(10),
HS(10),QS(10)
COMMON/RECPT/NR,XR(400),YR(400)
COMMON/RSCIDX/RSC(60)
```

OUTPUT:
```
COMMON/CONC/GLCGS,NGLCF,GLC(4000)
```

PROCEDURE: The data check option (IDATAC) is read in, and the subroutines DCLSIN, SRCIN, and RCPTIN are called to read and echo the remaining input data. If the run is a data check only, execution is terminated. Otherwise, receptor, source, and dispersion class information is written to the random access GLC file which will be used by the program FRQDTN.

DCLSIN

PURPOSE: This subroutine reads dispersion class information necessary to create the GLC file.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,IIDF,IOF
COMMON/WIND/DWD,PI

OUTPUT: COMMON/CLASS/NWD,NST,NWS,NMH,WDIR(16),WSPD(6),
HMIX(6),STAB(6)
COMMON/RSCIDX/MWD,MST,MWS,MMH,WSPDB(6),HMIXB(6),
STABB(6), DUMA(38)
COMMON/WIND/DWD,PI

PROCEDURE: The following information is read and echoed:

1. Title (TITLE);
2. Number of classes for each dispersion parameter: wind direction (NWD), stability (NST), wind speed (NWS) and mixing height (NMH); and
3. Class upper boundaries of each dispersion parameter, and representative values for each class to be used in calculating the GLC values.

The bearings delineating wind direction sectors are generated based on the indicated number of wind direction class.

Dispersion class information is written to common block RSCIDX which passes source, receptor, and dispersion information to the GLC file.

SRCIN

PURPOSE: This subroutine reads source layout information and stack emission parameters.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,IIDF,IOF

OUTPUT: COMMON/RSCDIX/DUMA(30),MSC,XSS(10),YSS(10),DUMB(9)
COMMON/SOURCE/NSC,XS(10),YS(10),DS(10),VS(10),
TS(10),HS(10),QS(10)

PROCEDURE: The following information is read and echoed:

1. Number of sources (NSC);
2. X and y co-ordinates for each source (XS,YS); and
3. Stack and emission information for each source [diameter (DS), exit velocity (VS), exit temperature (TS), stack height (HS) and pollutant emission strength (QS)].

Source information is written into common block RSCIDX which passes source, receptor, and dispersion information to the GLC file.

RCPTIN

PURPOSE: This subroutine reads receptor layout information.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,IIDF,IOF

OUTPUT: COMMON/RSCIDX/DUMA(25),NRGX,NRGY,DS,XOR,YOR,DUMB(30)
COMMON/RECPT/NR,XR(400),YR(400)

PROCEDURE: The number of gridpoints in the x-direction (NRGX), y-direction (NRGY), and specified receptors (NRS) are read in. The total number of receptors (NRGX*NRGY+NRS) is checked to ensure that the program dimension of 400 is not exceeded. If grid calculations are indicated (NRGX and NRGY non-zero), then grid spacing (DS) and coordinates of origin (XORIG, YORIG) are read and grid point locations calculated. If specified receptors are indicated (NRS non-zero), the coordinates of each receptor (XR,YR) are read. All receptor locations are echoed.

OPENMS

PURPOSE: This subroutine readies the random access GLC file for use. It is a CYBER system subroutine; it is likely that on other computer systems, this subroutine will be replaced or deleted.

INPUT: IGLCF,NREC2,0

OUTPUT: IGX

WRITMS

PURPOSE: This subroutine writes receptor, source, and dispersion class information to the second last record of the random access GLC file for use by the program FRQDTN. This subroutine is a CYBER system subroutine which likely will be replaced or deleted on other computer systems.

INPUT: !GLCF,RSC,60,NREC!

PBLCLS

PURPOSE: This subroutine determines stability of the planetary boundary layer.

INPUT: COMMON/ENVR/ZI,U400,WT

OUTPUT: COMMON/SIGMA1/SIGT,SIGE,LAGV,LAGW,ZIL,UST
COMMON/SIGMA3/Z,ZO,F,C1,C2,C3,ALPHAS,N
COMMON/ENVR/ZI,V400,WT

PROCEDURE: The first call to PBLCLS is to the entry point SETUP. Constants in DATA statements are accessed and echoed. Subroutine TABLE is then called which creates a table of values of Monin-Obukhov length L.

Subsequent calls to PBLCLS first calculate values of mixing heights in neutral and stable conditions. Values of L are calculated explicitly or by calling TABLE 1, an entry point in subroutine TABLE. Standard deviations of lateral and vertical wind fluctuations are calculated and Lagrangian length scales are specified.

PBLCLS is called from GLCGEN once for each dispersion class.

TABLE

PURPOSE: This subroutine sets up a table from which values of Monin-Obukhow length L can be calculated.

INPUT: XL,U,WT,USTAR
COMMON/SIGMAZ/GT,VK

OUTPUT: USTAR,XL

PROCEDURE: The first call to TABLE creates a table of L values which is accessed by subsequent calls to this routine. Later calls to TABLE are via entry point TABLE1. Based on values for the right-hand-side of the equation, the correct value of L is bracketed and then determined by linear interpolation. The friction velocity is also calculated.

PLUME

PURPOSE: This subroutine calculates plume rise using the formulation of Briggs.

INPUT: COMMON/STACK/DSTK,VSTK,TSTK,HSTK,QSTK
COMMON/ENVR/HM,UW,FLUX
COMMON/SIGMAI/SIGT,SIGE,RLAGV,RLAGW,ZIL,UST

OUTPUT: COMMON/PLMCH/HP
COMMON/SIGMA/XSIG,SIGMY,SIGMZ,DXY,DXZ,XT

PROCEDURE: Plume rise is calculated according to stability. Plume rise under unstable, neutral, and mechanically dominated stable conditions is calculated using Briggs' unstable formulation. Plume rise under thermally dominated stable conditions is calculated using the stable formulation. Final plume rise XF is assumed to occur at 2 km downwind. The transition distance between source and environmentally-dominated diffusion processes XT is calculated. The minimum XT is assumed to be 800 m.

Plume spread is constrained to be at least as fast as that predicted by Pasquill. Distance corrections (DXY,DXZ) are calculated, based on enhanced dispersion in the source-dominated region.

SIGMA

PURPOSE: This subroutine calculates plume sigmas.

INPUT: COMMON/SIGMAI/SIGT,SIGE,RLAGV,RLAGW,ZIL,UST
COMMON/SIGMA/XSIG,SIGMY,SIGMZ,DXY,DXZ,XT

OUTPUT: COMMON/SIGMA/XSIG,SIGMY,SIGMZ,DXY,DXZ,XT

PROCEDURE: The effective distance from the source to receptor (XEY,XEZ) is calculated as the sum of the actual distance XSIG and the distance correction for enhanced source-region dispersion (DXY,DXZ) found in subroutine PLUME. Plume standard deviations are then calculated based on Pasquill F(x) with $X^{1/2}$ distance variation.

GAUSS

PURPOSE: This subroutine calculates a Gaussian ground level concentration along the plume centerline.

INPUT: COMMON/SIGMA/XSIG,SIGMY,SIGMZ,DXY,DXZ,XT
COMMON/ENVR/HM,UW,FLUX
COMMON/STACK/DSTK,VSTK,TSTK,HSTK,QSTK
COMMON/PLMCH/HP

OUTPUT: COMMON/CONC/GLCGS,NGLCF,GLC(4000)

PROCEDURE: In stable conditions, 1 reflection from the surface is allowed, but only when the ratio of plume height to vertical standard deviation is less than three.
In convective conditions, if the ratio of vertical standard deviation to mixing height is greater than 1.6, the plume is assumed to be uniformly mixed in the vertical and the centerline GLC is a linear function of plume standard deviation and mixing height.
If the plume is not uniformly mixed, multiple reflections at the mixing height are allowed until the effect of additional reflections is negligible.

GLCOUT

PURPOSE: This subroutine writes GLC values to the random access file and printer.

INPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,IIDF,IOF
COMMON/CLASS/NWD,NST,NWS,NMH,WDIR(16),WSPD(6)
HMIX(6),STAB(6)
COMMON/CONC/GLCGS,NGLCF,GLC(4000)
IWD,IWS,IST,IMH
```

