AIRSHED MANAGEMENT SYSTEM FOR THE ALBERTA OIL SANDS

VOLUME III

VERIFICATION AND SENSITIVITY STUDIES

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 dispersion 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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I. INTRODUCTION

Volume 3 of the documentation for the Gaussian frequency distribution model outlines the sensitivity and verification studies performed to the spring of 1981. The review includes both the model response and sensitivities, an assessment of the uncertainties in the data base currently utilized and a comparison with observed air quality data in the Athabasca Oil Sands area. Detailed descriptions of the model formulation and of the generation of the data base are included in Volumes 1 and 2 of the documentation. It is assumed that the reader of Volume 3 is familiar with the general characteristics of the model and the data base and will have access to the previous two volumes for detailed reference.

In the following sections, the verification techniques are initially reviewed to determine which are meaningful for frequency distribution models in the Athabasca Oil Sands area. There are many possible evaluation techniques, but many of these do not produce relevant information for model evaluation. An evaluation procedure was adopted which involved an assessment of component uncertainties so that the results of formal statistical tests could be properly interpreted.

The specification of model and data base accuracy for defined applications is required for proper use of a modelling system; thus, Volume 3 concludes with a summary of the levels of uncertainty that can be expected and with recommendations for model and data base improvements. The results of the sensitivity and verification studies can quantify the relative importance of improvements of various model and data system components; thus, the basis for the uncertainty estimates and the recommendations can be easily reviewed and the impact of alternative studies on model performance evaluated.

2. EVALUATION CONSIDERATIONS FOR FREQUENCY DISTRIBUTION MODELS

2.1 OVERVIEW

Specification of the accuracy levels that can be expected is an integral part of any model. Models can be very powerful scientific and management tools if used within their ranges of applicability; however, they can be very misleading if used beyond. Evaluating the accuracy and applicability of a model and of a data base used to drive the model is not straightforward. The selection of relevant tests requires care since many standard parametric and non-parametric tests may give computationally correct but virtually meaningless results.

One of the most important considerations in the selection of appropriate model and data base tests is the intended use of the model. A model designed to predict extreme values has very different constraints than one designed to predict mean values. The spatial and temporal resolution within a frequency distribution model may be limited by the model formulation and data base accuracies and will also be a function of distance from source and the geographical region in which the model is applied. If the model use involves any evaluation of the ground level concentration (GLC) values in the presence of specified mixing conditions (e.g., summer convective conditions), then the model should be capable of predicting correct GLC levels under those conditions.

The long-term, average GLC value is one of the important outputs for frequency distribution models. Its importance arises from the need to assess long-term accumulative effects of both air quality and soil and water acidification or toxification due to deposition. The average is cumulative; therefore random errors in GLC values may be of little importance, provided that the averaging period is sufficiently long. The length of the necessary averaging period depends upon the frequency of occurrence of GLC events which contribute most to the average GLC value. In the Athabasca Oil Sands area, as will be discussed below, the average GLC values at existing monitors are usually dominated by infrequent events; thus, the necessary averaging period for GLC values at a particular receptor may be much greater than one month. The type of random error also affects the averaging requirements. If a major error source is imprecise knowledge of the wind direction, then spatial averaging may be as important as time averaging.

Other important model products are the magnitude and frequency of poor air quality episodes. The typically infrequent occurrence of events at a given monitor means that a distribution of episodes can be attained only by considering a time interval of duration greater than one month. Due to uncertainty in wind direction and the sparsity of monitors, case study comparisons of predicted and observed values at a given monitor at a given time are of dubious value.

In the Athabasca Oil Sands area, there are some particular problems and constraints. The region is snow-covered for close to one half of the year; thus, the surface energy budget and the resulting atmospheric stability and turbulent mixing can be expected to vary significantly from non-snow surfaces. Most of the existing processed air quality data were collected when Suncor was the only significant source. Newer oil sands plants can be expected to have higher effective stack heights and much reduced particulate emissions in comparison with the Suncor emissions during the time period of the present data base. In particular, the effective stack heights of new plants may exceed the convective mixing height more frequently than does the Suncor source. Plume level winds, as measured by minisondes, were found to correlate poorly with low-level winds and winds from the 152 m tower in the Athabasca valley. There was also evidence of large-scale, topographical steering of the wind direction. As a result, the specification of reliable wind directions will be difficult and the applicability of a single wind direction for all sources in the Athabasca Oil Sands area may be questionable.

2.2 THE USE OF STATISTICAL TESTS ON MONTHLY MEANS

Monthly mean GLC values are often used as a basis for statistical tests to evaluate a frequency distribution model. It is worthwhile, however, to consider whether such tests are effective and meaningful evaluation tools.

The error level in wind direction critically affects the monthly mean at a given receptor. The frequency distribution of winds for each major dispersion process must be reasonably correct or else the predicted values cannot match the observed values even with a perfect model. If the GLC values are dominated by infrequent episodes, then one month may be insufficient time to obtain a long-term, representative frequency distribution of such events. Frequency distribution models usually discretize the wind direction and perform some type of averaging across the sectors. This process approximates an averaging over many realizations; however, many must occur within the averaging period so that observed values at a receptor can converge to a sector-averaged GLC value. A single month may not be sufficient time.

If the above statistical averaging problems can be overcome, there remains the problem of possible misleading agreement between observed and predicted monthly values. Gross errors in GLC predictions for particular mixing processes may be masked. For example, the observed GLC values in winter may occur during strong winds whereas a model might predict GLC values due to convective mixing which may not exist. The monthly averages may be approximately correct but for the wrong reasons. Even if the monthly means are the only desired output, such errors may be very important if the nature of the sources changes. Such a model might lead to the conclusion that a particular height of stack will dramatically reduce the GLC value, while, in fact, it may not.

The application of statistical tests to the Athabasca Oil Sands region presents particular problems. The wind directions are not well defined and the monthly mean concentrations are dominated by infrequent episodes of high concentrations. For such a system, statistical tests on the hourly time series of predicted and observed values and on the monthly means themselves may be dominated by common zero GLC values. The hourly residuals will usually be either the predicted or observed values. In addition, the observed GLC data suffer from serious limitations. The uncertainty level of the sensors is usually greater than the monthly means. In the case of the Syncrude stations, the air quality data mean values are specified to the nearest 10 ppb. The largest monthly concentration found in all the stations was 13 ppb. Even a rank correlation of stations, given the sensitivity to infrequent events and uncertainty in observed data, may be meaningless. Combined space and time averaging, as suggested by Nappo (1974), may be useful when the air quality data are in a computer-compatible format; however, even then, plumes may not be observed due to the sparse network of monitoring stations, with resulting systematic errors in predicted values.

In summary, simple statistical tests on individual receptors are considered to have a limited role in the evaluation of a frequency distribution model in the Athabasca Oil Sands. Significant errors may be overlooked that could lead to inappropriate conclusions when the model is used as a management tool. The actual correlation values observed may be poor indicators of the model performance or of the relative performance of various models. The use of probabilities for the wind direction may be promising. The estimated uncertainties in the wind direction could be used to define the region in which the plume has a given probability of occurring. Over a sufficiently long time interval, a frequency distribution would be generated that could be compared with the observed distribution using one of the parametric tests described below. This approach assumes that the wind direction errors are random and it also would tend to smooth out any real anisotropy. The required time interval, however, would need to be much longer than a month and the problem of misleading agreement would still arise unless several frequency distributions were generated corresponding to distinct mixing mechanisms (e.g., mechanical vs. convective mixing). Although a probability approach may have some limitations for verification purposes, it does appear to be a worthwhile improvement to the model output.

2.3 OUTLINE OF EVALUATION PROCEDURES ADOPTED

Model evaluation is critical for the appropriate model operation and interpretation of results; however, it was argued in the previous section that statistical tests have major limitations. As a result, alternative or supplementary evaluation procedures are needed.

The first stage in the procedure to evaluate the model system adopted was to examine the model structure and sensitivities. This analysis clarifies how the model differs from other Gaussian frequency distribution models. It also leads to an evaluation of relative uncertainties and the best direction for further effort. Such an understanding is important in assessing the validity of applying the model in another area, or of incorporating components of the model into "worst case" or other types of models.

The second stage is an assessment of the uncertainties in the data base. Quantitative assessment is possible for some data by examining the cumulative frequency distributions of the empirically derived parameters specifying the generated data set. Quantitative uncertainties can then be compared with the sensitivities of the model and with typical discretizations used in the model.

Finally, the model results can be compared to observed values in a staged approach. The time series of predicted and observed GLC values at various receptors can be compared to assess what physical processes (e.g., high wind speed) are important and whether those processes are being simulated correctly, without concern for the timing or number of events. If the actual processes are poorly simulated, then the error level can be compared to error estimates resulting from the sensitivity study to assess where the problems likely exist.

Once the simulation uncertainties for the processes are established, the problems of the frequency and timing of events can be considered. Specific case studies can be examined to assess the impact of uncertainties in the time series data base. The formal statistical tests can be used as tools in this evaluation procedure but within the context of an understanding of the applicability and meaning of the results.

3. ACCURACY OF THE TIME SERIES DATA BASE AND ITS IMPLICATIONS

3.1 CONSIDERATIONS FOR ACCURACY REQUIREMENTS

Any uncertainties in the time series file parameters can have an affect on the results generated by the Gaussian frequency model. Parameters of particular concern are those that can enter directly into the model formulations, such as wind speed, wind direction and mixing height. The level of accuracy required in these parameters depends upon the selection of discrete dispersion classes and the user application of model results.

The Gaussian frequency distribution model generates ground level concentrations at selected receptors for discrete dispersion classes. Typical class boundaries that may be user selected are given in Table 1. Since discrete plume dispersion classes are used, limited scatter in the input parameters is not important. The scatter can become important, however, when it is large enough to shift the "true value" across one or more class boundaries. Systematic errors in the data should be removed as much as possible to remove any biasing to higher or lower dispersion classes.

The Gaussian model itself can be a limiting factor in the specification of the accuracy required for the data. The model assumes that meteorological conditions are homogeneous in time and space. In reality, the average wind can vary with height and location. The time series data should be designed to be representative of average conditions in the plume layer, even though it is not always clear exactly how to choose representative values.

The accuracy of the time series data base required is also governed by the user application of the model results. For example, if the user is interested in long-term averages, more scatter in the time series values can be accepted than if the user is interested in evaluating case studies.

Scatter or uncertainty in the data may have no net effect on the estimation of monthly, seasonal, or annual average concentrations if the data are not systematically biased towards higher or lower values and there are enough realizations of concentrations within the

Table 1. Typical dispersion class boundaries.

Parameter	Discrete Value Used	Range of Values Represented
Wind speed	2.0	0 to 3.0
(m/s)	4.0	3.0 to 5.0
	6.5	5.0 to 8.0
	10.0	8.0 to 12.0
	15.0	12.0 to 18.0
	25.0	> 18.0
Wind direction (degrees)	16 compass points	22.5° segments
Mixing height	100	0 to 200
(m)	300	200 to 400
	500	400 to 600
	700	600 to 800
	900	800 to 1000
	1100	> 1000
Heat flux	0.20	0.15
(°C m/s)	0.10	0.15 to 0.05
	0.02	0.05 to 0.00
	-.005	0.00 to -0.01
	-.015	-0.01 to -0.02
	-.030	< -0.02

averaging period to overcome the random scattering. The wind and mixing height data in the time series file are based on median values. If all values contribute to the concentrations in a linear fashion, and if the distribution of values is symmetric about the median, then median values should have limited systematic errors and provide adequate long-term averages. However, if there are critical threshold values, then problems may possibly arise. For example, if the plume rise is sufficiently large to take the plume just above the median mixing height, then adoption of a median mixing height would predict GLC values of zero. If actual mixing height values are larger than the median value, the plume can be trapped leading to non-zero GLC values.

The evaluation of a case study requires more accurate data since individual, hourly averaged values are often of concern. Since a receptor is often specified, the evaluation is clearly wind direction dependent; a difference of a few degrees can lead either to the prediction or the absence of a particular event. The mixing heights presented in the time series file are seasonal median values, the use of which, for a particular case study, would have limitations.

The data in the time series file should be useful in model testing of typical GLC values for all types of dispersion conditions. For example, GLC values for afternoon convective mixing conditions should occur at approximately the same frequency if there are not systematic errors in the model or in the data base. Median values should be adequate to assess whether there are major systematic errors. The same median values should lead to high wind speed conditions at the same frequency as observed and permit further model testing.

There are certain limitations in the data, the importance of which can be assessed by comparing the scatter or uncertainty to typical discrete ranges selected by a user. The ranges given in Table 1 were used in this evaluation.

3.2 WIND DATA

The time series wind data were derived for an average plume height of 400 m. A power law relationship may be used to estimate the sensitivity of wind speed to the selected plume height. For neutral atmospheric conditions, a power law exponent of 0.14 indicates that a wind speed variation of ±4% is associated with a plume height variation of ±100 m. For stable conditions, a power law exponent of 0.3 indicates that the wind speed variation for the same plume height variation is ±8%. This type of variation indicates that the selection of a 400-m plume height is not a critical assumption.

Discussions concerning derived time series winds compare the derived values with the actual values given by the pibal observations, and compare the uncertainties to typical user defined wind dispersion classes.

3.2.1 Comparison Between Observed and Derived Wind

An indication of the uncertainty in deriving 400-m winds may be obtained by comparing derived 400-m winds with the observed 400-m pibal winds. The pibal winds involve a combined spatial and temporal averaging associated with the ascent of the pilot balloon. These wind estimates will be subject to the low frequency wind variability and so will scatter about the hourly averaged value. At present, the pibal winds are the only direct wind measurements at 400-m, and so must be used as the observed wind for verification of the derived 400-m winds.

Visual comparisons between derived and observed wind roses are presented in Figures 1 and 2. The derived wind roses were obtained by using the derived directional median values of the empirical power law exponents, P, and the turning angles, Q, discussed in Volume 2 of this report. The visual agreement between the winter wind roses is poor; the agreement is much better for spring, summer, and autumn.

A more detailed comparison between the observed and derived frequency of occurrence of wind for a given direction is presented in Table 2. For easterly wind directions ranging from NNE to S, the derived frequencies are, on the average, underestimated by a factor of about 1.8. For westerly winds ranging from SSW to WNW, the derived frequencies are, on the average, overestimated by a factor of about 1.2. For north-northwesterly and northerly winds, the derived winds are overestimated by a factor of 1.6.

Table 2. A comparison between observed and derived 400-m wind directions.

	Annual Percent Frequency of Occurrence		
Wind Direction	Observed	Derived	Observed
N	6.2	12.1	1.95
NNE	5.6	3.4	0.61
NE	2.9	2.1	0.72
ENE	1.7	0.5	0.29
E	3.0	0.6	0.20
ESE	3.2	2.4	0.75
SE	5.3	2.3	0.43
SSE	6.1	4.8	0.79
S	8.4	4.5	0.54
SSW	6.9	11.2	1.62
SW	8.3	8.5	1.02
WSW	11.8	12.7	1.08
W	13.7	16.3	1.19
WNW	8.2	9.4	1.15
NW	4.6	3.8	0.83
NNW	4.1	5.2	1.27

Thus, the use of the derived winds may underestimate the frequencies of occurrence of certain events to the west of a source and overestimate them to the south; there may also be a slight overestimation in the frequency of occurrence to the east of the source.

3.2.2 Correlation Coefficient Between Observed and Derived Winds

A correlation coefficient was evaluated to provide an indicator of the degree of agreement between the derived and observed winds (Leahey and Hansen 1980). The coefficient used is defined by

$$R^2 = 1 - \frac{\Sigma(N_o - N_p)^2}{\Sigma(N_o - \bar{N})^2} \qquad (1)$$

where N_o = number of observed data in each class

N_p = number of predicted data in each class

N = average number of data in each class given, by the total number of data divided by the number of wind classes in the wind rose. The number of wind classes has a value of 96 for this report.

The adopted correlation coefficient is a comparison with a random distribution. If the value of R^2 is close to zero, then there is no skill; if R^2 is close to unity, then there is good skill.

Three sets of P and Q values were assessed for each season. The first set consisted of 32 directional median values as presented in the circumpolar graphs (Figures 10, 11, 13, 14, 16, 17, 19 and 20 in Volume 2). The second set consisted of the seasonal median P and Q values for the sectors shown in the cumulative frequency diagrams (Figures 12, 15, 18 and 21 in Volume 2). The third set was obtained by adjusting the P and Q values for each sector until the value of R^2 was maximized. In the second and third sets, values of P and Q were assumed to vary linearly at the boundaries between sectors.

Table 3 presents the sets of P's and Q's obtained for each season by the minimization procedure. It also presents for comparison, the set of median values obtained from the cumulative frequency

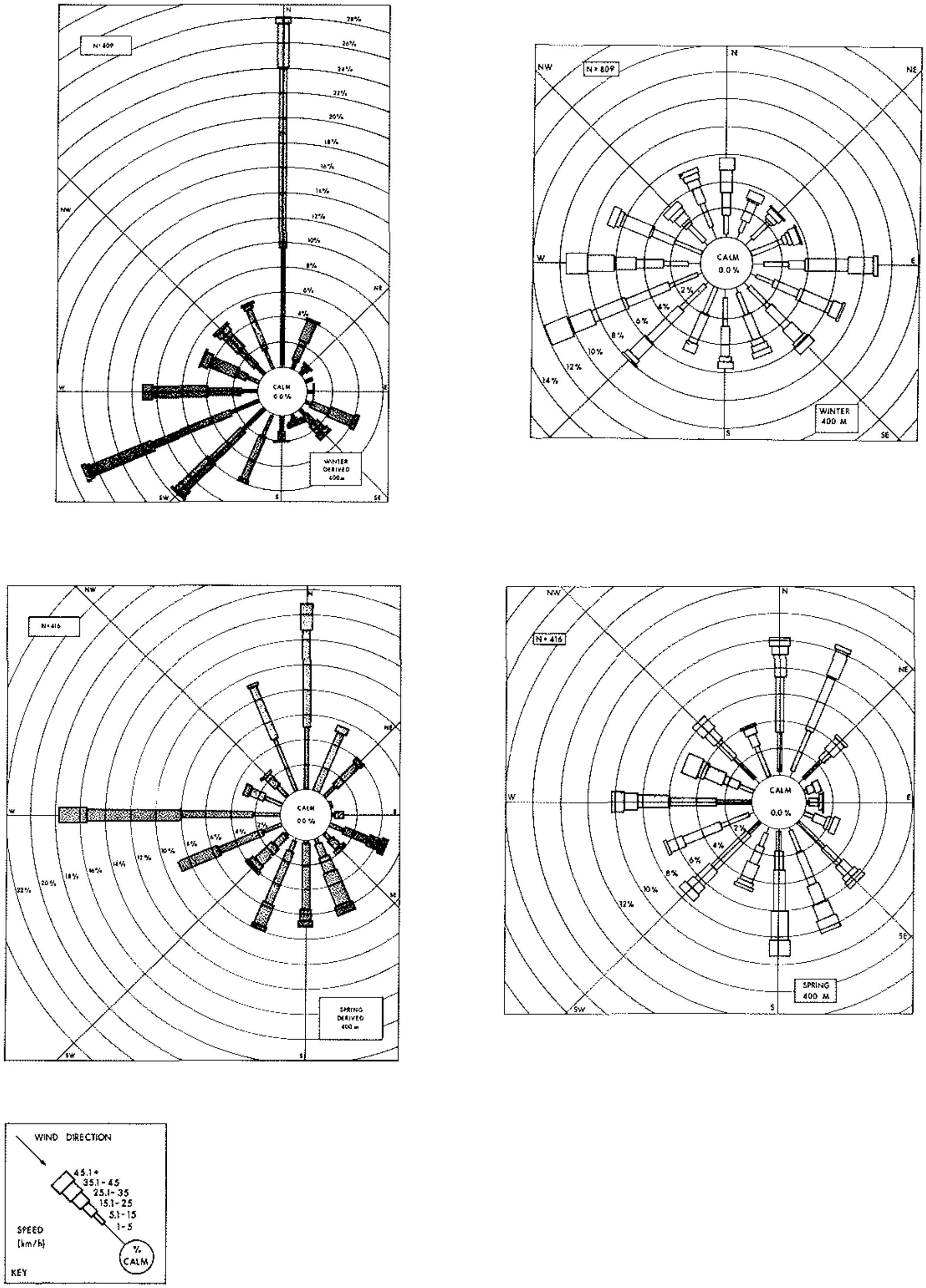

Figure 1. Comparison between observed and derived 400-m winds using median directional values of P and Q for winter and spring.