PROCEDURE: The random access file index is calculated for the current dispersion class. The subroutine WRITMS is called to store the current GLC values in the GLC file.

CLOSMS

PURPOSE: This subroutine closes the random access GLC file. It is a CYBER system subroutine that likely will be replaced or deleted on other computer systems.

INPUT: IGLCF

7.2 FRQDTN DESCRIPTION

7.2.1 Overview of FRQDTN Structure

Program FRQDTN is the operational part of the model and is the component that would be run by most users. It accesses the file of ground level concentrations produced by GLCGEN and the hourly time series files of meteorological parameters produced by TIMSER.

A brief summary of the program structure follows. User defined input data are read. The source and receptor layout are regenerated and source strengths are specified. A record is read from the times series file. Wet deposition and a GLC weighting factor are calculated. A dispersion classification is assigned and the appropriate value read from the GLC file. A GLC is calculated and the frequency distribution information is updated. After each month of data, dry deposition is determined and a monthly summary of results is printed. When all months have been examined, a summary for the total period is printed. Figure 7 shows the calling structure of the program and Figure 8 illustrates the loop structure within the program.

7.2.2 Subroutine Description

The present section gives a short description of each subroutine, and lists all common blocks used in that subroutine. An "input" common block is defined as one that brings a value to a variable in the subroutine, while an "output" common block is one that is being written onto by the subroutine. Thus, if a common block appears in both the input and output lists, it means that the variables that it carries are modified inside that subroutine. Table 8 summarizes the flow of all the common blocks through the different program units.