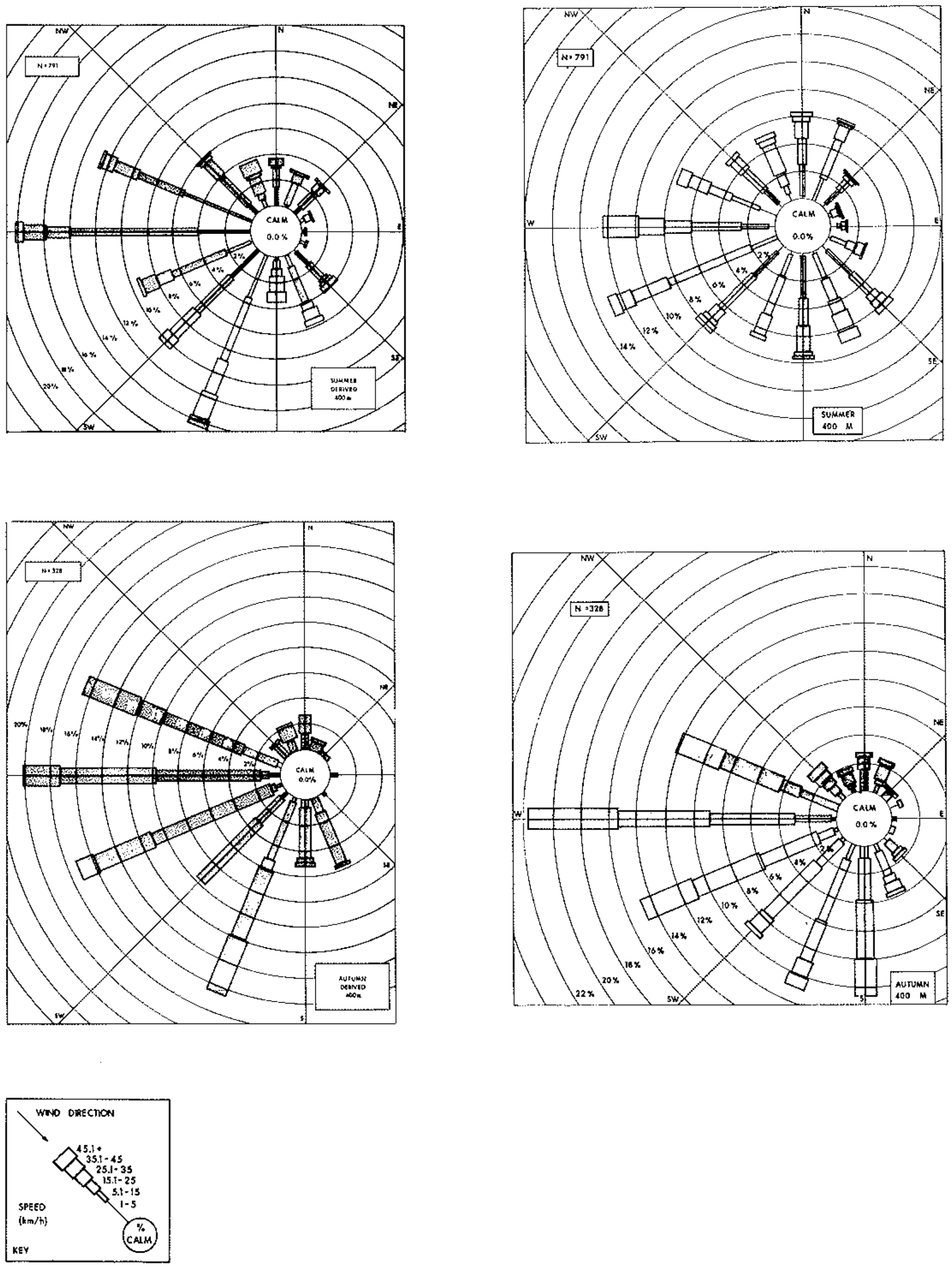

Figure 2. Comparison between observed and derived 400-m winds using median directional values of P and Q for summer and autumn.

Table 3. Seasonal values of P and Q for the indicated sector as derived from error minimization procedures. Median values of P and Q are also shown.

Season	Sector	n	Best Fit		Median Values	
			P	Q	P	Q
Winter	I NW NNE	296	0.35	-20	0.60	-30
	II NE ESE	28	-0.60	70	-0.35	60
	III SE WNW	485	0.00	35	0.25	25
Spring	I NW NNE	131	0.20	-25	0.15	-20
	II NE WNW	285	0.15	15	0.10	20
Summer	I NNW NE	94	-0.25	5	-0.20	0
	II ENE SE	68	-0.15	5	-0.10	0
	III SSE NW	629	0.05	25	0.00	20
Autumn	I NNW NE	21	0.00	0	0.00	5
	II ENE ESE	0	N/A	N/A	N/A	N/A
	III SE NW	307	0.00	25	0.00	20

diagrams; usually the two sets are similar, the exception being the P values during winter months.

Table 4 gives the number of data used for each seasonal wind rose, and correlation coefficients associated with each set of P's and Q's. The agreement between predicted and observed winter wind roses is poor; the agreement for the other seasons is better. It is of interest to note that the first set of P's and Q's containing 32 values usually resulted in larger standard errors than the use of the other two sets, which have fewer values of P and Q. The best correlation between predicted and observed wind roses occurs in the autumn where only three parameters are used.

Figures 3 and 4 show a comparison between the derived and observed wind roses using the best fit value of P and Q shown in Table 3. The main differences between these wind roses and those presented in Figures 1 and 2 can be noted in winter and summer. During the winter, the use of the best fit values distributes the derived north winds equally between north and north-northeast directions. In the summer, the best fit values shift the southerly winds to south-southwest.

3.2.3 Comparison with the Discretizations of the Wind Classes

An analysis of the cumulative probability distribution diagrams presented in Volume 2 of this report can be used to provide an indication of the effects of scatter in the values of P and Q on the selection of typical user-defined wind dispersion classes presented in Table 1.

The cumulative probability distributions derived for Q values were used to determine the fraction of the time the winds were within the same direction sector and within ± 1 wind direction sectors. Table 5 presents the results for both an 8- and a 16-point wind direction compass. On the average, for an 8-point compass, the wind directions should be within the same sector 46% of the time and within ± 1 sector 81% of the time. For a 16-point compass, the correct wind should be within the same sector 25% of the time and within ± 1 sector 58% of the time. These figures indicate that the wider the

Table 4. Statistics related to the comparison of observed and predicted wind roses.

Season	Number of Data	R^2_a	R^2_b	R^2_c
Winter	809	-3.2	-2.7	-1.7
Spring	416	-0.7	-0.4	-0.2
Summer	791	-0.2	-0.4	0.3
Autumn	328	0.3	0.2	0.4

Subscript notes:

a. prediction using directional median values

b. prediction using sector median values

c. prediction using sector best fit values

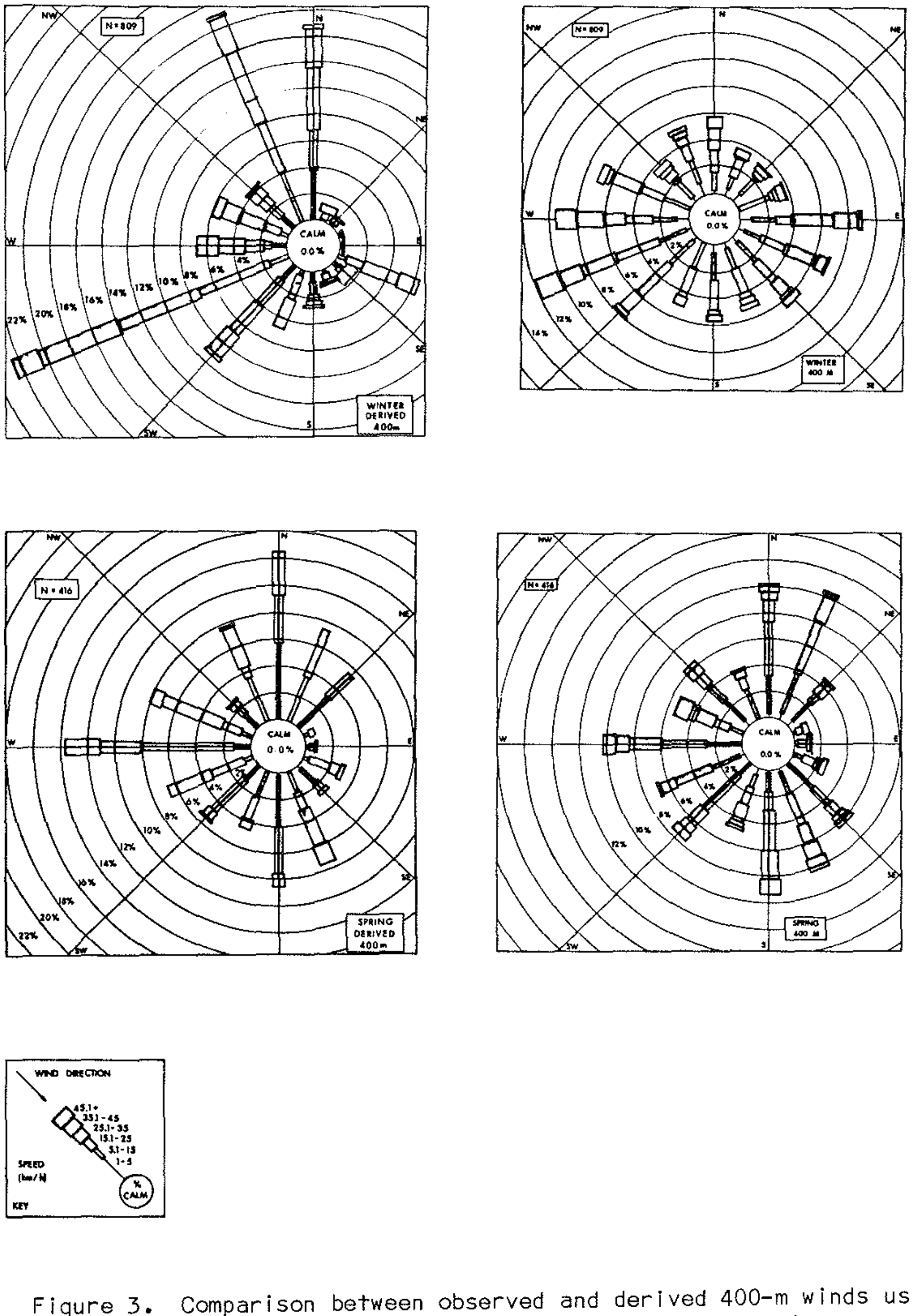

Figure 3. Comparison between observed and derived 400-m winds using best fit values of P and Q for winter and spring.

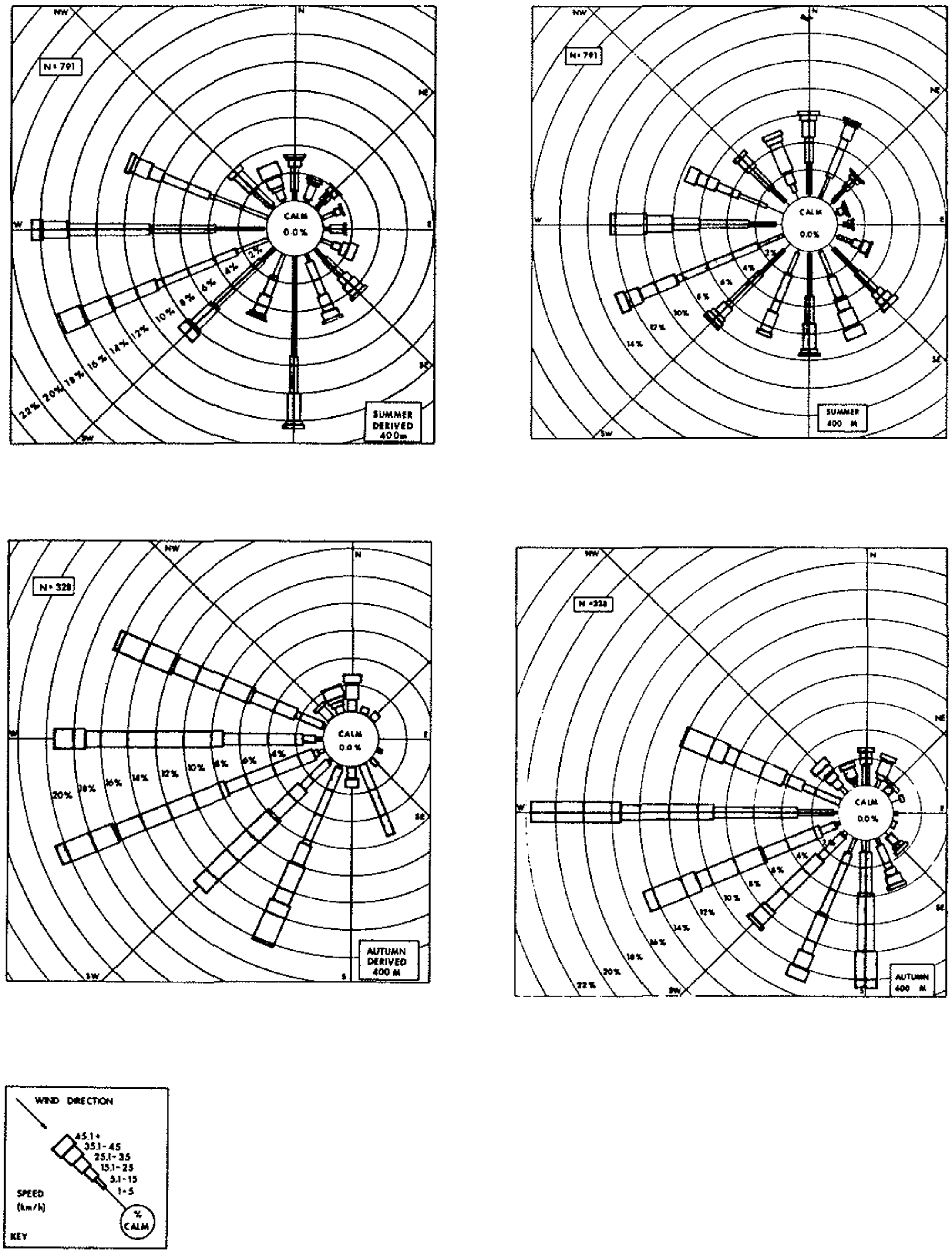

Figure 4. Comparison between observed and derived 400-m winds using best fit values of P and Q for summer and autumn.

Table 5. Percent of time that derived winds are within the same wind direction sector and within ±1 sector.

Season	Sector	8-Point Compass [a]		16-Point Compass [b]	
		Same	±1	Same	±1
Winter	I	15	48	6	22
	II	50	90	20	69
	III	50	78	20	55
Spring	I	40	84	20	53
	II	42	80	20	51
Summer	I	62	90	38	74
	II	33	83	11	48
	III	38	80	20	51
Autumn	I	65	83	45	74
	II	-	-	-	-
	III	65	94	45	80
Average		46	81	25	58

a. The 8-point compass direction sectors are 45° in width. A random wind direction would be in the same sector 13% of the time and within ± sector 38% of the time.

b. The 16-point compass direction sectors are 22.5° in width. A random wind would be in the same sector 6% of the time, and within ± sector 19% of the time.

direction sector, then the greater the probability of the derived 400 m winds being in the correct sector. The use of an 8-point compass is comparable to the uncertainty in the data base.

The wind speed class boundaries given in Table I range from about 75 to 125% of the middle value assumed in the dispersion calculations. This 25% variation corresponds to ranges in the wind speed power law profile of (Pm - 0.20) to (Pm + 0.26), where Pm is the median value given in the cumulative probability distribution diagrams presented in Volume 2. These diagrams were analyzed to determine how frequently the power law exponent fell within this range. The results are presented in Table 6. The table indicates that, on the average, the derived 400-m winds should be within ±25% of the actual 400-m winds about 40% of the time. About 60% of the time, the uncertainty in the wind speed can cause a shift from one wind speed class to another.

3.3 MIXING HEIGHTS

Typical user-selected mixing heights have a range of ±100 m for the classes less than 1000 m. Mixing depths greater than 1000 m are grouped into one class. An evaluation of the mixing height data frequency distribution was used to determine the frequency with which observed values less than 1000 m were within ±100 m of the time series values. For all observed time series values greater than 1000 m, perfect agreement was assumed. On the average, about 29% of the observed values were found to agree with the time series values.

During the winter, when the time series values were less than 400 m, the agreement between the time series values and the observed values was 45%. During the summer, when some time series values were found equal to 1,000 m, the agreement was 32%. The agreement during the spring and autumn was found to be about 23%.

The time series values are based on seasonal median values, and the same diurnal variation was assumed for each season. The values given in the time series can be useful for the estimation of long-term averages, but may be limited in their usefulness in examining case studies.

Table 6. Percent of time that wind speed is within ±25% of the median value[a].

Season	Sector	Percent
Winter	I	38
	II	56
	III	30
Spring	I	20
	II	36
Summer	I	40
	II	35
	III	40
Autumn	I	42
	II	-
	III	62
Average		40

[a] Corresponds to percent of time that exponent value in power law profile is within (Pm - 0.20) and (Pm + 0.26), where Pm is the median value.

3.4. HEAT FLUX

The heat flux values are used to help define turbulence classes and are derived from the net radiation values in the time series file. The determination of net radiation values are based on astronomical geometry and empirical formulations, evaluated using data processed by Kumar (1978).

Since the heat flux values are determined indirectly, the assessment of their accuracy is discussed in the section on model sensitivity.

3.5 SUMMARY

The use of the derived 400 m winds can lead to certain directional biasing. This conclusion was based on comparing the derived wind data with the observed pibal data, and may not provide a complete indication of any uncertainties due to the instantaneous nature of the pibal data. The scatter in the derived wind directions appears to be comparable to the use of 8-point compass wind directions. For a 16-point compass, the uncertainty is increased.

About 40% of the time, the derived winds should be within typical user-selected wind speed classes; about 60% of the time, the uncertainty in the wind speed can cause the wind to shift by one or more wind speed classes.

About 29% of the time, actual mixing heights were found to be within the limits of the median values specified by a typical user. This implies that, for case studies, the mixing height values may be of limited use.

Both the derived winds and mixing heights showed considerable uncertainties. At the present stage of the model and data base development, it was decided to examine model sensitivities before assessing where priority should be given for data base improvements.

4. SENSITIVITY STUDIES

4.1 OVERVIEW OF SENSITIVITY STUDIES

Sensitivity studies consist of assessing the amount of change in the results of a model to changes of user-supplied input or to changes of the internal model formulations. Sensitivity studies have several important functions. They can clarify the interactions of various components and formulations within a model system. They can quantify uncertainties in the model output due to assumptions, empirical parameters or input data. Perhaps most importantly, they can lead to an evaluation of limiting errors and so establish priorities for future efforts to improve model predictions.

In the present study, sensitivity studies were performed for both the model itself and the final model predictions. The sensitivity studies on the model consisted of examining the size of variations of various performance indicators when selected parameters were varied. The indicators printed by GLCGEN included intermediate values of stability parameters and computed wind fluctuations as well as ground level concentrations. This type of sensitivity study leads to evaluations of the relative importance of uncertainties in a variety of parameters or input data. The sensitivity studies in the whole model/data bank system involved comparisons of concentration predictions with observed values when a real-time series of meteorological data was utilized.

Selecting the most relevant sensitivity studies to perform and to present is often difficult. The procedure adopted in this program was to test parameters in the formulation that would tend to have a significant effect or to test parameters whose value were poorly known. The sensitivity to major input data was also undertaken to assess the importance of input uncertainties to the various levels of results. In the following sections, the sensitivity studies involving the dispersion formulation in GLCGEN are presented first; then the integrated system of model and data base is examined.

4.2 SECTOR-AVERAGING

4.2.1 Characteristics and Limitations of Sector-Averaging

Sector-averaging is a calculational technique used to generate smooth concentrations across the discretized angular sectors used for analysis in GLCGEN. It changes a Gaussian distribution along a single centre-line into a rectangular distribution across a calculational sector. As discussed in Volume I, averaging over wider sectors permits the use of a relatively small time series data base to generate GLC values which can more closely approximate results for longer time series undergoing similar sector-averaging. However, sector-averaging implicitly involves enhanced lateral dispersion. With sector-averaging applied to one particular episode, the model may predict lower GLC values but spread over a wider region than observed. The magnitude of the effect of this implicit lateral dispersion will depend upon the angular width of the sectors, the ambient lateral dispersion and the downwind distance from source. At long downwind distances when vertical mixing is complete (e.g., in a limited convective mixing situation), the centre-line concentration from the model will vary approximately as $X^{-1/2}$, due to lateral dispersion. The sector averaged concentration will vary approximately as X^{-1}. As discussed in Volume I, low frequency wind direction changes can, in some circumstances, smooth out the centre-line GLC values in a manner analogous to sector-averaging. Thus, the observed GLC values, when averaged over several hours, may range from the centerline GLC value to one similar to a sector-averaged value depending upon the magnitude of the low frequency wind direction changes.

Sector-averaging has two major approximations: (1) the GLC values for an episode are approximated by a rectangular distribution rather than a Gaussian distribution; and, (2) the width of the distribution is approximated by the sector width at any given downwind distance.

The use of a rectangular distribution will change the frequency distribution of GLC values. The peak values will be underestimated by an amount depending upon the adopted width of the plume. There will also be a reduced number of occurrences of the very low concentrations associated with the edges of the plume. For verification purposes, the truncation of low-level GLC values, due to the signal-to-noise ratio of the monitoring sensors, will generally be an equally serious problem; the limited number of monitoring stations will tend to result in the maximum GLC value also being missed. For the assessment of possible environmental impact, the meandering of the wind direction will tend to smooth out the average GLC values. The missing low-level values will probably be an acceptable approximation, povided that the total deposition is consistent. Thus, the adoption of a rectangualr distribution does not appear to be a major problem for either verification or environmental assessment applications, provided that a realistic plume width is adopted.

The adopted width of the distribution in sector-averaging may not be a good approximation for some of the model applications. The width of the rectangular distribution for the plume is determined by the selection of an 8- or 16-point compass. The width scales linearly with downwind distance from each source. For long-term averages, this approximation is acceptable; however, the frequency distribution may be sufficiently modified to cause problems in the assessment of maximum GLC values, particularly at larger downwind distances.

4.2.2 Possible Alternatives to Sector-Averaging

There are several alternatives to sector averaging, three of which are discussed below, which would not require major model changes.

The width of the rectangular distribution would be linked to the plume sigma-y which is already available in the model. Fractional occurrences defined by the ratio of plume width to sector width would then be used to maintain mass continuity. For frequency distribution, the number of occurrences would be a floating point number, rather than an integer; otherwise, no changes are necessary. For the generation of a time series, the fractional occurrences at each receptor would be integrated until they exceeded unity. At that time, an event would be said to occur and the integral of fractional occurrences would be reduced by one. For a sufficiently long time series, there should be no correlation between the magnitude of the GLC value and the timing of the fractional occurrences exceeding unity (prompting an event to be allocated). The use of plume widths and fractional occurrences would entail the storage of a plume width value along with the GLC value in the large matrix of GLC values generated in GLCGEN. Also, a storage array would be needed in FRQDTN for accumulated fractional occurrences for each receptor.

Another alternative to sector-averaging involves using a random number generator to give a specific wind direction within a sector. A random number between 0 and 1 would be multiplied by the sector angular width to generate a wind direction movement from a sector boundary. A Gaussian formulation could be used by applying the lateral offset term in FRQDTN; the centre-line GLC and plume sigma-y would have to be stored in GLCGEN. This approach has the disadvantage that the use of 8- or 16-point compasses would still cause an arbitrariness unrelated to the time variance of the wind direction. Persistence within a sector would be ignored.

Using a Markov process for changes in wind direction could allow for persistence as well as yielding a more realistic frequency distribution. A random wind direction would be generated as above; however, the adopted wind direction would be a weighted average of this random direction in the sector and the adopted wind direction at the previous time in the time series. A Markov process introduces persistence in the form of an auto-correlation. The weighting coefficient can scale with the number of wind direction classes to remove the arbitrariness of the number of sectors. It can also vary with meteorological conditions and averaging time in order to match observable auto-correlation statistics. The Markov process technique should give realistic frequency distributions and also a time series which reflects the true persistence in the wind field.

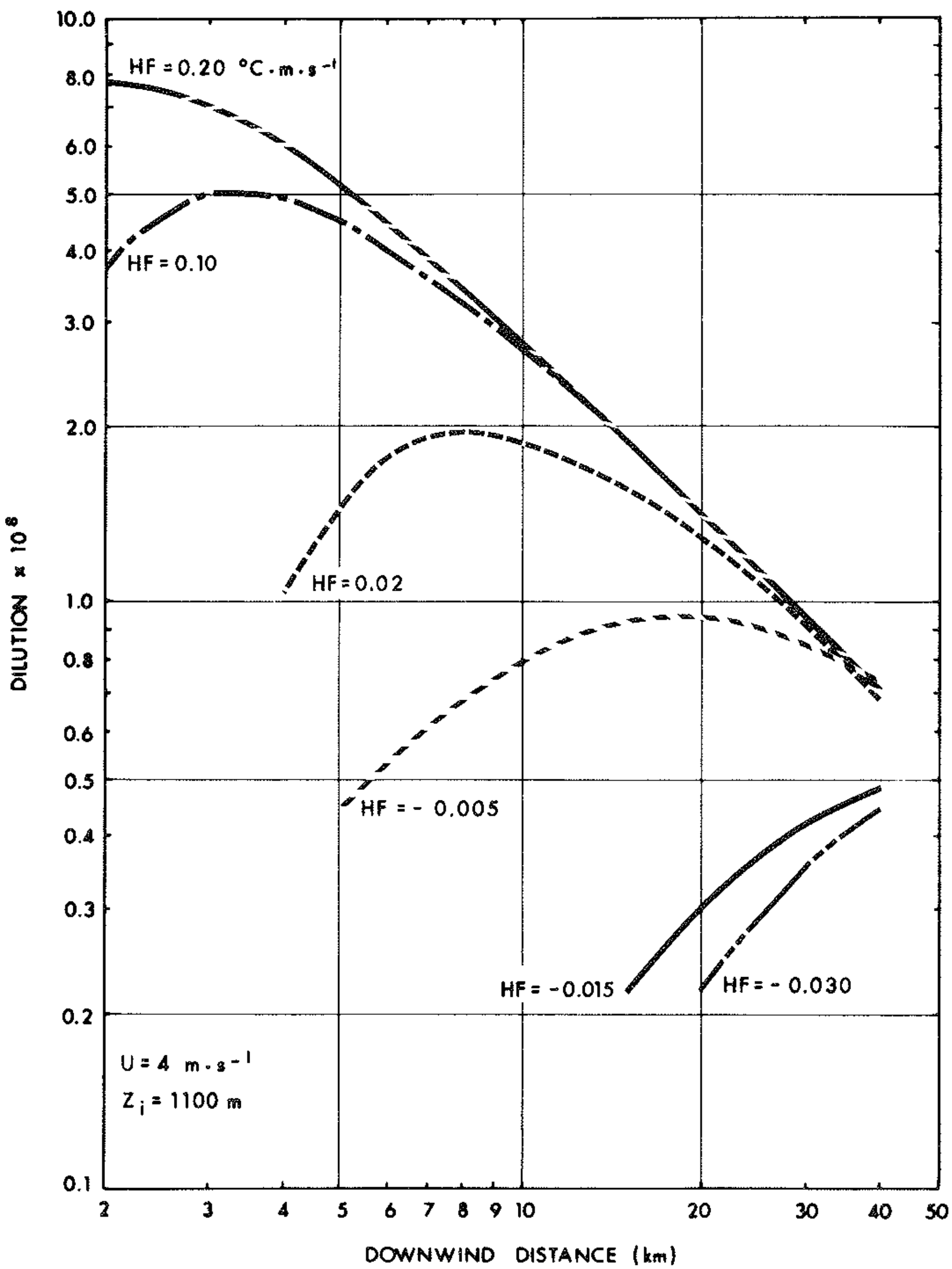

Figure 5. Sensitivity of sector-averaged GLC values (dilution) on heat flux for a wind speed of 4 m/s and a convective mixing height of 1100 m.

4.3 MODEL RESPONSE TO INPUT VARIABLES

The first stage in sensitivity studies was to examine how the model formulation responds to variations in the basic meteorological data. This study consisted of analyzing the GLC file for the basic run of GLCGEN by varying one parameter while keeping the others steady. This testing can be considered as "an algorithm" integrity check to ensure that the model behaves as expected. These studies also show the rate of change of the various intermediate parameters and the GLC values with changes of the primary input data. Results of these studies indicate the relative importance of uncertainties of the input data and clarify the interactions of the input data within the dispersion formulation. The source characteristics are those of the main Suncor powerhouse stock.

4.3.1 Effect of Heat Flux Variations on the GLC Values

The changes in GLC values (sector-averaged) resulting from changes in heat flux when wind speed and mixing height are held constant are shown in Figure 5. For U = 4 m/s, the GLC values decrease steadily with decreasing heat flux for downwind distances to 40 km. The centre-line GLC values are also shown in Figure 6 for purposes of comparison. In the absence of sector-averaging, the largest negative heat flux classes (i.e., stable) show the largest GLC values, which occur at more than 40 km downwind. These large values would be predicted to occur in steady conditions in the absence of any low-frequency meandering of the wind direction and in absence of any directional shear effects.

The interaction of several effects is shown in Figure 7 for the correponding GLC values for U = 6.5 m/s. For this larger wind speed, there are larger GLC values for moderate negative heat fluxes than for slightly negative heat fluxes. The σ_E values are less for the moderate negative heat fluxes; however, the plume rise is also less, due to the larger temperature gradient that can exist in more thermally stable conditions. As outlined in Volume I, both σ_E and $\partial\theta / \partial z$ will scale to powers of the stability parameter, μ_*. For U = 6.5 m/s, the ratio of plume rise to stack height and the range of

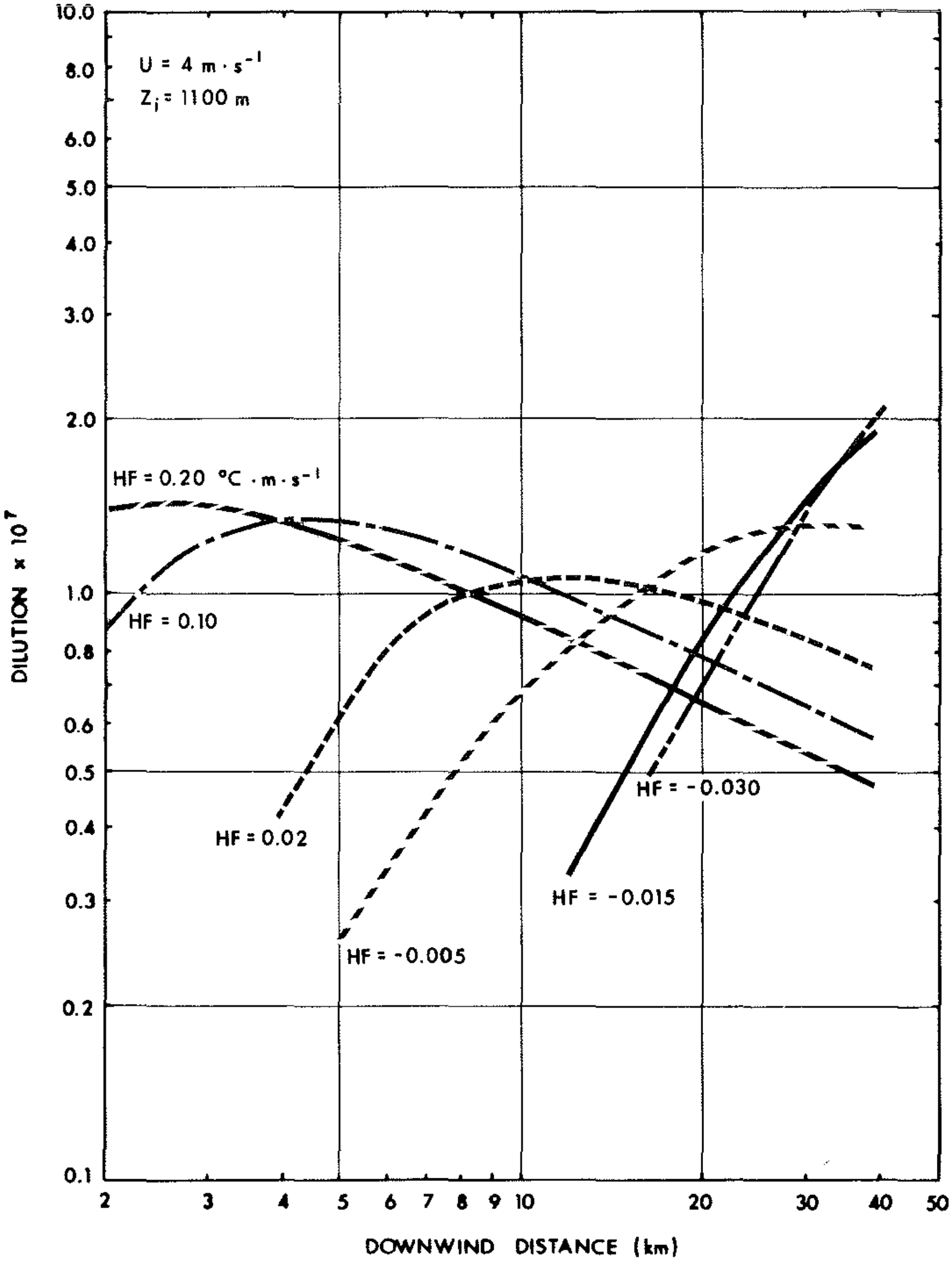

Figure 6. Sensitivity of plume centre-line GLC values (dilution) on heat flux for a wind speed of 4 m/s and a convective mixing height of 1100 m.

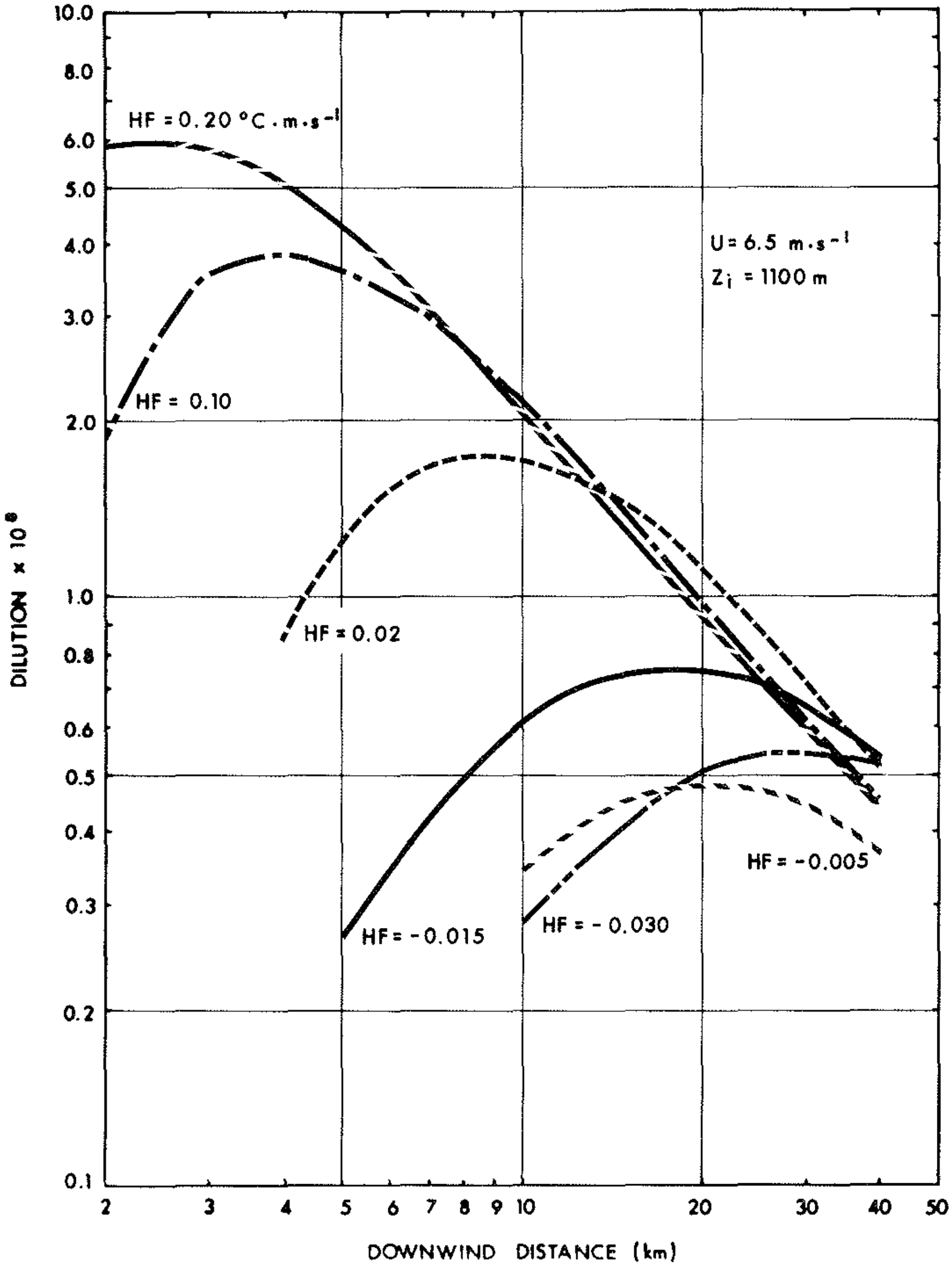

Figure 7. Sensitivity of sector-averaged GLC values (dilution) on heat flux for a wind speed of 6.5 m/s and a convective mixing height of 1100 m.

μ_* is such that the plume rise change is more important than the σ_E change, (σ_E approaching its neutral limit). There is little difference (<3%) in the GLC values for slightly and moderately negative heat fluxes. This small difference is due to the dominance of mechanical turbulent effects over stability effects for both σ_E and plume rise.

4.3.2 Effect of Wind Speed Variations on the GLC Values

The wind speed affects both the plume rise and dispersion, except in convectively dominated situations where $\sigma_w \propto w_*$, where σ_w is the standard deviation of the vertical velocity fluctuations. Thus, the rate of downwind mixing is not a function of wind speed for these unstable conditions. As the wind speed increases, the mixing becomes mechanically dominated and σ_w varies linearly with u. These effects are shown in Figure 8, where the differences between U = 6.5 and U = 10 m/s are relatively small. At even greater wind speeds, the total plume rise becomes dominated by the physical stack height and so the increased mixing gives rise to larger maximum concentrations closer to the source.

4.3.3 Effect of Mixing Height Variations on the GLC Values

Mixing height, Z_i, is utilized in the dispersion formulation only for convective conditions. The scaling velocity for unstable conditions, w_* , is defined as

$$w_* = (g\overline{w\theta}Z_i/T)^{1/3} \qquad (2)$$

Thus, the amount of mixing as described by σ_E and σ_A will scale with $Z_i^{1/3}$.

The model also adopts the approximation that if the total plume rise exceeds the mixing height class boundary by more than 100 m, the plume is ignored.

The model has a "reflective" upper boundary at the mixing height. Thus, if the plume rise is just within the upper boundary defined by the Z_i class boundary, then the maximum GLC values can be

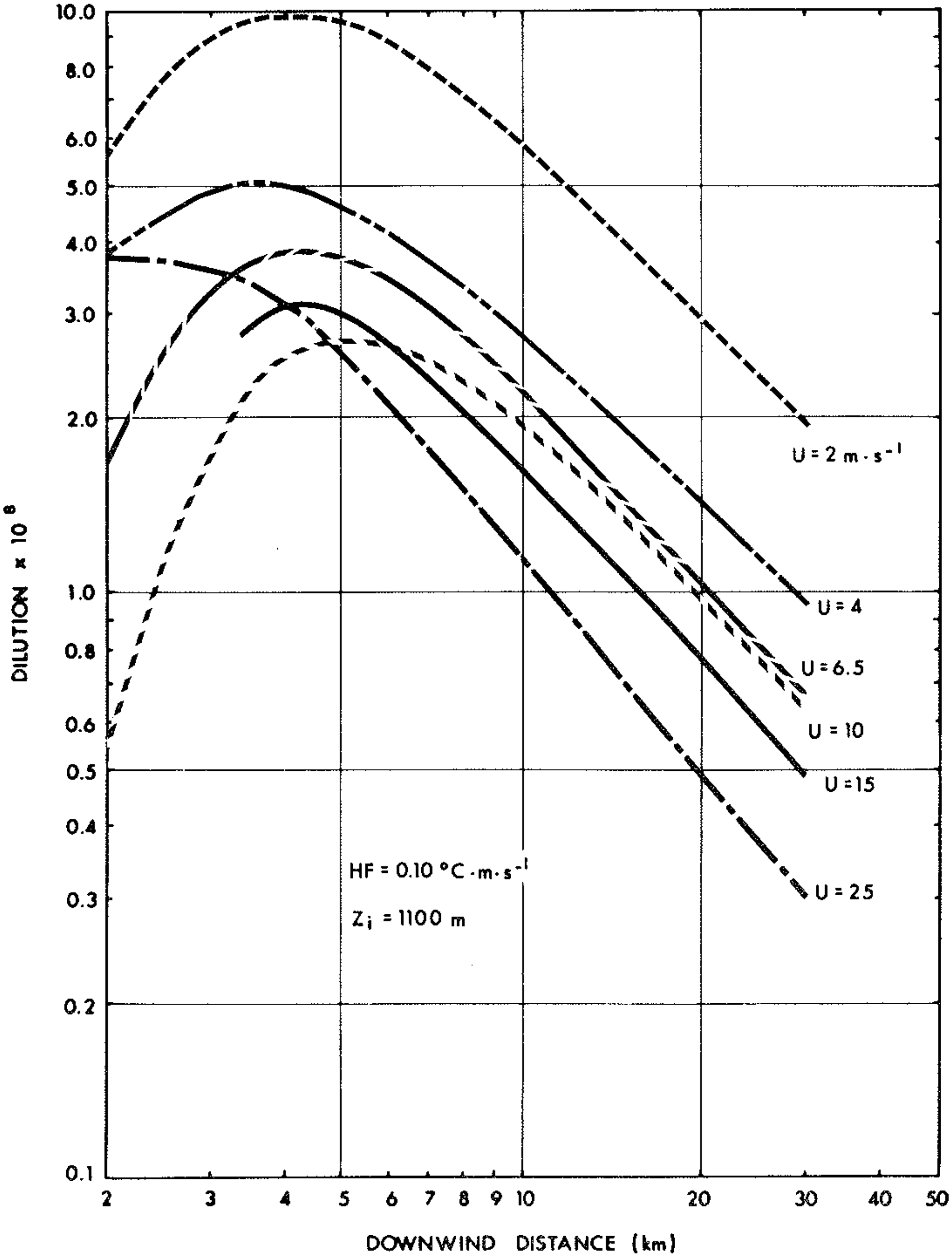

Figure 8. Sensitivity of sector-averaged GLC values (dilution) on convective wind speed for a heat flux of 0.10°C·m/s and a convective mixing height of 1100 m.

significantly increased. Note, however, that because vertical mixing also scales with Z_i, the increased GLC values are not twice the values for unlimited mixing except at downwind distances greater than about 10 km. Examples of the net result of these two effects are shown in Figures 9 and 10.