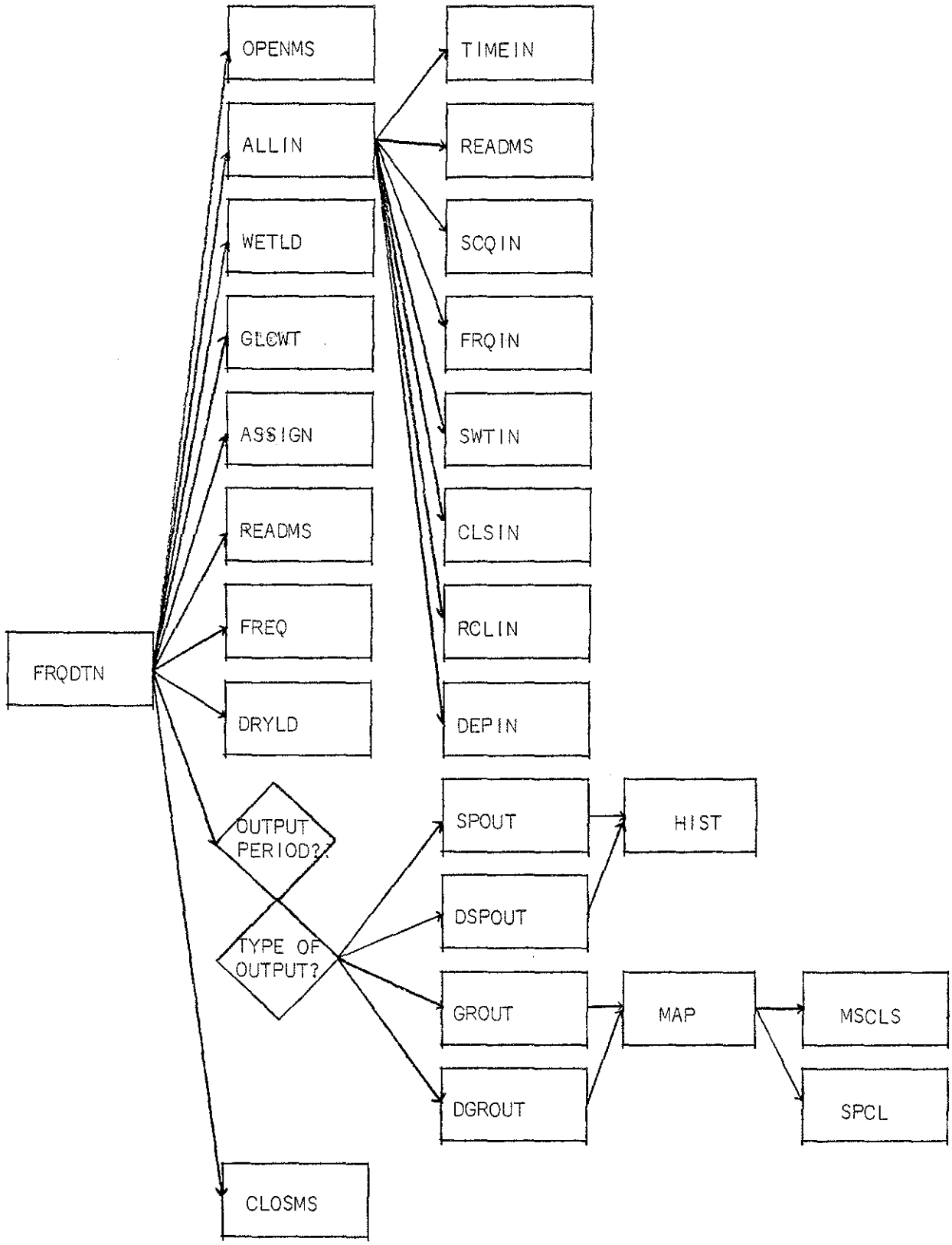

Figure 7. Subroutine call structure in FRQDTN.

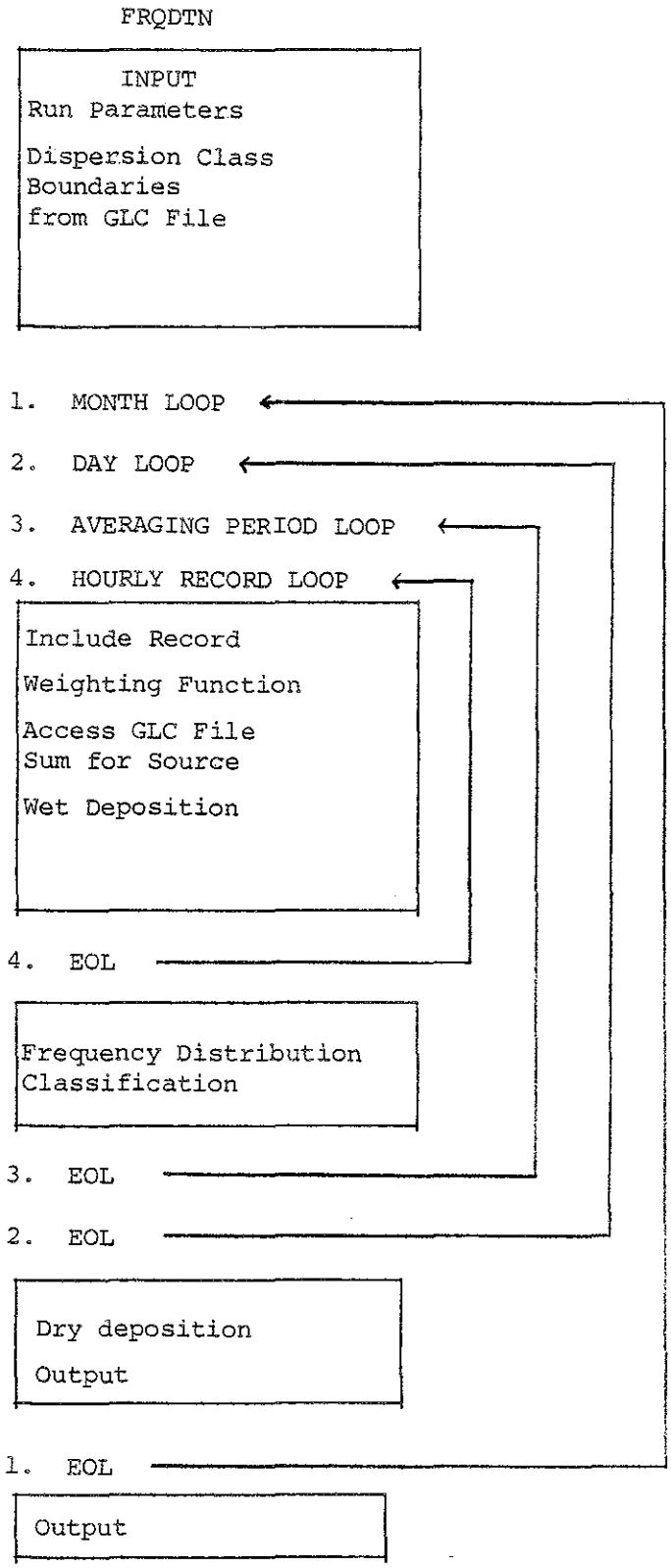

Figure 8. FRQDTN block flowchart.

Table 8. Subroutine-block common and subroutine-parameter list relationships in the program FRQDTN[a].

Common Block Name	Subroutine																						
	FRQDTN	ALLIN	TIMEIN	SCQIN	FRQIN	SWTIN	CLSIN	RCLIN	DEPIN	WETLD	GLCWT	ASSIGN	FREQ	DRYLD	GROUT	SPOUT	DGROUT	DSPOUT	MAP	MSCLS	SPCL	HIST
FILE	O	I	I	I	I	I	I	I	I						I	I	I	I	I	I		I
TSFILE	I		O																			
GLCF	I							O														
METHR	O								O					I								
OPT	I				O				O													
PSORT	IO					O					I	I										
TDIFF	O												IO									
PERIOD	O														I	I	I	I				
TIME	O											I	I									
AVGPD	O												IO									
TDAY	I		O																			
SOURCE	I			O					I	I									I		I	
FREQ	IO				O								IO		I	I						
WEIGHT						O					I											
RECPT	I							O	I	I			I	I		I		I				
RSCIDX		O		I			I	I														
TITLE		O													I	I	I	I				
UNITS				O	I					I				I	I	I						
DCLS							O		I	I		I										
RGRID								O							I		I		I	I	I	
RCORD								O	I													
WET									O	I												
MAPA															O		O		I	I		
SPCL																			IO		IO	
CLSMB																			IO	IO		
Parameter List										O	O	O		IO	I	I	I	I		I	I	I

[a] I: Common block inputs a value to the subroutine
O: Common block is written to by the subroutine

FRQDTN

PURPOSE: This program analyses a time series of meteorological data, relying on pre-calculated values of GLC based on a dispersion classification scheme, and generates frequency distributions of ground level concentrations and deposition.