The combined effects of Z_i upon the volume available for dilution and upon the rate of mixing have a significant impact upon the interpretation of air quality data from some of the monitoring sites. Note that at a downwind distance of about 4 to 5 km (the approximate distance of the monitors Mannix and Fina from the Suncor main stack), there is very little dependence of GLC upon mixing height. Thus, sensitivity studies of the ratio of observed to predicted GLC values to variations in Z_i will show little sensitivity, except for the effect of the plume rising above the mixing height and hence being excluded from the calculation.

4.4 MODEL RESPONSE TO SELECTED MODEL PARAMETERS

Within the model formulations, many parameters were utilized and assigned best-estimate values. The rationale and data base for the parameter values were discussed in Volume I. The following sections examine the sensitivity of model predictions for selected parameters which have both significant uncertainty in value and major impact upon the GLC values.

4.4.1 Neutral Plume Rise Coefficient, C_l

The specification of plume rise has received considerable attention in the last few years (Briggs 1975; Slawson et al. 1980; Djurfors and Netterville 1980). The formulation recommended by Briggs (1975) for neutral conditions was adopted in the present model. The plume height, HP, becomes

$$HP = HS + C_l F^{1/3} X_f^{2/3} U^{-1} \qquad (3)$$

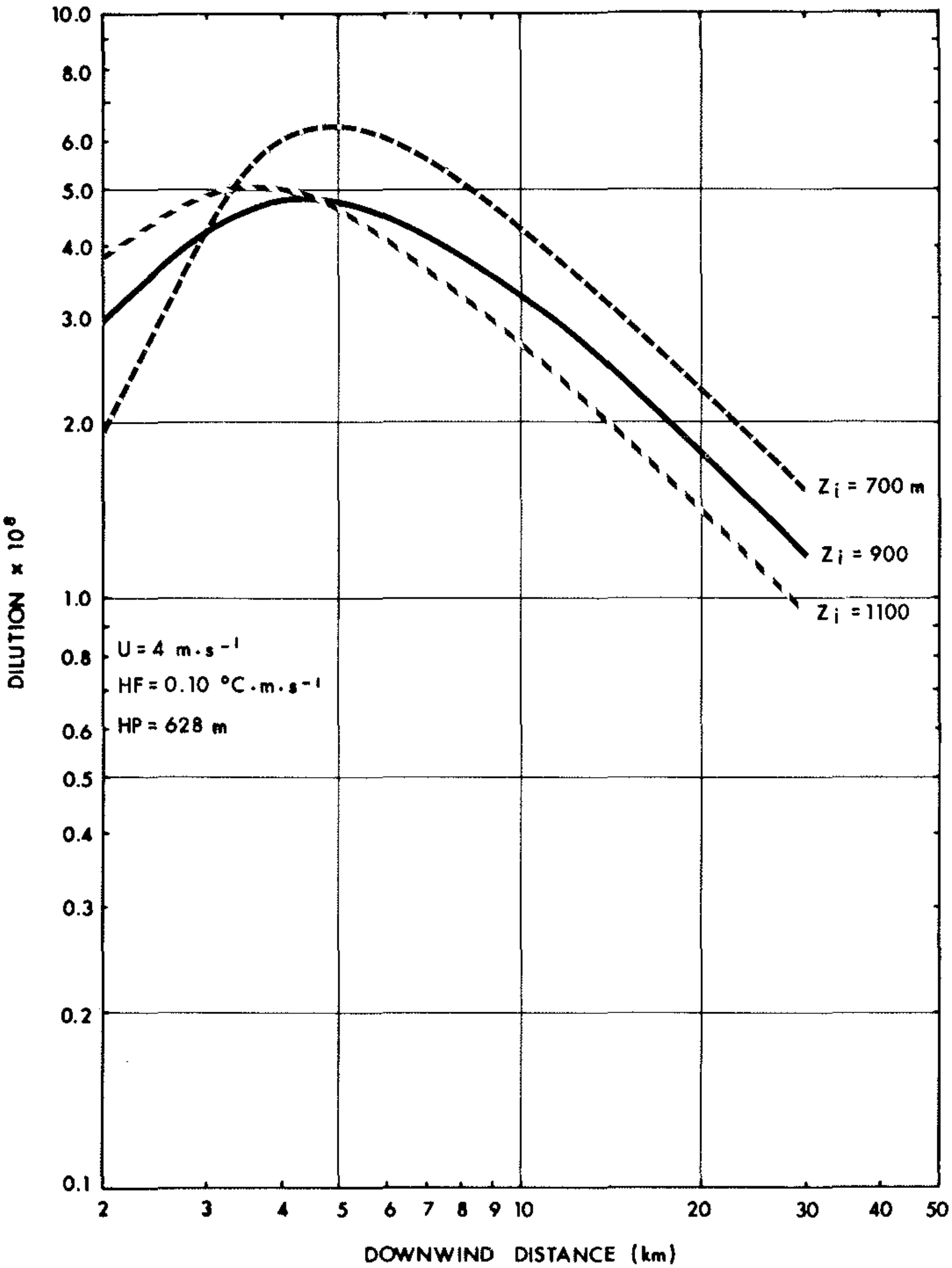

Figure 9. Sensitivity of sector-averaged GLC values (dilution) on convective mixing height for a wind speed of 4 m/s, a heat flux of 0.10°C·m/s and a plume height of 628 m.

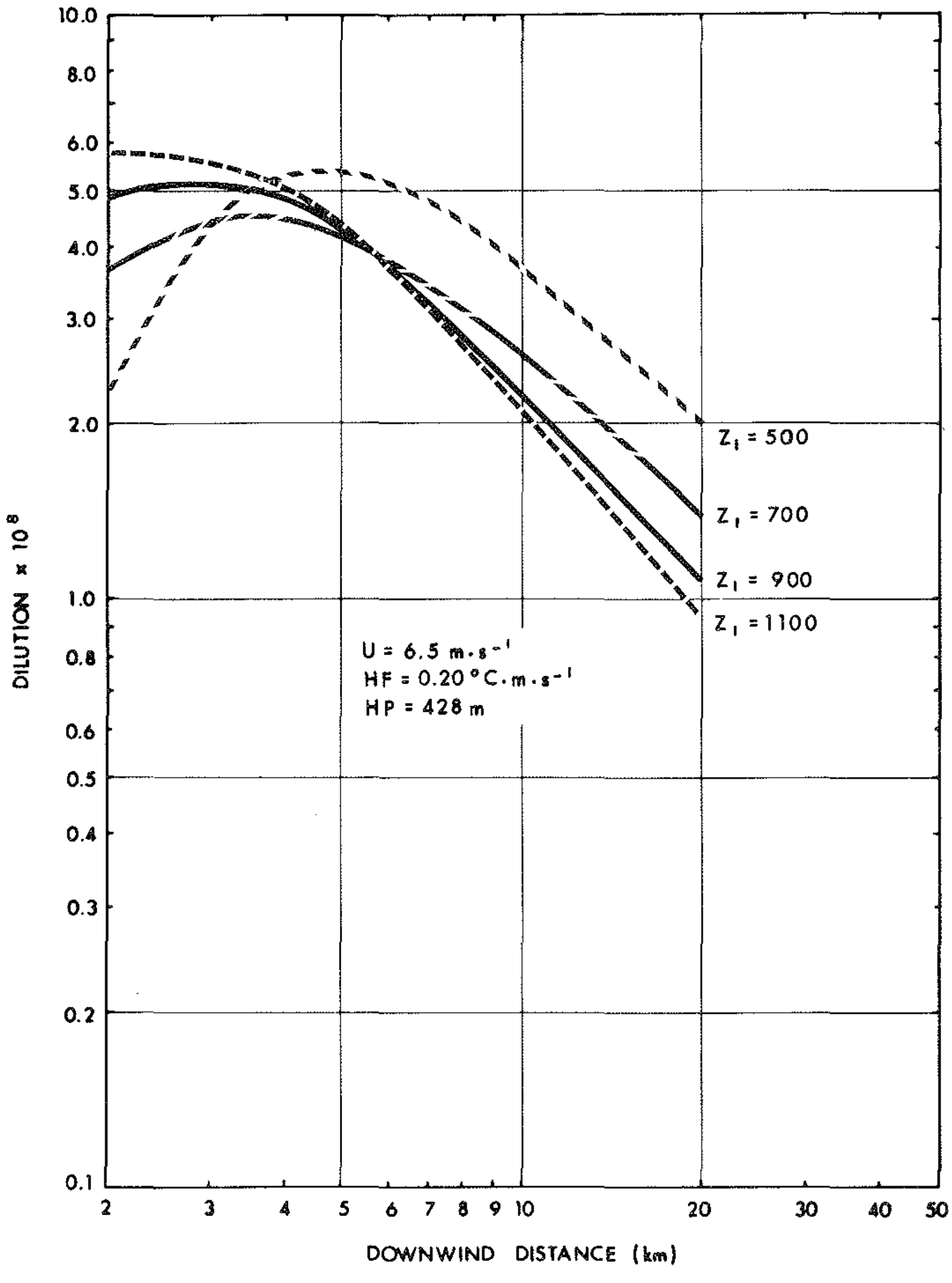

Figure 10. Sensitivity of sector-averaged GLC values (dilution) on convective mixing height for a wind speed of 6.5 m/s, a heat flux of 0.20°C·m/s and a plume height of 428 m.

where: HS = the physical stack height

F = the stack buoyancy parameter

u = the wind speed

X_f = the downwind distance for final plume rise, and

C_l = the neutral plume rise coefficient.

The details of the formulation were presented in Volume I. Briggs (1975) recommended a value of C_l = 1.6 based upon a survey of available observations. Davison and Leavitt (1979) reviewed observations taken as part of AOSERP sponsored studies and concluded that C_l = 1.4 gave better agreement. It was noted, however, that the observations may be subject to significant measurement uncertainties.

The variation of sector-averaged GLC values for C_l values of 1.4 and 1.6 are presented in Figures 11 and 12, for a source with the physical characteristic of the Suncor main stack. Comparisons of the change with both wind speed and heat flux changes are included to indicate the relative importance of the effect. Within the region of 4 to 10 km from the source, a change of C_l from 1.4 to 1.6 decreases the maximum GLC by about 25%, and moves the maximum about 1.5 km farther from the source. In this range, the change is roughly equivalent to a wind speed change from 6.5 to 10 m/s; however, the change in C_l is only about 20% as important as a wind speed change from 6.5 to 4 m/s. At higher wind speeds, the contribution of the plume rise to the total plume height decreases; therefore, the effect of C_l variations becomes less important. The effect of a heat flux change from 0.1 to 0.2 °C m/s has an effect similar in magnitude, but opposite in sign, to the variation of C_l from 1.4 to 1.6 for downwind distances greater than about 4 km. The change, however, from moderately to slightly convective (0.10 to 0.02) is over a factor of two greater the C_l change. In convective conditions, the difference in sector-averaged GLC values becomes progressively smaller at larger downwind distances and is generally less than 10% beyond 10 km. The sensitivity of the GLC values to plume height is characteristic of all Gaussian models.

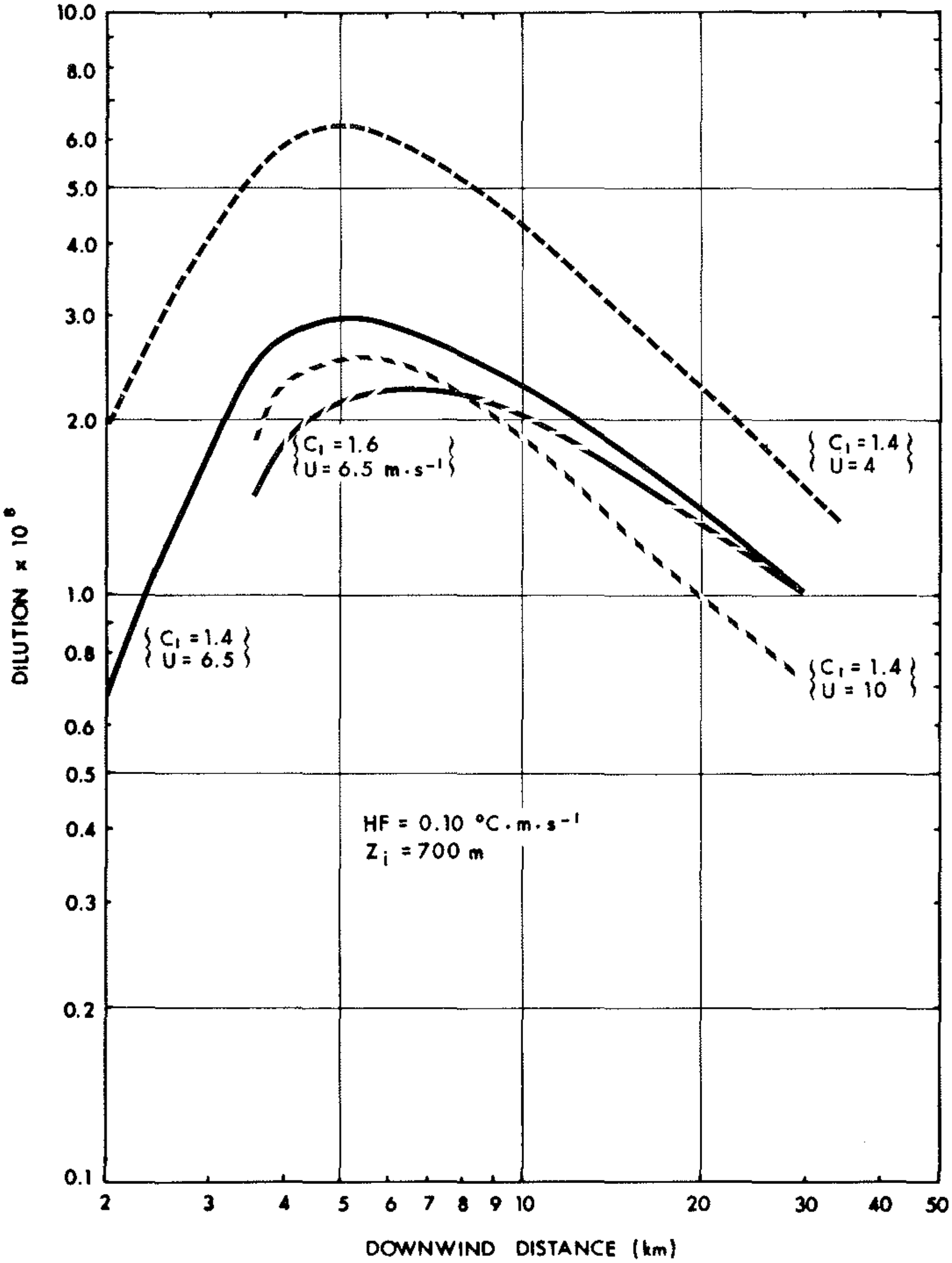

Figure 11. Sensitivity of sector-averaged GLC values (dilution) on the neutral plume rise coefficient, C_1, for a convective mixing height of 700 m and a heat flux of 0.10°C m/s.

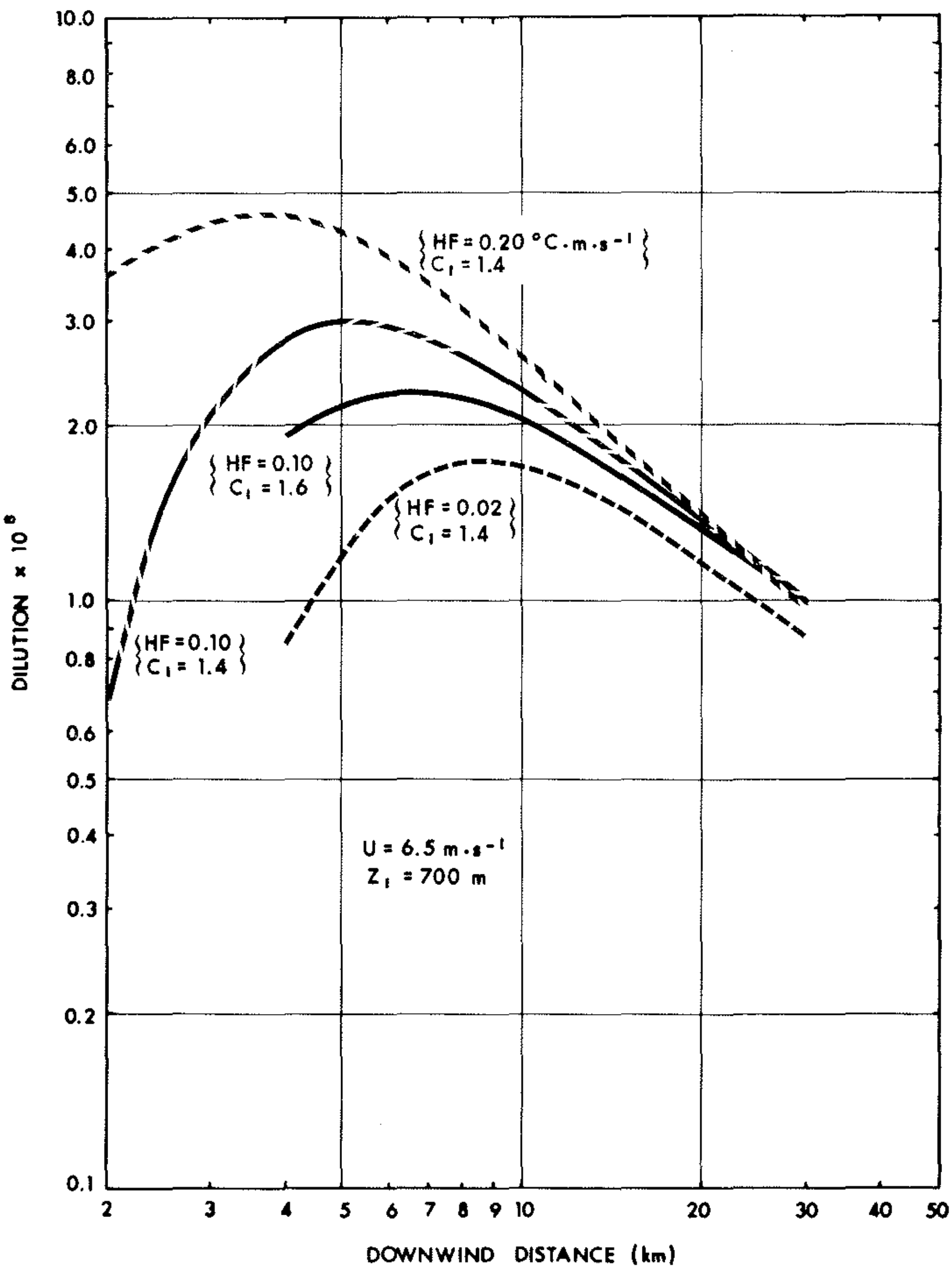

Figure 12. Sensitivity of sector-average GLC values (dilution) on the neutral plume rise coefficient, C_1, for a convective mixing height of 700 m and a wind speed of 6.5 m/s.

A variation of downwind distance for final plume rise, X_f, affects the GLC values exactly the same as a variation of C_1. The change of C_1 from 1.4 to 1.6 is equivalent to a change in X_f from 2,000 to about 2,400 m.

4.4.2 Stable Plume Rise Coefficient

The stable plume rise coefficient, C_2, appears in the stable plume rise formulation, following Briggs (1975)

$$HP = HS + C_2 \left(\frac{F}{US} \right)^{1/3} \qquad (4)$$

where S is a stability parameter, the square of the Brunt-Vaisalla frequency. The value of C_2 adopted in the model is 2.6 following Briggs (1975); however, the observational data quoted by Briggs indicated considerable scatter and so the value of C_2 must be considered as uncertain. In the model, the stable plume rise formulation is adopted whenever the transition distance calculated by the stable formulation is less than the transition distance calculated by the mechanical formulation. For the Suncor plume, the transition to mechanically controlled transition distance, and hence plume rise, occurs at about U = 10 m/s with a dependence on the magnitude of the negative heat flux.

The sector-averaged GLC values for C_2 values of 2.6 and 2.3 are compared in Figures 13, 14, and 15. A decrease in C_2 from a value of 2.6 to 2.3 increases the maximum sector-averaged GLC value by about 20 to 25% for moderate winds. At higher wind speeds (greater than about 10 m/s, the mechanical mixing becomes sufficiently large that the neutral plume rise formulation is adopted. The effects on the location and magnitude of the GLC values, due to variations in the heat flux and wind speed, vary markedly depending upon the absolute values of the wind and heat flux. In general, the heat flux and wind speed variations shown in Figure 13, 14, and 15 can lead to much more significant variations in the location and magnitude of the GLC values than the simulated C_2 variation.

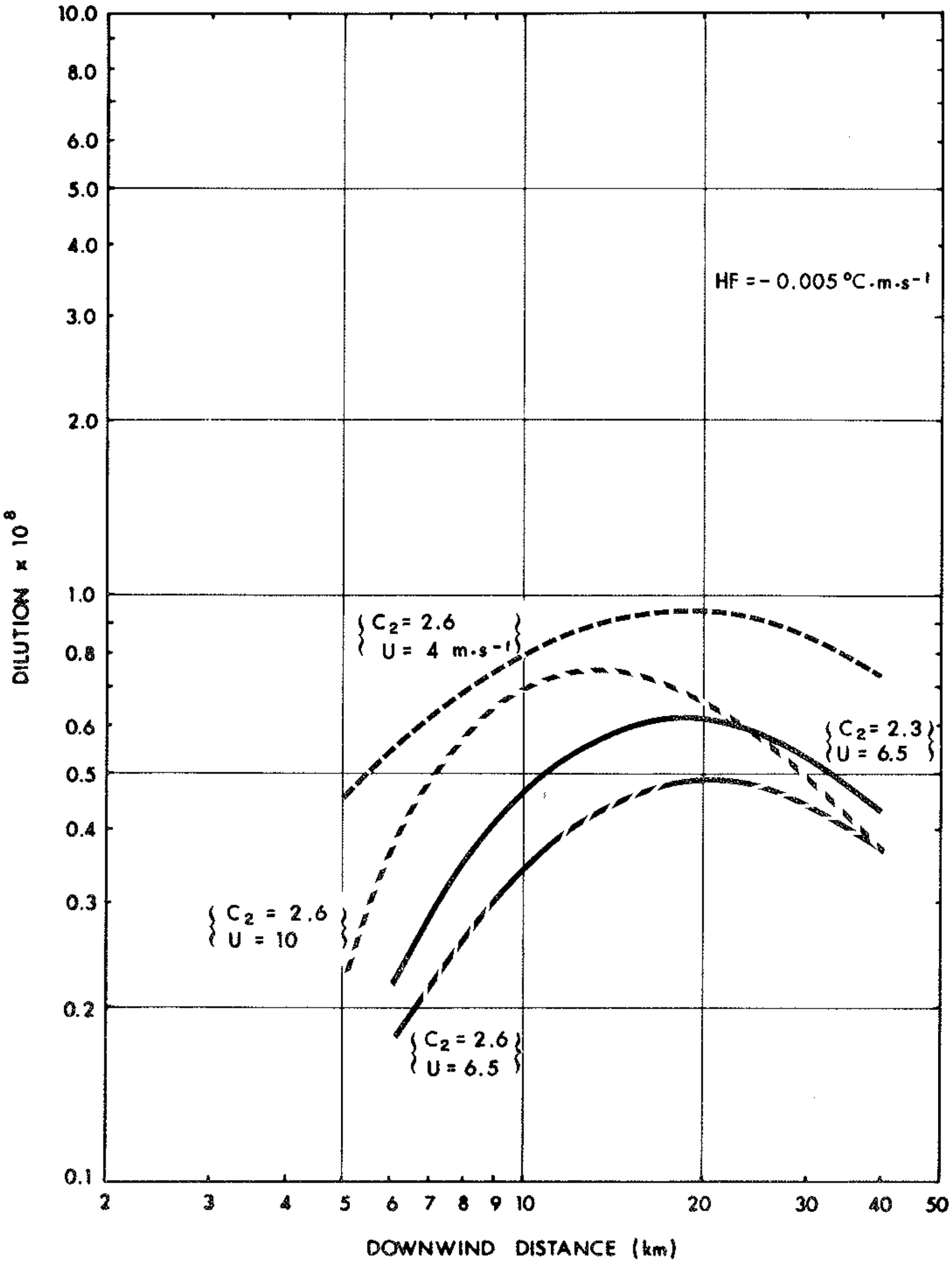

Figure 13. Sensitivity of sector-averaged GLC values (dilution) on the stable plume rise coefficient, C_2, for a heat flux of -0.005°C·m/s.

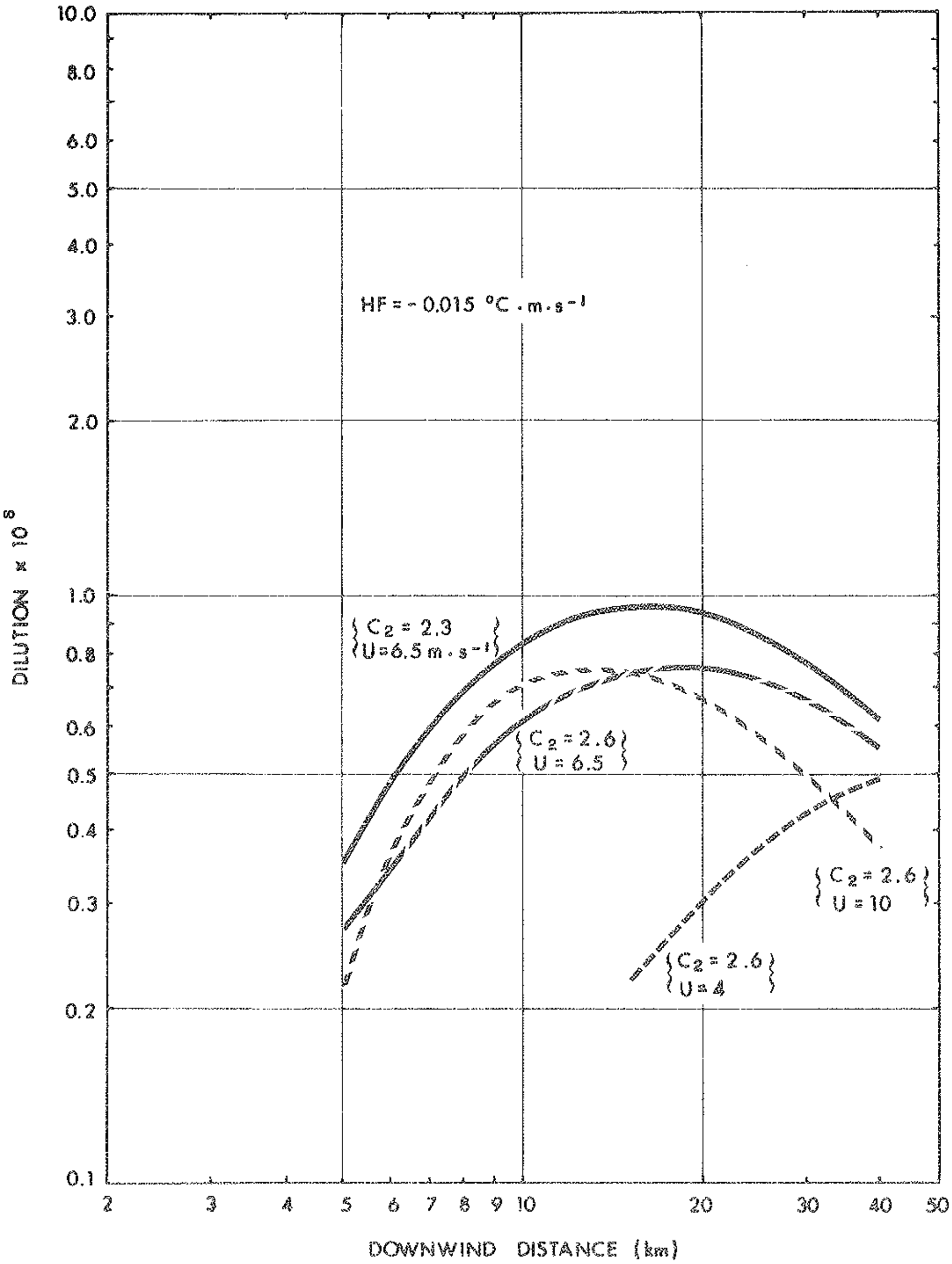

Figure 14. Sensitivity of sector-averaged GLC values (dilution) on the stable plume rise coefficient, C_2, for a heat flux of $-0.015°C \cdot m/s$.

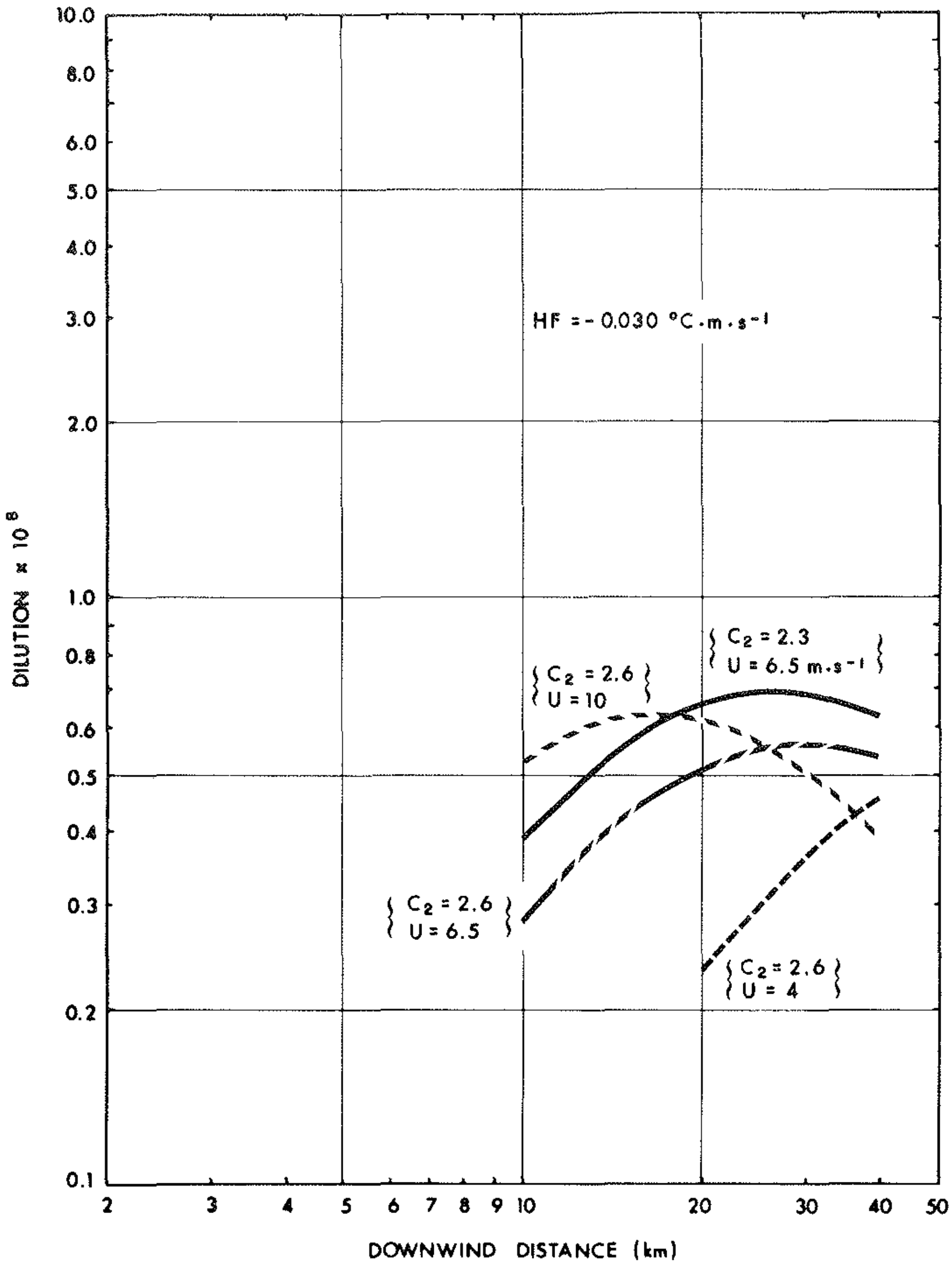

Figure 15. Sensitivity of sector-averaged GLC values (dilution) on the stable plume rise coefficient, C_2, for a heat flux of -0.030°C·m/s.

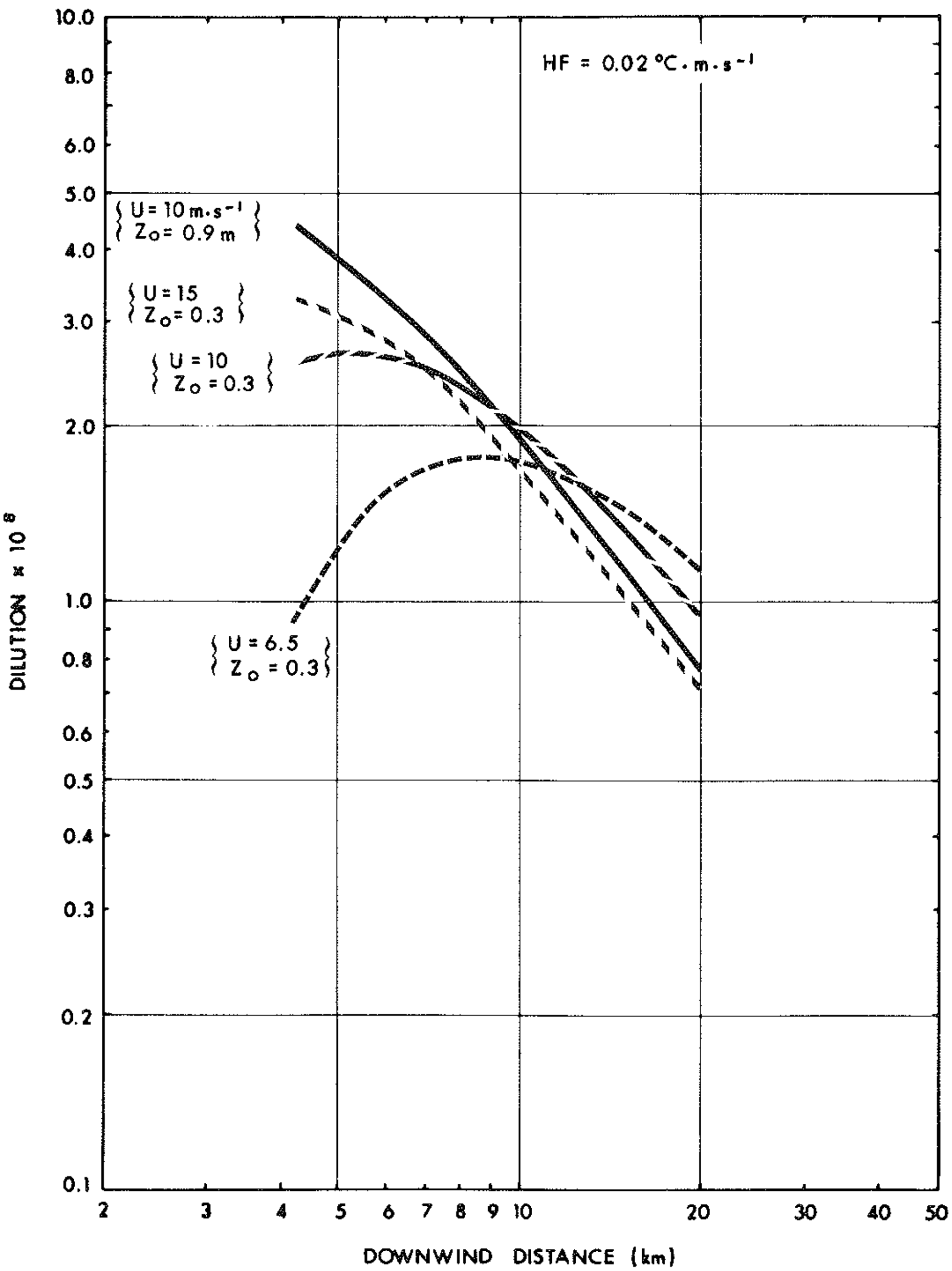

Figure 16. Sensitivity of sector-averaged GLC values (dilution) on roughness length, Z_o, for a heat flux of 0.02°C·m/s.

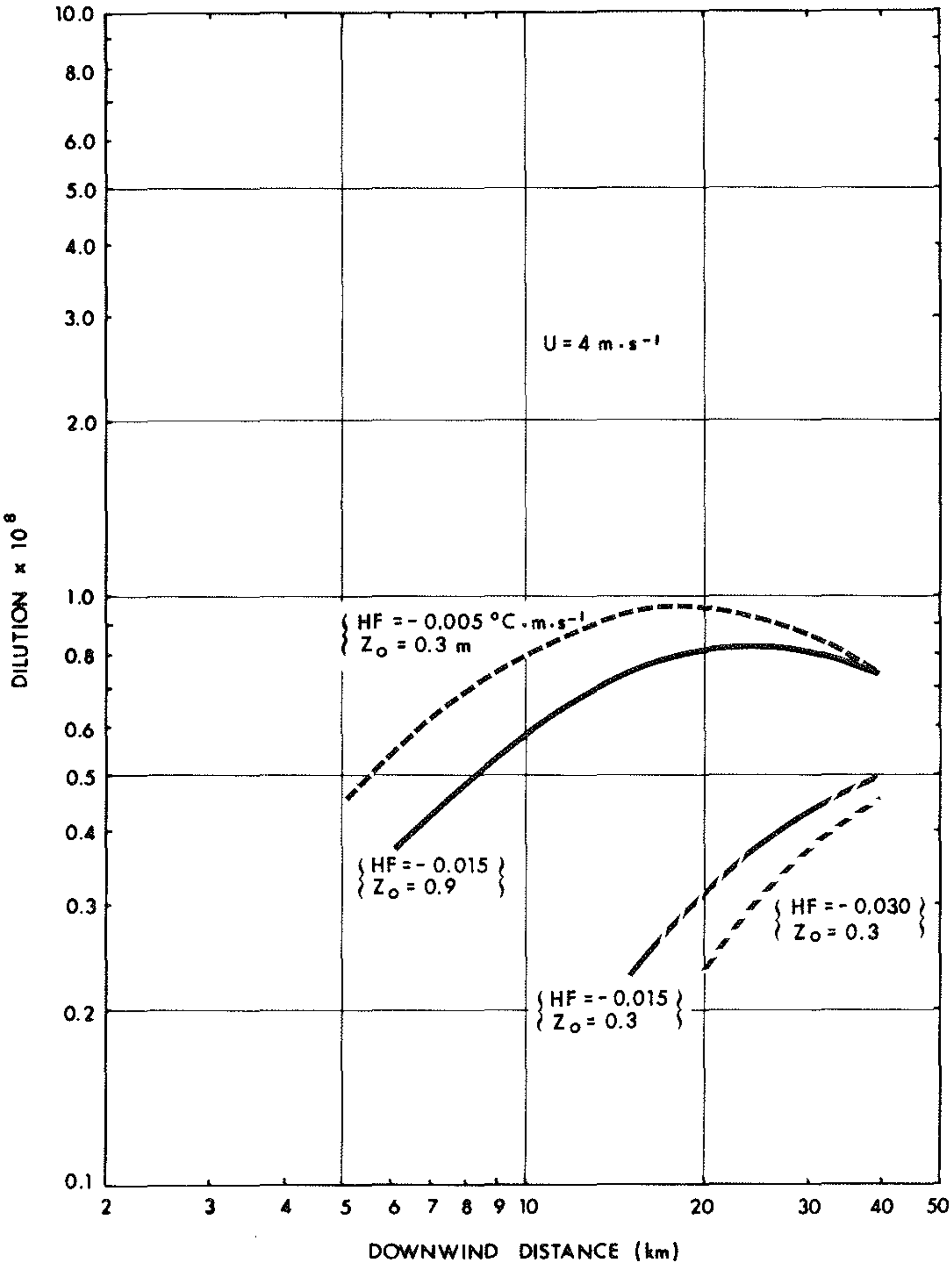

Figure 17. Sensitivity of sector-averaged GLC values (dilution) on roughness length, Z_o, for a wind speed of 4 m/s.