INPUT:
```
COMMON/RECPT/NR,NRSP,IRPT(20)
COMMON/TSFILE/NFILE,IFILE(20)
COMMON/GLCF/NGLCF
COMMON/OPT/MOPT(4),IOPT(4),MDOPT(3),IDOPT(3)
COMMON/PSORT/NPARM,ISORT(20),PARAM(20)
COMMON/TDAY/NAPD,NAVG,INCL(24)
COMMON/FREQ/NCCLS,NTCLS,CCLS(10),TCLS(10),CFREQ(400,10)
TFREQ(400,10),GLCPK,CFREQM(400,10),TFREQM,(400,10)
COMMON/SOURCE/NSC,XS(10),YS(10),QS(10)
```

OUTPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/METHR/WD,U,P
COMMON/DY/VG(12),NWET
COMMON/PSORT/NPARM,ISORT(20),PARAM(20)
COMMON/TDIFF/TLAST
COMMON/PERIOD/IP(12),IPERIOD(12,2)
COMMON/TIME/IYR,IMON,IDAY,IHRS
COMMON/AVGPRD/NAP,GLCAP(20)
COMMON/FREQ/NCCLS,NTCLS,CCLS(10),TCLS(10),CFREQ(400,10)
TFREQ(400,10),GLCPK,CFREQM(400,10),TFREQM(400,10)
```

PROCEDURE: FRQDTN first calls the CYBER system subroutine which readies the random access GLC file. Subroutine ALLIN is then called to read all input data, and to read dispersion class, source, and receptor information from the GLC file.

The program then enters its major loop through which it cycles once each month. Various monthly arrays are initialized. The secondary loop in a day, is then entered; the tertiary loop for the number of hours in the averaging period in entered immediately thereafter. A recod is read from the appropriate time series file, and the meteorological parameters reordered if necessary. Wet deposition is calculated by subroutine WETLD if precipitation is reported for the hour. Subroutine GLCWT is called to calculate weighting functions for the GLC. Subroutine ASSIGN is called which matches a dispersion class in the GLC file, and returns a file index. System subroutine READMS uses the index to return a GLC for each source-receptor combination. The program then loops through the sources and receptors and generates a GLC at each receptor due to multiple sources. The tertiary loop ends with the weighting function being applied to the GLC and the GLC being summed over the averaging priod. At the end of the averaging period, subroutine FREQ is called which increment the appropriate frequency distribution classes. This procedure continues for each averaging period in the day. At the end of each month, subroutine DRYLD is called to compute dry deposition, and GLC and deposition arrays are incremented.

Appropriate output subroutines are then called, dependent upon whether receptors are defined on a grid or at specified locations. This ends the major loop of the program. When all calculations are concluded, the output routines are again called the output GLC's, frequency distributions, and deposition. The final call to CYBER system subroutine CLOSMS closes the random access GLC file.

OPENMS

PURPOSE: This subroutine opens the random access file of information created by the program GLCGEN. It is a CYBER system subroutine; on other computer systems this subroutine may need to be replaced or deleted.

INPUT: IGLCF

OUTPUT: IGX

ALLIN

PURPOSE: This subroutine controls reading and echoing of all input parameters for the run.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,ITSF,IDATAC

OUTPUT: COMMON/RSCIDX/RSC(60)
COMMON/TITLE/TITLE(20)

PROCEDURE: The title and data check option are read. The subroutines TIMEIN, READMS, SCQIN, RQIN, SWTIN, CLSIN, RCLIN, and DEPIN are called to read and echo the remaining input data, and to generate output indicating which options have been specified for the analysis. If the run is meant merely to echo input data and to display the choice of output options, the run is terminated in this subroutine.

TIMEIN

PURPOSE: This subroutine determines which meteorological time series data records will be used in the frequency distribution analysis.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,ITSF

OUTPUT: COMMON/TSFILE/NFILE,IFILE(12)
COMMON/TDAY/NAPD,NAVG,INCL(24)

PROCEDURE: Parameters are read indicating:

1. Which files of meteorological time series to use;
2. Which records (hours) of each file to use; and
3. Number of records to combine for calculating a time averaged GLC.

Information echoing the input data and indicating the selected options is printed.

SCQIN

PURPOSE: This subroutine determines source information for the analysis.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/RSCIDX/DUMA(30),MSC,XSS(10),
YSS(10),DUMB(9)

OUTPUT: COMMON/SOURCE/NSC,XS(10),YS(10),QS(10)
COMMON/UNITS/IUNIT,CUNIT(2,7),ISCU,
CONVERT

PROCEDURE: Information is read for emission scaling of each source, input emission units, output concentration units, and the conversion factor between input and output units for the analysis. The information is echoed along with the source coordinates used to create the GLC file. Information on number of sources and their locations is passed from common block RSCIDX to SOURCE. Source strengths are pre-scaled according to the units of concentration.

FRQIN

PURPOSE: This subroutine determines frequency distribution information for the analysis.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/UNITS/IUNIT,CUNIT(6,7)ISCU,CONVERT

OUTPUT: COMMON/OPT/MOPT(4),IOPT(4),MDOPT(3),IDOPT(3)
COMMON/FREQ/NCCLS,NTCLS,CCLS(10),
TCLS(10),CFREQ(400,10),TFREQ(400,10),GLCPK,
CFREQM(400,10),TFREQM(400,10)

PROCEDURE: The following input data are read:

1. Number of frequency distribution classes of ground level concentration and time between GLC episodes;
2. The upper boundaries for each class of the frequency distributions; and
3. Output options for displaying monthly or total period average ground level concentrations and frequency distributions.

The input data are echoed and the selected output options are listed.

SWTIN

PURPOSE: This subroutine reads information for reordering parameters on the meteorological time series and for weighting the calculated GLC.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,ITSF

OUTPUT: COMMON/PSORT/NPARM,ISORT(20),PARAM(20)
COMMON/WEIGHT/NBWT,IBWT(20),PTHL(10),
PTHU(10),INDW(10)

PROCEDURE: The following input data are read:

1. Number of meteorological parameters on the time series file;
2. Indices indicating the order in which the meteorological parameters appear;
3. Number of meteorological parameters to be included in weighting analysis for GLC;
4. Index of each meteorological parameter to be included in weighting;
5. For each meteorological parameter, lower and upper threshold values defining the range to be weighted; and
6. Weighting index specifying relationship between weight and meteorological parameters.

Output is generated echoing the input data and indicating the options selected.

CLSIN

PURPOSE: This subroutine regenerates the dispersion classes used in creating the GLC file.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/RSCIDX/MWD,MST,MWS,MMH,WSPB(6)
HMIXB(6),STABB(6),DUMA(38)

OUTPUT: COMMON/DCLS/NWD,NST,NWS,NMH,WSPD(6)
HMIX(6),STAB(6)

PROCEDURE: Information for number of classes and representative data values for each class used in calculating the GLC file is transferred from the common block RSCIDX (GLC file information) to the common block DCLS (frequency distribution analysis information).

A summary of the dispersion classes is listed.

RCLIN

PURPOSE: This subroutine specifies the layout for receptors where GLC information is required.

INPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/RSCIDX/DUMA(25),NRGX,NRGY,DS,XOR,YOR,NSC,
DUMB(29)
```