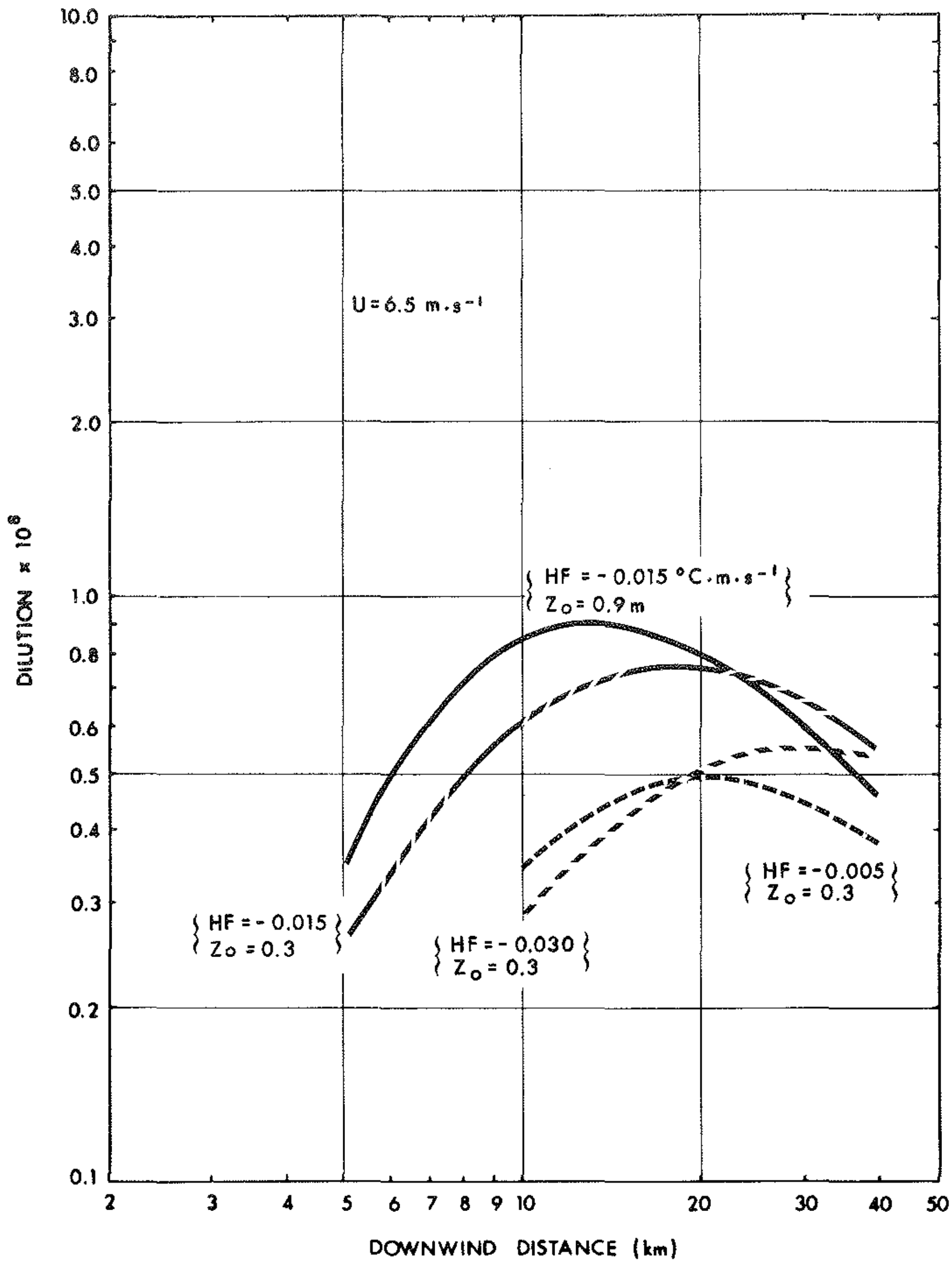

Figure 18. Sensitivity of sector-averaged GLC values (dilution) on roughness length, Z_o, for a wind speed of 6.5 m/s.

4.4.3 Roughness Length

The roughness length, Z_o, is a major determinant of the amount of mechanical turbulent energy produced by the mean wind. In the present model, the roughness length enters into the calculation of the friction velocity, u_*, which is the scaling velocity in mechanically dominated turbulence. From Volume I, the expression for U_* is

$$u_* = kU \left\{ \log \left(\frac{Z}{Z_o} \right) + f \left(\frac{Z}{L} \right) \right\}^{-1} \qquad (5)$$

where:

k	=	von Karman's constant
f(Z/L)	=	a function of Z/L to be specified
L	=	the Monin-Obukhov length
Z	=	the height at which u_* is evaluated (10 m)

In positive heat flux conditions, when f(Z/L) was taken as zero, then u_* could be calculated immediately. However, in convectively dominated situations, the scaling velocity was w_*, which is independent of the mechanical energy contribution. In these unstable cases, Z_o should have little effect. In stable conditions, f(Z/L) was taken as $\alpha Z/L$ where α is a constant. Since L varies as u_*^3, the calculation of u_* and L were not explicit, and the effect of Z_o on the GLC values in stable conditions was not a simple analytic expression.

The appropriate value for the roughness length was discussed in Volume I, based upon measured values at somewhat similar sites in other parts of the world. From this review, a value of $Z_o = 0.3$ m was adopted. Other investigators have suggested a value of $Z_o = 1.0$ m for the Athabasca Oil Sands region (R. Angle, Alberta Environment, personal communication, 1980). The sector-averaged GLC values for Z_o values of 0.3 and 0.9 m were compared for both convective and stable conditions.

The significance of the Z_o uncertainty depends upon the mixing conditions. In convectively dominated situations, there is no

Z_o effect. The scaling velocity is w_* which is independent of the roughness length. The effects of varying Z_o in mechanically dominated situations with a positive heat flux are shown in Figures 16, 17, and 18. The larger Z_o value results in more mechanical mixing which produces larger concentrations closer to the source (<8 km), and smaller concentrations at greater distances. At a distance of 5 km from the source, the change in Z_o from 0.3 to 0.9 increases sector-averaged GLC values by over 40%. The effect is greater than changing the wind speed from 10 to 15 m/s, but is much less than a wind speed change from 10 to 6.5 m/s. At long distances (>15 km), the larger Z_o value results in about 20% smaller GLC values.

In stable conditions, the scaling parameter for the wind direction and wind elevation angle fluctuations is μ_* , where, as discussed in Volume 1,

$$\mu_* = \frac{u_*}{fL} \tag{6}$$

The μ_* values for Z_o values of 0.3 and 0.9 m are shown in Table 7. A factor of three change in Z_o gives a factor of about two change in μ_* . Note that at very low wind speeds, the value of μ_* becomes independent of heat flux, because of the need to impose a minimum value on L in such cases. In stable, thermally dominated conditions, the values of σ_E and σ_A show a similar increase of a factor of 2 for an increase of a factor of 3 in Z_o. However, at wind speeds of 6.5 m/s and larger, mechanical effects become more important, and the increase in σ_A and σ_E is closer to 50% when Z_o is increased from 0.3 to 0.9 m, as shown in Tables 8 and 9.

In stable conditions, increasing Z_o from 0.3 to 0.9 causes much larger GLC values. The magnitude of the increase depends strongly upon the wind speed, as shown in Figures 13, 14, and 15. If the wind speed decreases from 6.5 to 4 m/s, the maximum GLC values for Z_o = 0.9 change by only about 10%, although they are displaced about 10 km farther downwind. However, for Z_o = 0.3, the maximum sector-averaged GLC values are displaced, perhaps 50 km farther downwind and are reduced by about 30%.

Table 7. Values of the stable scaling parameter, μ_* , as a function of roughness length, Z_o.

Wind Speed (m/s)	Z_o = 0.3 m Heat Flux Values (°C·m/s)			Z_o = 0.9 m Heat Flux Values (°C·m/s)		
	-0.005	-0.015	-0.030	-0.005	-0.015	-0.030
2	31.1	31.1	31.1	39.2	39.2	39.2
4	8.2	33.9	62.2	3.7	12.2	30.6
6.5	2.9	9.1	19.5	1.4	4.1	8.5
10	1.2	3.7	7.4	0.6	1.7	3.5
15	0.5	1.6	3.2	0.3	0.8	1.5

Table 8. σ_e values as functions of Z_o in stable conditions.

U	$Z_o = 0.3$ Heat Flux Values (°C·m/s)			$Z_o = 0.9$ Heat Flux Values (°C·m/s)		
	-0.005	-0.015	-0.030	-0.005	-0.015	-0.030
2	2	2	2	2	2	2
4	5	2	2	9	4	2
6.5	7	5	3	10	8	5
10	7	7	6	10	10	9
15	7	7	7	10	10	10

Table 9. σ_A values as functions of Z_o in stable conditions.

U	$Z_o = 0.3$ Heat Flux Values (°C• m/s)			$Z_o = 0.9$ Heat Flux Values (°C• m/s)		
	-0.005	-0.015	-0.030	-0.005	-0.015	-0.030
2	5	5	5	5	5	5
4	11	5	4	17	9	5
6.5	13	10	7	18	18	16
10	13	13	11	18	18	17
15	13	13	13	19	18	18

In summary, the magnitude of the changes in the sector-averaged GLC values is significant for the Z_o variations examined. Efforts should be undertaken to generate better Z_o estimates for the Athabasca Oil Sands area.

4.4.4 Free Convective Scaling Constants

For conditions of positive heat flux, the expressions for wind direction and elevation angle fluctuations, Z_o and σ_E, used in the model are

$$\sigma_A = \frac{u_*}{U} \left\{ 12 + 0.5 \left(\frac{Z_i}{L} \right) \right\}^{1/3} \qquad (7)$$

$$\sigma_E = \text{MAX} \left\{ \frac{0.6\ w_*}{U} , \frac{1.3\ u_*}{U} \right\} \qquad (8)$$

In the limit of free convection, the expressions become

$$\sigma_A = \frac{0.8\ w_*}{U} \qquad (9)$$

$$\sigma_E = \frac{0.6\ w_*}{U} \qquad (10)$$

where w_* is given by Equation (2). The experimental evidence for these expressions was presented in Volume I. It was noted that the numerical coefficients in the expressions for σ_A and σ_E were not experimentally well defined; in addition, any systematic changes in the vertical have not been found consistently by different groups. In general, there was an indication that $U \sigma_E$ probably reached a maximum in the middle of the convectively mixed PBL and its value may be less (perhaps 0.4 w_*) towards the bottom of the free convection region of the PBL.

The values of the constants defining the values U, σ_E/w_*, and $U\sigma_A/w_*$ can be indirectly varied by examining the σ_E and σ_A values, and their corresponding GLC values, for different heat fluxes. If the plume rise is nearly the same, then a change in the heat flux,

$\overline{w\theta}$, changes the value of w_*; therefore, it can be used as an effective change in the free convection scaling constants. For example, at U = 4 m/s, the heat flux value HF = 0.1 can be treated as HF = 0.2 with a free convection constant for σ_E of $0.6\ (0.5)^{1/3} = 0.48$. The plume rise is the same, although the transition point occurs about 360 m farther downwind. The sigma matching leads to a difference in effective downwind distance of about 170 m. Thus, except for an offset of 170 m, the case of HF = 0.1 can be treated as HF = 0.2, with a free convective scaling parameter of 0.48 for σ_E.

The decrease in the σ_E values, due to a decrease of the free convective constant from 0.60 to 0.48, scales linearly with the constant and so is about 20%. The decreased σ_E values result in a lower maximum GLC value farther from the source. The effect on both sector-averaged and centre-line GLC values was presented earlier in Figures 11 and 12. The sector-averaged maximum GLC value is about one-third lower. The centre-line concentration is decreased only about 5%; however, the maximum occurs at 4 rather than 2.5 km downwind. At 5 km downwind, the sector-averaged GLC values differ by 15% and continue to diminish in difference farther downwind. Since σ_E is independent of the wind speed in free convection, the same results should apply at other wind speeds, as long as the mixing is thermally dominated.

As mentioned in Volume I, a value of the free convective constant for $_E$ of 0.4 may be possible. An analysis similar to the one above, except involving HF = 0.02 and 0.10, would correpond to a simulation using a free convection constant value of 0.35. In that situation, the differences would be very large at distances less than about 15 km downwind. At 5 km, the difference would be a factor of about 3 for HF = 0.1°C m/s; even the centerline concentration values at 5 km would be greater than a factor of two smaller.

In summary, if the free convection constant for σ_E is within about 20% of the adopted value, the effects of this uncertainty on the predicted concentrations are relatively small. However, if the adopted value is in error by 40% or more, the effects are severe at small downwind distances. A comparison of observed and predicted GLC values in convective cases at the monitors Mannix and Fina is presented below, and indications are that any error in the free convection scaling constant is probably small.

4.5 EFFECTIVE DOWNWIND DISTANCE AND PLUME SIGMAS

The model incorporates the concept of an effective downwind distance to allow for the effects of source-dominated dispersion on the plume sigma values. The plume sigmas in the source-dominated region are scaled with plume rise in accordance with the formulations recommended by Briggs (1975) and utilizing constants consistent with observations in the Athabasca Oil Sands area (Davison and Leavitt 1979). At the transition distance to environmentally dominated dispersion, the plume sigmas are compared to values that would have been predicted if Taylor's statistical theory had been used. An effective downwind distance, X_e, is defined such that the plume sigma value at X_e calculated using an $X_e^{1/2}$ statistical formulation matches the plume sigma at the transition point. The effective distance offset defines the distance at which a source dispersing according to $X^{1/2}$ would have to be located in order to generate the plume sigma at the transition point. This calculational technique permits use of a simpler dispersion formulation while including the effects of source-dominated dispersion, and also, to a large extent, the effects of the change from X^1 to $X^{1/2}$ dispersion rates in the statistical theory.

The concept of effective downwind distance has a significant effect primarily in light and moderate winds in stable conditions. At the slow environmental dispersion rates in such conditions, the effects of source-induced dispersion during plume rise may be the equivalent of many kilometres of dispersion from a passive source. For example, at U = 4 m/s, effective downwind distance increment for σ_z is 10.4 km for a moderately negative heat flux of -0.015 °C•m/s. This distance increment means that, at the transition distance to environmentally dominated turbulence, the σ_z value is equivalent to a σ_z at 10.4 km calculated by the dispersion formulation

$$\sigma_Z = \sigma_E \, (0.5 \, \ell_w)^{1/2} \, X^{1/2} \qquad (11)$$

At subsequent downwind distances, the σ_Z value is calculated according to the above formulation, with an effective downwind distance (in metres) of

$$X_e = X + 10400 \qquad (12)$$

The effect of such a formulation is that at downwind distances less than the effective distance increment, the σ_Z curve is flat and gradually rises to an $X^{1/2}$ at long downwind distances.

In Figures 19, 20, and 21, σ_Z is plotted as a function of three downwind distances. There are different curves for different wind speeds since the stability parameter defining σ_E is a function of heat flux, wind speed, and mixing height (in convective conditions). The effective downwind distance concept is most noticeable for U = 4 m/s in stable conditions, because of the low environmental dispersion rates.

In stable conditions, the simple power law used to generate surface level winds (10 m) may be increasing the predicted levels of σ_Z. In order to generate the stability parameters, a value of the friction velocity, u_* , had to be generated. As outlined in Volume 1, the friction velocity was evaluated in the surface layer using

$$u_* = kU \left\{ \log\left(\frac{Z}{Z_o}\right) - \Psi_u\left(\frac{Z}{L}\right) \right\}^{-1} \qquad (13)$$

This expression was evaluated at a height of Z = 10 m. The value of U at 10 m was approximated from the 400 m level wind using a simple power law

$$U_{10} = U_{400} \left(\frac{10}{400}\right)^P \qquad (14)$$

where P was assigned a value of 0.14. This value of P is quite reasonable for neutral and convective conditions, but in progressively more stable conditions, larger values of P should be used. For very stable conditions, a value of P = 0.3 would be more appropriate. A variable value of P could be utilized in the model by use of a simple

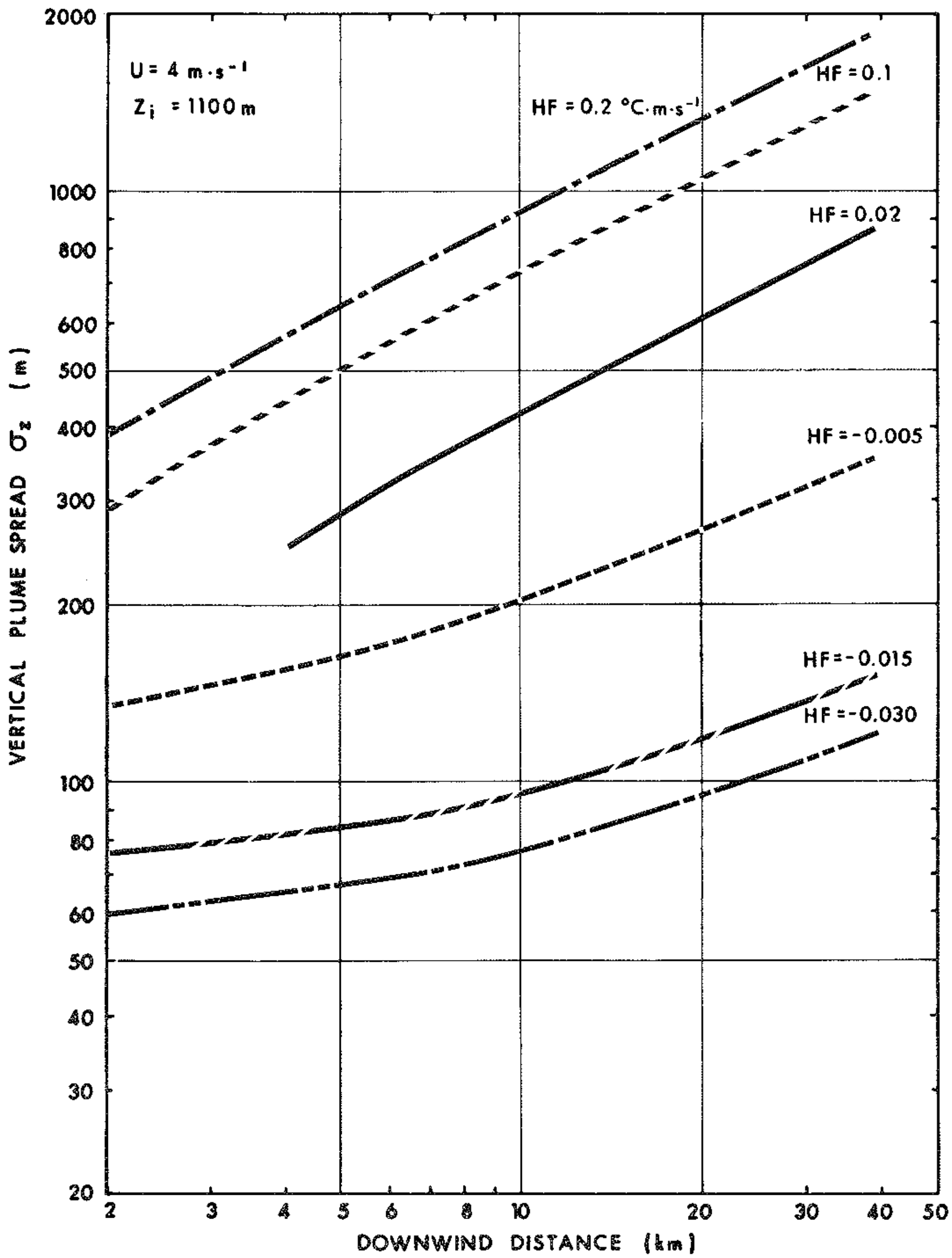

Figure 19. Sensitivity of vertical plume spread, σ_z, as a function of downwind distance and heat flux for a wind speed of 4 m/s.

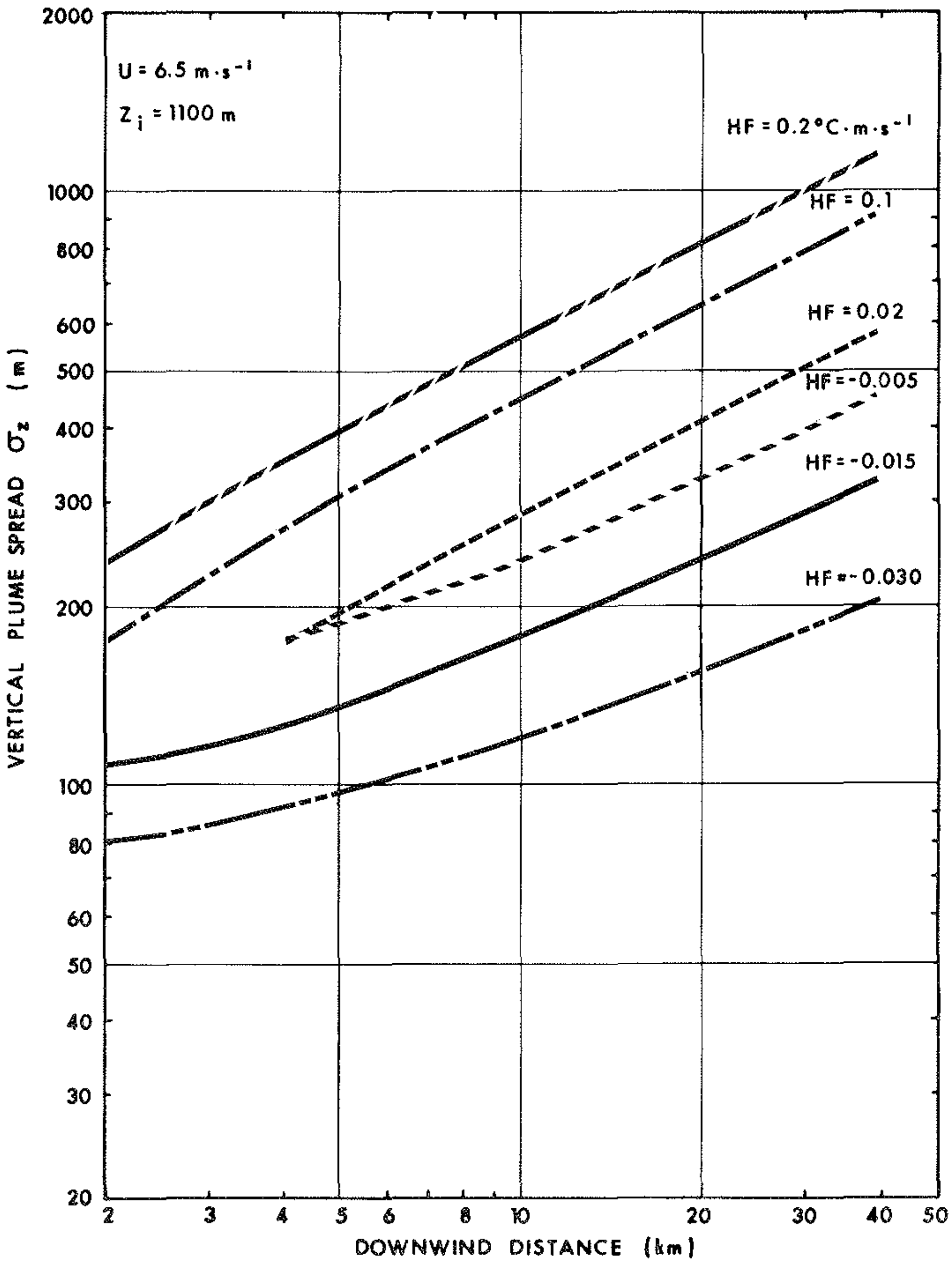

Figure 20. Sensitivity of vertical plume spread, σ_z, as a function of downwind distance and heat flux for a wind speed of 6.5 m/s.

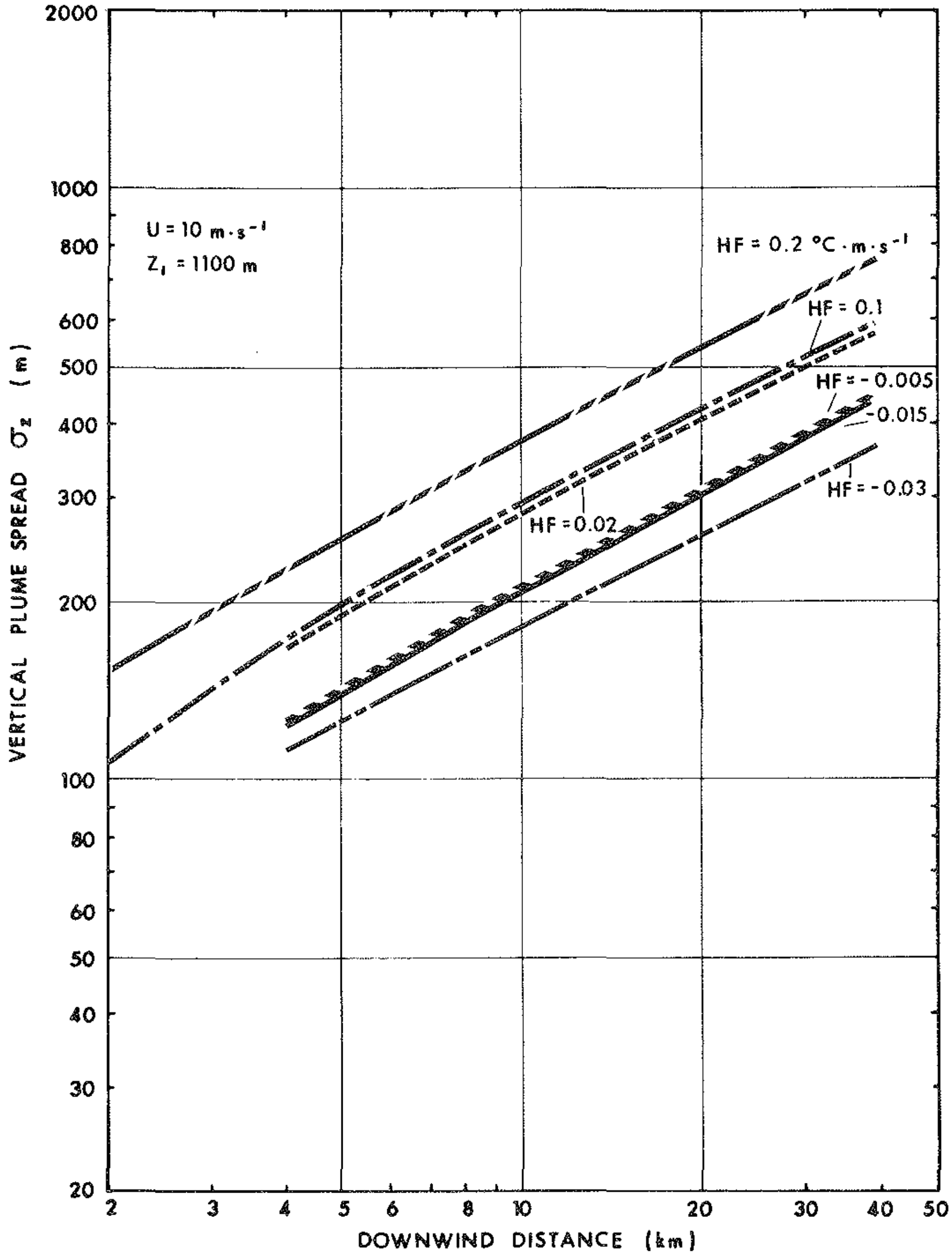

Figure 21. Sensitivity of vertical plume spread, σ_Z, as a function of downwind distance and heat flux for a wind speed of 10 m/s.

iterative technique. The effect of keeping P = 0.14 is to overestimate u_*, and hence the amount of mechanical mixing in more stable conditions. For U = 10 m/s in Figure 21, the largest negative heat flux case would have a curve close to the curve for U = 6 m/s if a value of P = 0.3 were adopted.

In very stable conditions, however, decoupling of the flow may occur. For such cases, the boundary layer parameterization is not valid. If, however, the plume rises into the decoupled layer (which is very likely), a simple Gaussian formulation is inadequate.

5. COMPARISON OF PREDICTED AND OBSERVED VALUES

5.1 CHARACTERISTICS OF THE OBSERVED AIR QUALITY DATA

Ground level SO_2 concentrations are available from 10 air quality monitoring stations operated by Syncrude and Suncor. The location of these stations relative to the plants are shown in Figure 22. The one Syncrude and five Suncor stations have been in operation since 1976, and the remaining four Syncrude stations since mid-1977. Observed monthly average SO_2 concentrations at these stations have been summarized in a report prepared by Strosher (1980). Monthly average values ranged between 0 and 13 ppb.

The observed data have some serious limitations in their use for model verification. As discussed by Strosher (1980), the instrumental accuracy is about 5 ppb and there is a possible 5 ppb offset uncertainty. Strosher recommended truncating values less than about 20 ppb from the calculation of monthly statistics. This procedure would ensure a suitable frequency distribution of concentrations during episodes; however, frequent low-level concentrations would be ignored. The problem is basically one of having a marginal ability to measure the time series of concentrations. The problem becomes more severe at greater distances from the sources, as the lower concentrations cause continued deterioration of the signal-to-noise ratio. The discretization of the monthly averages in the presently processed data set can lead to misleading correlations. In particular, the stations operated by Syncrude have monthly averages reported by Strosher (1980) only to the nearest 10 ppb. Since monthly averages ranged from 0 to 13 ppb, resolution of 10 ppb leads to virtually meaningless correlation results.

The existing air quality data base is not available in a computer-compatible format. As part of this program, the SO_2 GLC values at one-half hour resolution were digitized from hardcopy for the monitors Fina and Mannix for the four months in 1977 corresponding to the meteorological time series data file: January, April, July and October. These digitized data were converted to hourly records by

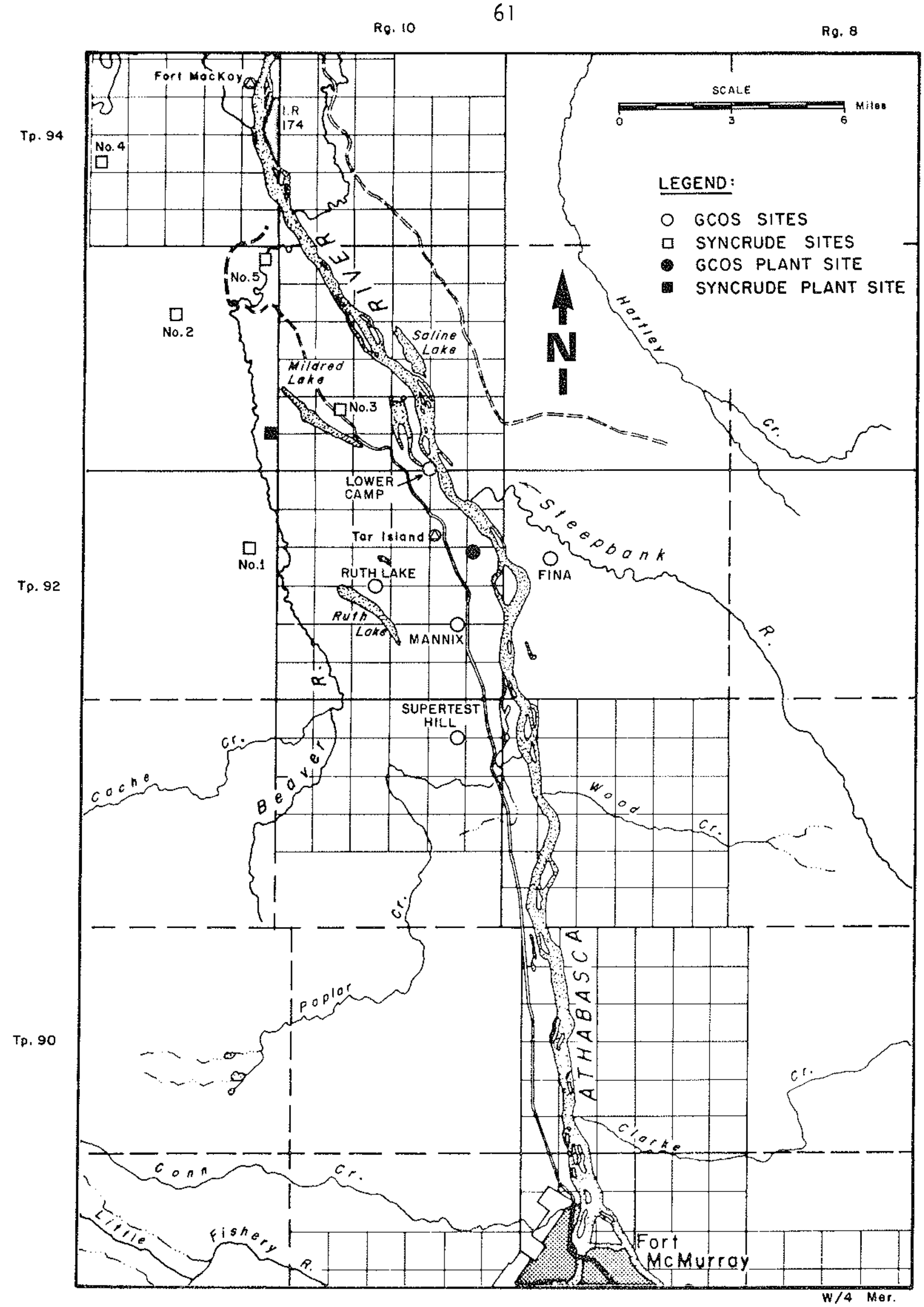

Figure 22. Map of continuous ambient air monitoring stations.

box-car averaging, and were then available for comparison with model predictions for both statistical and time series analyses. Converting the air quality data base from hardcopy to a computer-compatible format was beyond the scope of the present project. Without a computerized data bank, extensive statistical analysis could not be undertaken; rather, previous analyses had to be adopted for this project.

Strosher (1980) analyzed the one-half hour SO_2 data for all the monitoring stations and developed frequency distributions according to the following classes:

Class	Concentration (ppm)
1	0.0
2	0.001 to 0.060
3	0.061 to 0.170
4	0.171 to 0.200
5	0.201 to 0.340
6	0.341

As was discussed earlier, the first and second classes are not well defined, due to the measurement uncertainties of about ± 0.01 ppm. The fraction of observations in Class 2 depends upon qualitative interpretation by the observer of what constituted a zero reading. The number of values in classes 4 to 6 were usually very small. Since these were the only previously processed frequency distributions available, they were utilized for some formal statistical comparisons between predicted and observed values. The statistical problems of using a frequency distribution with such non-uniformly populated classes is discussed below.

Strosher (1980) presented evidence of significant observer bias. The SO_2 concentrations are recorded in hardcopy analog form by a TECO-43 sensor, with offset and accuracy uncertainties of about 5 ppb each. These analog traces were abstracted by hand onto tables by making visual one-half hour averages. Strosher noted that a change in observer resulted in a systematic change in recorded values, due to the observers evaluation as to what constituted a zero reading and what should be taken as a 5 or 10 ppb reading. These uncertainties are not significant when specific air quality episodes are examined, but they can seriously affect the value adopted for the "observed" monthly mean.

5.2 STATISTICAL METHODS

The verification studies of the frequency distribution model involved, in part, the use of certain statistical tests. These included the estimation of correlation coefficients, and the application of the chi-squared (X^2) and Kolmogorov-Smirnov (K-S) tests. A brief description of each follows.

5.2.1 Linear Correlation Coefficient

As a quantitative measure of the relationship between predicted and observed data sets, a correlation coefficient is often used. In this study, both linear and rank correlation coefficients were used.

The linear correlation coefficient assumes a linear relationship exists between the observed and predicted values. The coefficient is given by:

$$R = \frac{N \Sigma O_i P_i - \Sigma O_i \Sigma P_i}{\{N \Sigma O_i^2 - (\Sigma O_i)^2\}^{1/2} \{N \Sigma P_i^2 - (\Sigma P_i)^2\}^{1/2}} \quad (15)$$

where O_i and P_i are the observed and predicted values respectively, and N is the number of data pairs. Values of R near zero imply no linear correlation, R values near unity imply a perfect correlation, and negative values of R imply an inverse correlation.

5.2.2 Rank Correlation Coefficient

The rank correlation coefficient uses the rank instead of the actual predicted and observed values. Each value is assigned a rank using the numbers 1, 2, 3...N, according to its size. The ranking is then used to calculate the correlation coefficient from

$$P = 1 - \frac{6 \Sigma (V_i - U_i)^2}{\Sigma N (N^2 - 1)} \quad (16)$$

where V_i and U_i are the ranking of observed and predicted values, respectively. This relationship is also called the Spearman formula for rank correlation. Values of p near unity imply identical rankings of predicted and observed concentrations.

5.2.3 Pearson Chi-Square Test for Frequency Distribution

The X^2 test may be used to compare the goodness-of-fit between the predicted and observed frequency distribution. The X^2 value is calculated from the relationship

$$X^2 = \Sigma \left\{ \frac{(f_{pi} - f_{oi})^2}{f_{oi}} \right\} \quad (17)$$

where f_p and f_o are the frequencies of occurrence of predicted and observed concentration classes, respectively. The X^2 value can then be compared to values in standard tables to assess the degree to which the predicted and observed frequency distributions represent the same population. If the X^2 value is equal to zero, then the predicted and observed frequency distributions agree exactly. Large X^2 values indicate disagreement between the observed and predicted frequencies.

The application of the Pearson X^2 test is valid only if the following three criteria are met:

1. Each and every sample observation falls into one and only one class;
2. The N observations in the sample are independent; and
3. The sample size N is large.

For the present application in the verification of model predictions, the interpretation of the results of the Pearson X^2 test may be questionable. The hourly values of concentration are clearly not independent; episodes may last many hours. Another more serious aspect of the independent samples is associated with the time scale of synoptic systems. For example, if a high pressure area exists over a region for several weeks, resulting in clear skies and the corresponding dispersion characteristics, then the observed concentrations are not fully dependent. A month of data may have a few truly independent values.

The requirement for a large number of independent events is also a significant constraint for model verification involving the existing processed air quality data. The Strosher (1980) analysis pointed out the problems of zero-definition and how qualitative observer bias may have significantly modified the relative populations of the zero and near zero concentration classes. Thus, the lowest two classes in the Strosher (1980) analysis may not be suitable for testing. The concentration class of 0.06 to 0.17 ppm SO_2 appears to be well defined. However, the frequency distribution classes for concentrations greater than 0.17 ppm SO_2 were generally very sparsely populated. When values did occur, inspection of the time series of observed concentrations usually indicated, at most, one or two episodes each month. Thus, the actual number of independent samples in these frequency classes was very small.

For the present, the Pearson X^2 value has been utilized. Its use as quantitative indicator of similarity of frequency distributions is dubious; however, it can serve as a qualitative indicator of improvement in a sensitivity study.

5.2.4 Kolmogorov-Smirnov Test for Cumulative Distribution Functions

The Kolmogorov-Smirnov (K-S) test can be used to estimate the goodness-of-fit between predicted and observed cumulative distribution functions. The measure of the agreement is the maximum difference between the cumulative distribution functions for observed and predicted values; that is:

$$D = \text{MAX} \; \Sigma \left\{ F_o(x) - F_p(x) \right\} \quad (18)$$

where $F_o(x)$ and $F_p(x)$ are observed and predicted cumulative frequency distribution functions. The test can be applied to continuous functions or to discretized functions formed from the frequency distributions. Large values of D indicate disagreement between the predicted and observed results.

5.2.5 Comments on the Application of the Statistical Tests

The limitations of each statistical test should be considered when comparing model predictions with observations. These limitations are often sensitive to the nature of the data base. The present observed and predicted time series data sets are relatively sparsely populated with non-zero values at many monitoring locations. Some of the implications for the X^2 test have been discussed above; implications for the remainder of the tests will be briefly examined.

The linear correlation coefficient is independent of systematic changes in the magnitude of the predicted values. A multiplicative change to each predicted value will not change the value of the coefficient. Thus, linear correlation coefficients do not detect systematic errors. The linear correlation coefficient is sensitive to the timing of predicted and observed events. When predicted and observed events are consistently in phase, correlations are nearer unity than when the events are out of phase, even if the magnitude of the values is similar. Thus, the value of the linear correlation coefficient will depend, to a large extent, upon the accuracy of the wind direction data. The process of sector-averaging, which is inherent in a frequency distribution model, will degrade the linear correlation coefficient at a given receptor, particularly for hourly concentrations due to an averaging of wind directions.

A second implication exists for linear correlation coefficients and monthly mean ground level concentrations. A month of data, with relatively few non-zero values, combined with a model that correctly predicts the many zero values, even if missing the few important events, may result in relatively large linear correlation coefficients because of the phase influence. Thus a model may realize reasonable correlation statistics and adequate monthly mean GLC values, and yet not properly simulate the frequency and magnitude of the major GLC episodes, nor have the GLC values occurring during meteorological conditions in which they are observed. These implications severely limit the applicability of the linear correlation coefficient when comparing predicted with observed concentrations, or when comparing the results of different models.

The Spearman rank correlation coefficient also has significant limitations on its usefulness. As mentioned earlier, the uncertainties in the monthly averages and their discretized values can result in a statistical noise that can invalidate a rank comparison. Since the monthly averages are generally sensitive to a very few events, the wind direction uncertainty in the data base may dominate the difference in the predicted and observed monthly values. A much longer averaging period may be required.

The use of residuals between predicted and observed values was found to be of value. Although residuals do not constitute a formal statistical evaluation of the similarities of populations of values, they do provide a measure by which to evaluate alternative modifications to the formulation parameters in the model.

5.3 SOURCE SPECIFICATIONS

This section describes the source characteristics assumed during validation and sensitivity studies of the frequency distribution model. Emissions at Suncor for the years 1976 to 1978 were assumed to originate exclusively from the powerhouse and incinerator stacks; emissions from the flare stack and possible low-level sources were not included. Syncrude was assumed to be operational only during October 1978; potential emissions associated with construction and testing were not included.

Stack parameters and emission rates used in validation are shown in Table 10 and are based on values from Walmsley and Bagg (1977). The emission rates are consistent with Sandhu's (1979) estimates. Statistics on the variability of the Suncor SO_2 emissions from both the powerhouse and incinerator stacks from 1976 to 1978 have been compiled by Sakiyama (1981). Mean emissions were 216 t with a standard deviation of about 30 t, representing about 60% of the design (license) rate. The standard deviation reported is about 14% of the mean emission rate; in months when the plant operated normally (i.e, no days with very low emissions), the standard deviation was about 12% of the mean rate. Sakiyama also reported emission rate extremes. During an average month, the lowest daily emissions were about 60% of the mean rate and the highest daily emissions were about 125% of the mean rate.