OUTPUT:
```
COMMON/GLCF/NGLCF
COMMON/RECPT/NR,NRSP,IRPT(20)
COMMON/RGRID/NX,NY,XORIG,YORIG,DH
COMMON/RCORD/XR(400),YR(400),XRSP(20),YRSP(20)
```

PROCEDURE: The number of specified receptors is read. If not equal to zero, the coordinates of the receptors are then read. If the GLC file produced by GLCGEN contains GLCs for a grid of receptors, grid point locations are regenerated. If the grid is regenerated and specified receptor locations are required, the location of the nearest grid point to each receptor is determined.

The coordinates of receptor locations are listed.

DEPIN

PURPOSE: This subroutine reads information specifying deposition calculations to be performed and calculates preliminary information required for the deposition computations.

INPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/SOURCE/NSC,XS(10),YS(10),QS(10)
COMMON/RECPT/NR,NRSP,IRPT(20)
COMMON/DCLS/NWD,NST,NWS,NMH,WSPD(6),
HMIX(6),STAB(6)
COMMON/RCORD/XR(400),YR(400),XRSP(20),YRSP(20)
```

OUTPUT:
```
COMMON/DRY/VG(12),NWET
COMMON/OPT/MOPT(4),IOPT(4),MDOPT(3),IDOPT(3)
COMMON/WET/A,B,TH(400,10),CWL(400,10)
```

PROCEDURE: The type of deposition output for each monthly analysis and the total period is determined from input information.

Dry deposition velocities and wet deposition scavenging coefficients are assigned either by input or default. Statements echoing these constants and indicating the selected options are printed. Sector width and coordinate system angles are calculated for all source-receptor combinations.

WETLD

PURPOSE: This subroutine calculates sulphur loading due to wet deposition.

INPUT:
```
COMMON/METHR/WD,U,P
COMMON/SOURCE/NSC,XS(10),YS(10),QS(10)
COMMON/RECPT/NR,NRSP,IRPT(20)
COMMON/UNITS/IUNIT,CUNIT(2,7),ISCU,CONVERT
COMMON/DCLS/NWD,NST,NWS,NMH,WSPD(6),HMIX(6)
COMMON/WET/A,B,TH(400,10),CWL(400,10)STAB(6)
```

OUTPUT: WETDEP

PROCEDURE: This subroutine is called for each hour during which precipitation is indicated on the meteorological time series. Wet loading is calculated employing the irreversible capture technique.

GLCWT

PURPOSE: This subroutine determines a weight for the calculated GLC based on the magnitude of selected parameters for the current time series record.

INPUT: COMMON/PSORT/NPARM,ISORT(20),PARAM(20)
COMMON/WEIGHT/NBWT,IBWT(10),PTHL(10),
PTHU(10),INDW(10)

OUTPUT: WEIGHT

PROCEDURE: If weighting was not specified in the input data for the run, a weight of unity is returned. If weighting was specified for a number of time series parameters, the weight returned is the product of all individual parameter weights. Weighting parameters are calculated based on threshold values specified in the input data. If weight was specified for increasing parameter values, the weight is unity for all parameter values above the upper threshold, and zero for all parameters below the lower threshold. Weight specified for decreasing parameter values would be the opposite, i.e., zero for parameter values above the upper threshold, and unity for parameters below the lower threshold. Weight varies linearly for all values in the range between the upper and lower thresholds.

ASSIGN

PURPOSE: This subroutine determines which GLC dispersion class corresponds to the current record of the meteorological time series.

INPUT: COMMON/PSORT/NPARM,ISORT(20),PARAM(20)
COMMON/TIME/IYR,IMON,IDAY,IHRS
COMMON/DCLS/NWD,NST,NWS,NMH,WSPD(6),HMIX(6)STAB(6)

OUTPUT: INDEX

PROCEDURE: Wind direction, windspeed, net radiation, and mixing height are read directly from the time series record. Heat flux is calculated from net radiation. The classes into which each of these parameters fall are determined, and the GLC file index corresponding to the overall dispersion class is obtained.

READMS

PURPOSE: This subroutine reads the GLC file record for the current dispersion classification. It is a CYBER system subroutine designed to read random access files. It is likely that this subroutine will be deleted or changed on other computer systems.

INPUT: INDEX, IGLCF, NGLCF

OUTPUT: GLC

FREQ

PURPOSE: This subroutine calculates, for each receptor, the current time-averaged GLC and adds the value to the frequency distributions for GLC and time difference between peak episodes.

INPUT:
```
COMMON/IDIFF/TLAST(400)
COMMON/TIME/IYR,IMON,IDAY,IHRS
COMMON/AVGPRD/NAP,GLCAP(400)
COMMON/FREQ/NCCLS,NTCLS,CCLS(10),TCLS(10),CFREQ(400,10)
TFREQ(400,10),GLCPK,CFREQM(400,10),TFREQM(400,10)
COMMON/RECPT/NR,NRSP,IRPT(20)
```

OUTPUT:
```
COMMON/TDIFF/TLAST(400)
COMMON/AVGPRD/NAP,GLCAP(400)
COMMON/FREQ/NCCLS,NTCLS,CCLS(10),TCLS(10),
CFREQ(400,10),TFREQ(400,10),GLCPK,CFREQM(400,10),
TFREQM(400,10)
```

PROCEDURE: For each receptor, the time-averaged GLC is obtained. The appropriate frequency distribution class for the current month and total period is incremented. If the time-averaged GLC exceeds the peak value, the time interval since the last excedance is calculated, and the appropriate class of the time difference frequency distribution for the current month and the total period is incremented.

DRYLD

PURPOSE: This subroutine calculates sulphur loading due to dry deposition.

INPUT: COMMON/DRY/VG(12),NWET
COMMON/RECPT/NR,NRSP,IRPT(20)
COMMON/UNITS/IUNIT,CUNIT(2,7),ISCU,CONVERT
GLCMON,NMONTH,IF

OUTPUT: DRYDEP

PROCEDURE: For each receptor, dry deposition is calculated as the product of monthly average deposition velocity, GLC, and fraction of the month for which there is no preciptation.

SPOUT

PURPOSE: This subroutine provides output of average ground level concentration, frequency distribution and inverse cumulative frequency distribution of GLC, and frequency distribution of time difference between peak GLC for individual receptors.

INPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/PERIOD/IP(12),IPERIOD(12,2)
COMMON/FREQ/NCCLS,NTCLS,CCLS(10),TCLS(10)
CFREQ(400,10),TFREQ(400,10),GLCPK,CFREQM(400,10),
TFREQM(400,10)
COMMON/RECPT/NR,NRSP,IRPT(20)
COMMON/TITLE/TITLE(20)
COMMON/UNITS/IUNIT,CUNIT(2,7),ISCU,CONVERT
KOPT,NUM,CONCF,TDF,GLC,I1,I2
```

PROCEDURE: Preliminary calculations for arranging output information are performed. Depending on the output options specified, a table showing average concentration at all receptors is printed. Header information for frequency distribution tables is also printed. The subroutine HIST is called to print a histogram for the frequency distribution at each receptor.

HIST

PURPOSE: This subroutine plots a histogram for frequency distributions.

INPUT: COMMON/FILE/IRD,IPR,IGLCF,ITSF
NUM,NCLASS,FREQ,CLASS

PROCEDURE: The shape of the histogram curve is calculated from the frequency array and stored in an output array. The output array is then printed in the form of a histogram.

DSPOUT

PURPOSE: This subroutine provides output of dry, wet, and total deposition for specified receptor locations.

INPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/PERIOD/IP(12),IPERIOD(12,2)
COMMON/RECPT/NR,NRSP,IRPT(20)
COMMON/TITLE/TITLE(20)
DRY,WET,KOPT,I1,I2
```

PROCEDURE: If specified by the output option indices, average, dry, wet, and total depositions are printed for each receptor.

GROUT

PURPOSE: This subroutine provides output of average ground level concentration, frequency distribution, and inverse cumulative frequency distribution of GLC, and frequency distribution of time difference between peak GLC for an entire grid of receptors.

INPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/PERIOD/IP(12),IPERIOD(12,2)
COMMON/FREQ/NCCLS,NTCLS,CCLS(10),TCLS(10),CFREQ(400,10)
TFREQ(400,10),GLCPK CFREQM(400,10),TFREQ(400,10)
COMMON/TITLE/TITLE(20)
COMMON/UNITS/IUNIT,CUNIT(2,7),ISCU,CONVERT
COMMON/PGRID/NX,NY,XORIG,YORIG,DH
KOPT,NUM,CONCF,TDF,GLC,I1,I2
```

OUTPUT:
```
COMMON/MAPA/ARRAY(20,20)
```

PROCEDURE: Each type of output is handled individually in the following manner. The output option selection indices are checked for which type of output is specified. The information for all gridpoints is assigned to the map array, ARRAY. Header information is then printed and the subroutine MAP is called to print out the grid of values.

MAP

PURPOSE: This subroutine prints a two-dimensional array of frequency class symbols arranged in an x-y grid.

INPUT:
```
COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/SOURCE/NSP,XSP(10),YSP(10),QS(10)
COMMON/PGRID/NX,NY,XORIG,YORIG,DH
COMMON/MAPA/ARRAY(20,20)
COMMON/SPCL/ROW(125),NXINT,NYINT,NROW
COMMON/CLSMB/CLASS(20),SYMBOL(20),NC
```

OUTPUT:
```
COMMON/SPCL/ROW(125),NXINT,NYINT,NROW
COMMON/CLSMB/CLASS(20),SYMBOL(20),NC
```

PROCEDURE: An array of data is received from the calling program. The subroutine MCLS is called to assign the array values into classes and provide a symbol for each class. Map scale and axes are generated. Values of the map data between grid points are generated by second-order interpolation of grid point values. The subroutine SPCL is called to assign special map symbols for reference points if required. The map data are then output line-by-line.

MSCLS

PURPOSE: This subroutine generates classes of data, assigns a map symbol for each, and outputs a generated legend.

INPUT:
```
COMMON/IFILE/IRD,IPR,IGLCF,ITSF
COMMON/RGRID/NX,NY,XORIG,YORIG,DH
COMMON/MAPA/ARRAY(20,20)
COMMON/CLSMB/CLASS(20),SYMBOL(20),NC
IZERO
```

OUTPUT:
```
COMMON/CLSMB/CLASS(20),SYMBOL(20),NC
```

PROCEDURE: The maximum and minimum values in the output array are determined. Classes are generated based on the range of data, the number of classes NC, and IZERO, the index specifying a lower bound of either zero or the minimum value of data. A map legend is generated and printed.

SPCL

PURPOSE: This subroutine plots a special symbol (*) at reference points on the map.

INPUT: COMMON/RGRID/NX,NY,XORIG,YORIG,DH
COMMON/SOURCE/NSP,XSP(10),YSP(10),QS(10)
COMMON/SPCL/ROW(125),NXINT,NYINT,NROW
J

OUTPUT: COMMON/SPCL/ROW(125),NXINT,NYINT,NROW

PROCEDURE: All the reference points are scanned to determine the print row in which they will occur. If any points lie on the current row (J), the special symbol(*) is inserted at the x location of the point.

DGROUT

PURPOSE: This subroutine provides output of dry, wet, and total deposition for an entire grid of receptors.

INPUT:
COMMON/FILE/IRD,IPR,IGLCF,ITSF
COMMON/PERIOD/IP(12),IPERIOD(12,2)
COMMON/TITLE/TITLE(20)
COMMON/RGRID/NX,NY,XORIG,YORIG,DH
DRY,WET,KOPT,I1,I2

OUTPUT: COMMON/MAPA/ARRAY(20,20)

PROCEDURE: Each type of deposition is handled individually in the following manner. The output option selection indices are checked for the type of output specified. The information for all gridpoints is assigned to the map array, ARRAY. Header information is then printed and the subroutine MAP is called to print out the grid.

CLOSMS

PURPOSE: This subroutine closes the GLC file at the end of the frequency distribution analysis. It is a CYBER system subroutine designed to manipulate random access files. On other computer systems, this subroutine is likely to be changed or deleted.

INPUT: IGLCF

8. LIST OF AOSERP WIDE DISTRIBUTION RESEARCH REPORTS

Report	Project	Reference
1	PM	Alberta Oil Sands Environmental Research Program. 1976. First annual report, 1975. Alberta Oil Sands Environmental Research Program. AOSERP Report 1. 58 pp.
2	AF 4.1.1	Kristensen, J., B.S. Ott, and A.D. Sekerak. 1976. Walleye and goldeye fisheries investigations in the Peace-Athabasca Delta--1975. Prep. for the Alberta Oil Sands Environmental Research Program by LGL Ltd., Environmental Research Associates. AOSERP Report 2. 103 pp.
3	HE 1.1.1	McVey, W.W. 1976. Structure of a traditional baseline data system. Prep. for the Alberta Oil Sands Environmental Research Program by the University of Alberta, Population Research Laboratory. AOSERP Report 3. 26 + 266 pp.
4	VE 2.2	Stringer, P.W. 1976. A preliminary vegetation survey of the Alberta Oil Sands Environmental Research Program study area. Prep. for the Alberta Oil Sands Environmental Research Program by Intraverda Plant Systems Ltd. AOSERP Report 4. 108 pp.
5	HY 3.1	Strosher, M.T. and E. Peake. 1976. The evaluation of wastewaters from an oil sand extraction plant. Prep. for the Alberta Oil Sands Environmental Research Program by the University of Calgary, Environmental Sciences Centre (Kananaskis). AOSERP Report 5. 103 pp.
6	PM	Patterson, R. and A.M. Lansdown. 1976. Housing for the north--the stackwall system; construction report--Mildred Lake tank and pump house. Prep. for the Alberta Oil Sands Environmental Research Program by the University of Manitoba, Faculty of Engineering, Northern Housing Committee. AOSERP Report 6. 36 pp.
7	AF 3.1.1	Jantzie, T.D. 1977. A synopsis of the physical and biological limnology and fishery programs within the Alberta oil sands area. Prep. for the Alberta Oil Sands Environmental Research Program by Renewable Resources Consulting Services Ltd. AOSERP Report 7. 73 pp.

8	AF 1.2.1	Machniak, K. 1977. The impact of saline waters upon freshwater biota (a literature review and bibliography). Prep. for the Alberta Oil Sands Environmental Research Program by Aquatic Environments Ltd. AOSERP Report 8. 258 pp.
9	ME 3.3	Croft, B.R., A. Lamb, and R.N. Dawson. 1977. A preliminary investigation into the magnitude of fog occurrence and associated problems in the oil sands area. Prep. for the Alberta Oil Sands Environmental Research Program by Stanley Associates Engineering Ltd. AOSERP Report 9. 87 pp.
10	HE 2.1	Millar, J.F.V. 1977. Development of a research design related to archaeological studies in the Athabasca Oil Sands area. Prep. for the Alberta Oil Sands Environmental Research Program by the University of Saskatchewan. AOSERP Report 10. 69 pp.
11	AF 2.2.1	Flannagan, J.F. 1977. Life cycles of some common aquatic insects of the Athabasca River, Alberta. Prep. for the Alberta Oil Sands Environmental Research Program by Fisheries and Environment Canada, Freshwater Institute. AOSERP Report 11. 20 pp.
12	ME 1.7	Mercer, J.M. and R.B. Charlton. 1977. Very high resolution meteorological satellite study of oil sands weather: "a feasibility study". Prep. for the Alberta Oil Sands Environmental Research Program by the University of Alberta, Department of Geography. AOSERP Report 12. 44 pp.
13	ME 2.3.1	Davison, D.S., C.J. Fortems, and K.L. Grandia. 1977. Plume dispersion measurements from an oil sands extraction plant, March 1976. Prep. for the Alberta Oil Sands Environmental Research Program by Intera Environmental Consultants Ltd. AOSERP Report 13. 195 pp.
14		none
15	ME 3.4	Denison, P.J. 1977. A climatology of low-level air trajectories in the Alberta oil sands area. Prep. for the Alberta Oil Sands Environmental Research Program by Acres Consulting Services. AOSERP Report 15. 118 pp.

16	ME 1.6	Barge, B.L., R.G. Humphries, and S.L. Olson. 1977. The feasibility of a weather radar near Fort McMurray, Alberta. Prep. for the Alberta Oil Sands Environmental Research Program by Alberta Research Council, Atmospheric Sciences Division. AOSERP Report 16. 72 pp.
17	AF 2.1.1	Lutz, A. and M. Hendzel. 1977. A survey of baseline levels of contaminants in aquatic biota of the AOSERP study area. Prep. for the Alberta Oil Sands Environmental Research Program by Fisheries and Environment Canada, Freshwater Institute. AOSERP Report 17. 51 pp.
18	HY 1.1	Loeppky, K.D. and M.O. Spitzer. 1977. Interim compilation of stream gauging data to December 1976 for the Alberta Oil Sands Environmental Research Program. Prep. for the Alberta Oil Sands Environmental Research Program by Fisheries and Environment Canada, Water Survey Branch. AOSERP Report 18. 257 pp.
19	ME 4.1	Walmsley, J.L. and D.L. Bagg. 1977. Calculations of annual averaged sulphur dioxide concentrations at ground level in the AOSERP study area. Prep. for the Alberta Oil Sands Environmental Research Program by Atmospheric Environment Service. AOSERP Report 19. 40 pp.
20	HY 3.1.1	Strosher, M.T. and E. Peake. 1978. Characterization of organic constituents in waters and wastewaters of the Athabasca Oil Sands mining area. Prep. for the Alberta Oil Sands Environmental Research Program by the University of Calgary, Environmental Sciences Centre (Kananaskis). AOSERP Report 20. 71 pp.
21	PM	Alberta Oil Sands Environmental Research Program. 1977. Second Annual Report, 1976-77. Alberta Oil Sands Environmental Research Program. AOSERP Report 21. 62 pp.
22	PM	Smith, S.B., ed. 1979. Alberta Oil Sands Environmental Research Program Interim Report covering the period April 1975 to November 1978. Prep. by A.S. Mann, R.A. Hursey, R.T. Seidner, and B. Kasinska-Banas. AOSERP Report 22.

23 AF 1.1.2 Lake, W. and W. Rogers. 1979. Acute lethality of mine depressurization water to trout-perch and rainbow trout: Volume I. Prep. for the Alberta Oil Sands Environmental Research Program by Alberta Environment, Water Control Branch. AOSERP Report 23. 44 pp.

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28 VE 2.1 Turchenek, L.W. and J.D. Lindsay. 1978. Interim report on a soils inventory in the Athabasca Oil Sands area. Prep. for the Alberta Oil Sands Environmental Research Program by Alberta Research Council, Soils Division. AOSERP Report 28. 100 pp.

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31 VE 2.3 Thompson, M.D., M.C. Wride, and M.E. Kirby. 1978. Ecological habitat mapping of the AOSERP study area: Phase I. Prep. for the Alberta Oil Sands Environmental Research Program by Intera Environmental Consultants Ltd. AOSERP Report 31. 176 pp.

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33 TF 1.2 Nowlin, R.A. 1978. Relationships between habitats, forages, and carrying capacity of moose range in northern Alberta. Part I: moose preferences for habitat strata and forages. Prep. for the Alberta Oil Sands Environmental Research Program by Alberta Recreation, Parks and Wildlife, Fish and Wildlife Division. AOSERP Report 33. 63 pp.

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44 VE 3.1 Malhotra, S.S. and P.A. Addison. 1979. Interim report on symptomology and threshold levels of air pollutant injury to vegetation, 1975 to 1978. Prep. for the Alberta Oil Sands Environmental Research Program by Canadian Forestry Service, Northern Forest Research Centre. AOSERP Report 44. 13 pp.

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54 WS 2.3 Nix, P.G., J.W. Costerton, R. Ventullo, and R.T. Coutts. 1979. A preliminary study of chemical and microbial characteristics of the Athabasca River in the Athabasca Oil Sands area of northeastern Alberta. Prep. for the Alberta Oil Sands Environmental Research Program by Chemical and Geological Laboratories Ltd., Microbios Ltd., and Xenotox Services Ltd. AOSERP Report 54. 135 pp.

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60	WS 1.1.1	Neill, C.R. and B.J. Evans. 1979. Synthesis of surface water hydrology. Prep. for the Alberta Oil Sands Environmental Research Program by Northwest Hydraulic Consultants Ltd. AOSERP Report 60. 84 pp.
61	AF 4.5.2	Machniak, K. and W.A. Bond. 1979. An intensive study of the fish fauna of the Steepbank River watershed of northeastern Alberta. Prep. for the Alberta Oil Sands Environmental Research Program by Fisheries and Environment Canada, Freshwater Institute. AOSERP Report 61. 196 pp.
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63	ME 3.8.3	Davison, D.S. and E.D. Leavitt. 1979. Analysis of AOSERP plume sigma data. Prep. for the Alberta Oil Sands Environmental Research Program by Intera Environmental Consultants Ltd. AOSERP Report 63. 251 pp.
64	LS 21.6.1	Thomson, D.C., D.M. Ealey, and K.H. McCourt. 1979. A review and assessment of the baseline data relevant to the impacts of oil sands developments on large mammals in the AOSERP study area. Prep. for the Alberta Oil Sands Environmental Research Program by McCourt Management Ltd. AOSERP Report 64. 155 pp.
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74 AS 4.5 Angle, R.P. 1979. Air quality modelling and user needs. Prep. for the Alberta Oil Sands Environmental Research Program by Alberta Environment, Air Quality Control Branch. AOSERP Report 74. 34 pp.

75 WS 1.3.4 Hickman, M., S.E.D. Charlton, and C.G. Jenkerson. 1979. Interim report on a comparative study of benthic algal primary productivity in the AOSERP study area. Prep. for the Alberta Oil Sands Environmental Research Program by the University of Alberta, Department of Botany. AOSERP Report 75. 107 pp.

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85 HY 2.5 Akena, A.M. 1979. An intensive surface water quality study of the Muskeg River watershed. Volume I: water chemistry. Prep. for the Alberta Oil Sands Environmental Research Program by Alberta Environment. AOSERP Report 85. 187 pp.

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