Table 10. Suncor and Syncrude stack parameters and SO_2 emissions used in the verification runs.

Plant Stack	Suncor Powerhouse	Suncor Incinerator	Syncrude Main
Height (m)	107	107	183
Diameter (m)	5.8	1.8	7.9
Exit velocity (m/s)	17.5	17.0	23.7
Exit temperature (°C)	272	610	246
SO_2 emission (kg/s)	2.60	0.27	3.30

During April 1977, the entire plant was inoperative for about nine days; at various other times the incinerator was inoperative.

These statistics affect the model validation in several ways. First, they show that the emissions rates used during the validation computer runs were larger than the actual rates by about 15%, that is, by about one standard deviation. An uncertainty in the emission rate of about $\pm 20\%$ should include about 90% of the hours during which the plant is operating normally. This level of uncertainty is similar to the uncertainty in the specification of the meteorological variables. With the exception of case studies, the use of a mean value appears reasonable; it is thought unnecessary to include hour-by-hour emission estimates in a time series file.

Flaring represents a much more intermittent and ill-defined source associated with plant upset conditions. Sandhu (1979) reported flare emissions as 1% of Suncor total emissions in 1978. Sakiyama (1981) reported, for the Suncor plant, typically one or two days of flaring each month. High variability in source strengths and duration of release were indicated. In some cases, although flaring was reported, no dates, durations or amounts were given.

Observed GLC values of monitors Mannix and Fina during 1977 were examined for evidence of flaring. During the three days in July and January when flaring was reported, observed GLC values at these monitors were zero or significantly small (less than 50 ppb). No flaring was reported in April, but flaring was reported for all days in October, at a rate of less than 5 t/d. Thus, while flaring may be responsible for isolated episodes of high GLC values, both the lack of good flaring emission data and the sparsity of the monitoring network make identification of these episodes difficult. For the same reasons, verification of flaring influences on GLC values, in other than a case study mode, is also difficult.

In summary, for model verification, steady emission rates were used which were about 15% larger than those recently reported. Source variability is considered important for hour-by-hour verification at specific sites, or for case study analyses, but not as important when examining time- or space-averaged GLC values. Flare emissions were poorly defined and were not included in the present study, although they may be important in a case study approach.

5.4 HOURLY AVERAGE TIME SERIES

Hourly observed and predicted SO_2 concentrations were compared for two air quality stations, Mannix and Fina, for the year 1977. This year was selected to reduce any interference associated with the commencement of Syncrude operations in 1978. Data collected during 1977 were assumed to have a higher degree of quality control than the data of 1976, due to increased experience of the network maintenance and data reduction staff.

Mannix and Fina were selected for time series analysis because high monthly average concentrations were observed at these sites. In addition, the directions of the stations from Suncor are along and across the river valley; therefore, systematic wind direction errors may be more detectable. Observed SO_2 concentrations were available as half-hourly averages in hard copy. These data were digitized and then converted to hourly average values by using a 1-h boxcar averaging procedure. The results of the comparison of hourly predicted and observed values have been summarized in Tables 11 and 12 for Mannix and Fina, respectively. The predicted values shown in these tables were based on the actual 107-m stacks for the Suncor plant. The tables show the number of predicted and observed "events". An "event" was defined as two or more consecutive hours having SO_2 concentrations greater than or equal to 50 ppb.

Hourly observed and predicted SO_2 concentrations for Mannix and Fina are presented in the Appendix for the four 1977 months under evaluation. The following discussion summarizes the comparison of the predicted and observed hourly time series.

5.4.1 <u>January</u>

The model had a tendency to underpredict observed concentrations and frequencies at both stations. At Mannix, predicted and observed non-zero values were spread throughout the day; however, at Fina, the few predicted values occurred mostly in the afternoon

Table 11. A comparison of observed and predicted 1977 hourly average SO_2 concentrations for Mannix air quality monitoring site.

	1977			
	Jan.	Apr.[a]	July	Oct.
Mean Monthly Concentration				
Observed (ppb)	4.9	2.4	2.1	0.2
Predicted (ppb)	1.3	3.0	2.3	1.9
Residual (ppb)	-3.6	0.6	0.2	1.7
Concentrations Greater Than 10 ppb				
Observed (h)	74	37	67	6
Predicted (h)	45	43	28	34
Number of Events				
Observed	6	3	1	0
Predicted	0	4	3	1
Pearson Chi-Square Test				
X value	4	0.1	34	130
Kolmogorov-Smirnov Test				
D-value	0.060	0.008	0.053	0.038

[a] Observed and predicted statistics for April include 9 days when emissions were zero.

Table 12. A comparison of observed and predicted 1977 hourly average SO_2 concentrations for Fina air quality monitoring site.

	1977 Jan.	Apr.[a]	July	Oct.
Mean Monthly Concentration				
Observed (ppb)	3.1	3.5	3.4	3.0
Predicted (ppb)	0.4	2.0	4.3	6.5
Residual (ppb)	-2.7	1.5	0.9	3.5
Concentrations Greater Than 10 ppb				
Observed (h)	94	43	107	50
Predicted (h)	7	21	53	63
Number of Events				
Observed	2	4	2	2
Predicted	1	2	4	6
Pearson Chi-Square Test				
X^2 value	90	13	71	104
Kolmogorov-Smirnov Test				
D-value	0.118	0.036	0.083	0.046

[a] Observed and predicted statistics for April include 9 days when emissions were zero.

with one night-time exception, while the observed values were spread throughout the day. Predicted concentrations occurred in both convective and mechanically dominated conditions. Mechanically dominated concentrations were typically predicted to be 10 ppb or smaller; slightly convective concentrations reached 30 ppb. The one predicted night-time event at Fina occurred during wind speeds of 10 m/s and resulted in concentrations of about 50 ppb.

The observed events occurred principally in non-convective situations. In January, the number of daylight hours varies between about 6 and 8 h, and the number of net positive heat flux hours will be several hours less. As can be seen in the time series shown in the Appendix, the six major events observed at Mannix cannot be convectively related, and only one of the two events at Fina may be convectively related. The wind speeds on the time series file were less than 10 m/s during the episodes and often were about 5 m/s.

The underprediction, in terms of frequency of occurrences, may be attributed to at least four causes: incorrect wind direction at stack height, significant underestimation of wind speed, significant difference of the actual mixing depth from the climatological value and/or failure to identify a low-level source. Wind direction errors are definitely a major problem. A westerly wind is necessary to advect the Suncor plumes toward the Fina monitor; however, only about 25% of the non-zero concentration values observed at Fina were associated with a westerly wind on the input time series data file.

5.4.2 April

At Mannix, most of the observed non-zero values occurred more or less continuously during the first two days of the month, whereas the predicted values are largely associated with convective mixing and were distributed over seven days throughout the month. At Fina, there are at least three observed cases of convective mixing, with maximum values similar to the predicted values.

The magnitude of the observed and predicted concentrations showed close agreement in convective conditions, although the timing of events was not similar. At both Mannix and Fina, predicted concentrations during convective events reached 130 to 140 ppb; whereas, observed concentrations in mid-afternoon typically reached 140 to 160 ppb at Fina.

For 1 h at 1100 MST on 2 April, the observed SO_2 concentration at Fina was 500 ppb. This single hour is over three times larger than any other hourly observation or prediction in April at either Mannix or Fina. An inspection of predicted centre-line concentrations from intermediate GLCGEN results suggests that the maximum predicted GLC centre-line value would probably not exceed 300 ppb. Possible explanations for this anomaly, and other systematic discrepancies in the predicted values, are discussed in a later section.

The three major events observed at Fina occurred at times when the wind directions on the input data file were about 90° from the necessary westerly wind direction. The errors in wind direction will clearly keep the hourly based linear correlation coefficient small.

The wind directions during the 30-h event at Mannix were quite well predicted. During the stable conditions of the event, however, the wind speeds on the time series file were too low to induce significant mechanical mixing.

5.4.3 July

Observed concentrations at Mannix occurred almost entirely during afternoons; at Fina, the majority of observed values occurred during afternoons but many other values were spread throughout the day. Observed concentrations during convective hours at both stations are generally low, typically less than 50 ppb, with only three events greater than 100 ppb.

Predicted concentrations at both Mannix and Fina occurred almost exclusively during convective hours. Maximum concentrations were near 130 ppb. Predicted concentrations during convective conditions were typically somewhat larger than observed, and the predicted number of hours with concentrations greater than 10 ppb was approximately half the observed number. Thus, the relatively small difference between observed and predicted monthly mean GLC values appears somewhat fortuitous, as seen by the relatively large K-S value.

Wind direction appeared to be a major source of error for the prediction of the days of the month in which concentrations will occur. However, at Mannix, the paucity of days with concentrations, between 12 July and 27 July appeared to be quite well predicted. The observed concentrations during afternoon mixing conditions were less than during apparently similar conditions in April. This feature, combined with more frequent lower values, suggests that the wind direction may have been more variable in the July case.

5.4.4 October

The observed concentrations at Mannix were all zero, with the exception of 6 h on 28 October when the maximum value was 30 ppb. The predicted concentrations for Mannix occurred over two long, continuous time periods of 17 and 24 h, with a maximum GLC of about 100 ppb. The agreement in having almost entirely non-zero values is good. The reason for the agreement may be due to a good wind direction data file, since there were only two periods (corresponding to predicted concentrations) in the month when the necessary northerly winds were present in the input data file. The discrepancy between observed and predicted values may again be strongly due to the wind direction errors, or to an overprediction of wind speeds.

At Fina, there is better agreement between the observed and predicted concentrations and frequencies. Both predicted and observed concentrations occurred throughout the day. Predicted concentrations reached 130 ppb, and observed concentrations reached 115 ppb. Generally, predicted concentrations were approximately equal to observed concentrations, but occurred more frequently. The highest predicted concentrations were produced by trapping the plume in high wind speed conditions; they always occurred at 1000 or 1100 MST when convective mixing heights were 350 to 450 m. Overprediction of the frequency of events can probably be attributed to wind direction errors in the input time series data.

5.4.5 Discussion of Time Series Comparisons

The model was generally able to predict GLC values similar to values observed during both convectively and mechanically dominated situations. For the July 1977 comparisons, however, there appeared to be evidence of greater wind direction fluctuations in convective conditions than simulated. The maximum observed values in convective conditions were typically less than values in April.

The timing of events, and often the frequency of occurrence of events, were not well predicted. The data showed that a small number of episodes generally dominated the monthly averages. Errors in the wind direction dominated all other errors for the time series comparisons. Without a very good wind direction data file, the hourly based linear correlation coefficients will always be small, and even monthly averages at a given site will be questionable.

5.5 ANNUAL AND MONTHLY MEANS

5.5.1 Overview of Procedure

The serious limitations on the application of statistical tests to monthly mean GLC values have been outlined above. Primarily, the problems arise because a single month is too short an averaging period to produce representative values. There are usually a very small number of events which dominate the monthly mean GLC values. The prediction of these events requires very accurate wind direction information which is not available. Even if the wind direction data base could be improved, the sector-averaging or directional discretization, together with the discretization of the wind, heat flux, and mixing height, implies the need for many realizations to obtain results that are applicable at a given receptor. Single month averaging periods are not sufficiently long.

The comparison of predicted and observed concentrations averaged over many months was considered an appropriate test of the model and data base combined. The available time series file, as outlined in Volume 2 of this report, consisted of the four months, January, April, July, and October for the years 1976, 1977, and 1978.

The sensitivity of the mean monthly concentrations to variations in the physical stack height of the Suncor plant was also investigated. The Suncor plant, at an elevation of 225 m, is within the Athabasca River valley, while the Syncrude plant, at an elevation of 305 m, and most of the monitoring stations, are located out of the valley. To test the sensitivity of the effect of the lower elevation of the Suncor plant, monthly average concentrations were estimated using both the actual physical stack heights of 107 m and stack heights of 60 m.

A comparison of the observed and predicted average concentrations for the two assumed stack heights at the Suncor plant is shown in Tables 13 and 14. The Syncrude stations are compared separately, because the resolution of the monthly average GLC values are 10 ppb. The linear and rank correlation coefficients are shown in Tables 13 and 14, although their relevance is questionable. The time series of monthly averages for the Suncor and Syncrude stations are presented in the Appendix.

5.5.2 Comparisons with the Syncrude Stations

The observed values from the Syncrude stations are subject to major uncertainties, due to the 10 ppb resolution. For example, the observed monthly means for Station 1 were all taken as 0.0, with the exception of October 1977, when the first incremental value of 10 ppb was adopted as the monthly average. This single incremental value gives rise to an "observed" mean of 1.7 ppb over the six months of data. None of the other Syncrude stations had monthly values greater than 10 ppb; therefore, the variations in the average values for the Syncrude stations (except Station #3) in Tables 13 and 14 are due to varying numbers of months with the first increment of concentrations.

Strosher (1980) noted that the instrument used for the SO_2 measurements had an offset uncertainty of at least 5 ppb, and a measurement uncertainty of 5 ppb. He also suggested that there was significant observer bias during the abstraction of visual one-half

Table 13. A comparison of the observed and predicted monthly average SO_2 concentrations (ppb) with the Suncor stack heights taken as their actual physical height of 107 m.

Station	No. of Months (N)	Mean Observed (O)	Mean Predicted (P)	Residual (P-O)	R^a	P^b
Mannix	12	2.8	1.6	-1.2	0.19	0.34
Ruth Lake	12	1.8	0.3	-1.5	-0.05	0.05
Fina	11	4.4	3.2	-1.2	0.21	0.16
Lower Camp	6	2.1	0.8	-1.3	0.40	0.47
Supertest	11	1.8	1.7	-0.1	-0.16	-0.02
Average	10.4	2.6	1.5	-1.1	0.12	0.20
Syncrude 1	6	1.7	0.4	-1.3	-0.21	0.20
Syncrude 2	6	0.0	0.5	0.5	-	0.50
Syncrude 3	11	3.9	0.6	-3.3	-0.03	0.14
Syncrude 4	6	3.3	0.5	-2.8	-0.01	0.16
Syncrude 5	6	5.0	0.4	-4.6	0.53	0.37
Average	7.0	2.8	0.5	-2.3	0.06	0.27

[a] R is the value of the linear correlation coefficient.

[b] P is the value of the Spearman rank correlation coefficient.

Table 14. A comparison of the observed and predicted monthly average SO_2 concentrations (ppb) with the Suncor stack heights taken as 60 m.

Station	No. of Months (N)	Mean Observed (O)	Mean Predicted (P)	Residual (P-O)	R	P
Mannix	12	2.8	3.8	1.0	0.43	0.41
Ruth Lake	12	1.8	0.4	-1.4	-0.04	-0.04
Fina	11	4.4	7.1	2.7	0.19	0.10
Lower Camp	6	2.1	1.2	-0.9	0.39	0.50
Supertest	11	1.8	2.6	0.8	-0.50	-0.41
Average	10.4	2.6	3.0	0.4	0.09	0.09
Syncrude 1	6	1.7	0.6	-1.1	-0.07	0.20
Syncrude 2	6	0.0	0.6	0.6	-	0.50
Syncrude 3	11	3.9	0.9	-3.0	0.05	0.14
Syncrude 4	6	3.3	0.6	-2.7	0.11	0.16
Syncrude 5	6	5.0	0.4	-4.6	0.51	0.37
Average	7.0	2.8	0.6	-2.2	0.12	0.27

hour averages from the analog hard-copy traces of what constituted a 0 or a 10 ppb reading. The discrepancy would not be significant for measurement during episodes, but could have a major impact on the monthly means. The largest observed mean values in Tables 13 and 14 occurred for Syncrude Station #5, which is about 18 km northwest of the Suncor plant. This large value of 5 ppb is due to three of the six months of records available showing a monthly mean value at the first incremental level of 10 ppb. Station #2, about 5 km to the southwest of Station #5, is about 19 km from Suncor. Although the angular difference in the directions of Stations 2 and 5 from Suncor is less than 20°, Station #2 values were all 0.0 ppb.

At Syncrude Station #3, the observed monthly average GLC values were recorded to the nearest 1 ppb until July 1977 when the 10 ppb resolution was adopted. Of the six months after that time, two of the months, July 1977 and January 1978, had observed monthly means at the first incremental level of 10 ppb; three monthly means were zero, and one was missing. The monthly value recorded on April 1976 was 13 ppb, all remaining four monthly values were less than or equal to 4 ppb.

The above considerations suggest that the apparent discrepancies with the Syncrude stations are probably a combination of the month-to-month variability exhibited in the time series from Mannix and Fina, combined with a very coarse increment for GLC values, and an uncertainty in what constituted a zero value. It appears that model comparisons with the observed Syncrude data are limited by the uncertainties in the abstraction of the observed data. If the originally abstracted data were digitized and a truncation level of 10 or 20 ppb were adopted, as suggested by Strosher (1980), then model comparisons would be instructive. The cumulative effect of episodes of elevated GLC values could be compared to assist in model and data base validation. Observed long-term averages, however, would still be significantly uncertain due to the possible neglect of frequent low levels of concentrations which are lost in the signal-to-noise ratio of the sensor.

5.5.3 Comparisons with the Suncor Stations

The observed and predicted values at the Suncor stations are similar in magnitude when the limitations in both the observed GLC values and the model/data system are considered. The Suncor stations are all within about 5 km of the Suncor plant, except for Supertest, which is about 10 km south. The time histories of the observed monthly means generally show wide fluctuations. These fluctuations are partially due to the effects of a very small number of episodes occurring each month. The predicted values show a similar degree of fluctuations, but are not well correlated with the observed fluctuation. The lack of month-to-month correlation is understandable based upon the hourly time series for Mannix and Fina presented above.

The probable systematic errors in the frequency of wind directions has a significant impact upon the monthly mean concentrations at individual monitors. In Table 15, the average of the predicted monthly means over the available data set for the simulations using an average of the concentrations for the 107-m and 60-m stacks at Suncor are presented. These values are then modified by a factor which represents the changed frequencies of winds towards each receptor from Suncor due to the discrepancies between the generated wind file and its calibration base of minisondes. This correction factor may roughly compensate for systematic under- or overprediction of the wind direction frequencies. However, it does not remove most of the effects of random scatter of wind directions. There are significant changes at individual receptors, but the net effect over all stations is small. The variances of the two sets of residuals are the same.

The residual for the predicted-less-observed concentration values, when averaged over all five Suncor receptors, shows a systematic underprediction of about 1 ppb. Averaging over all receptors tends to diminish the importance of wind directional errors. Although adopting a physical stack height of about 80 m appears to give good overall results, it is premature to ascribe the model prediction discrepancies to the terrain effect. There are several other ways in which the predicted concentrations from the 107-m stacks might be increased to match observations. One major effect neglected is the

Table 15. Effect on residuals of applying a systematic correction to the wind direction frequency distribution. The predicted values are based upon the average of the concentrations for the 107- and 60-m stack simulations at Suncor.

Station	No. of Months of Data	Observed	Predicted	Modified	Residuals	
		O	P	PR	P-O	PR-O
Mannix	12	2.8	2.7	4.4	-0.1	1.6
Ruth Lake	12	1.8	0.4	1.2	-1.4	-0.6
Fina	11	4.4	5.2	4.4	0.8	0.0
Lower Camp	6	2.1	1.0	1.3	-1.1	-0.8
Supertest	11	1.8	2.2	1.1	0.4	-0.7
Average		2.6	2.3	2.5	-0.3	-0.1
Average Absolute Value of Residuals					0.8	0.7

contribution of the flare stacks, which were not included in the present runs due to their intermittent nature. To determine the cause of the systematic underprediction at the Suncor stations, it is necessary to combine the results of the sensitivity studies with the results of the time series analysis.

5.6 DISCUSSION OF PREDICTION DISCREPANCIES

The discrepancies in the predicted and observed GLC values can be compared to the changes that result from variations of input data and dispersion parameters as discussed in Section 4. The procedure adopted was to examine the plume sigma predictions compared to observations, and to summarize the mixing processes during which most discrepancies in GLC values arose. These results indicated the types of modificiations which could lead to better GLC predictions of monthly means, and those which could improve predictions during specific mixing processes.

5.6.1 Comparison of Observed and Predicted Plume Sigmas

For sector-averaged concentrations, the vertical plume dimension as specified by σ_z, is much more important than the lateral plume dimensions specified by σ_y. The vertical dispersion determines how quickly the emissions can mix down to the surface; therefore, for monitors as close as 5 km, a good σ_z specification is essential to predict realistic GLC values. Any discrepancies in σ_y tend to be lost in the sector-averaging. A limited comparison of the predicted $_z$ values with some measured sigma values from the Athabasca Oil Sands area is shown in Figures 23, 24, and 25. The comparison is only approximate, since a standard convective mixing height of 1100 m was adopted. Variations of the order of 30% can be expected for mixing height effects as discussed in the sensitivity studies. One set of sigma data is discussed in Davison and Leavitt (1979), the other in Slawson et al. (1980). The data were divided into approximate stability groups according to the temperature gradient. At U = 4 m/s (at plume height), the observed σ_z values (mostly from the March 1976 aircraft data collected by Davison et al. 1977) show an X-dependence

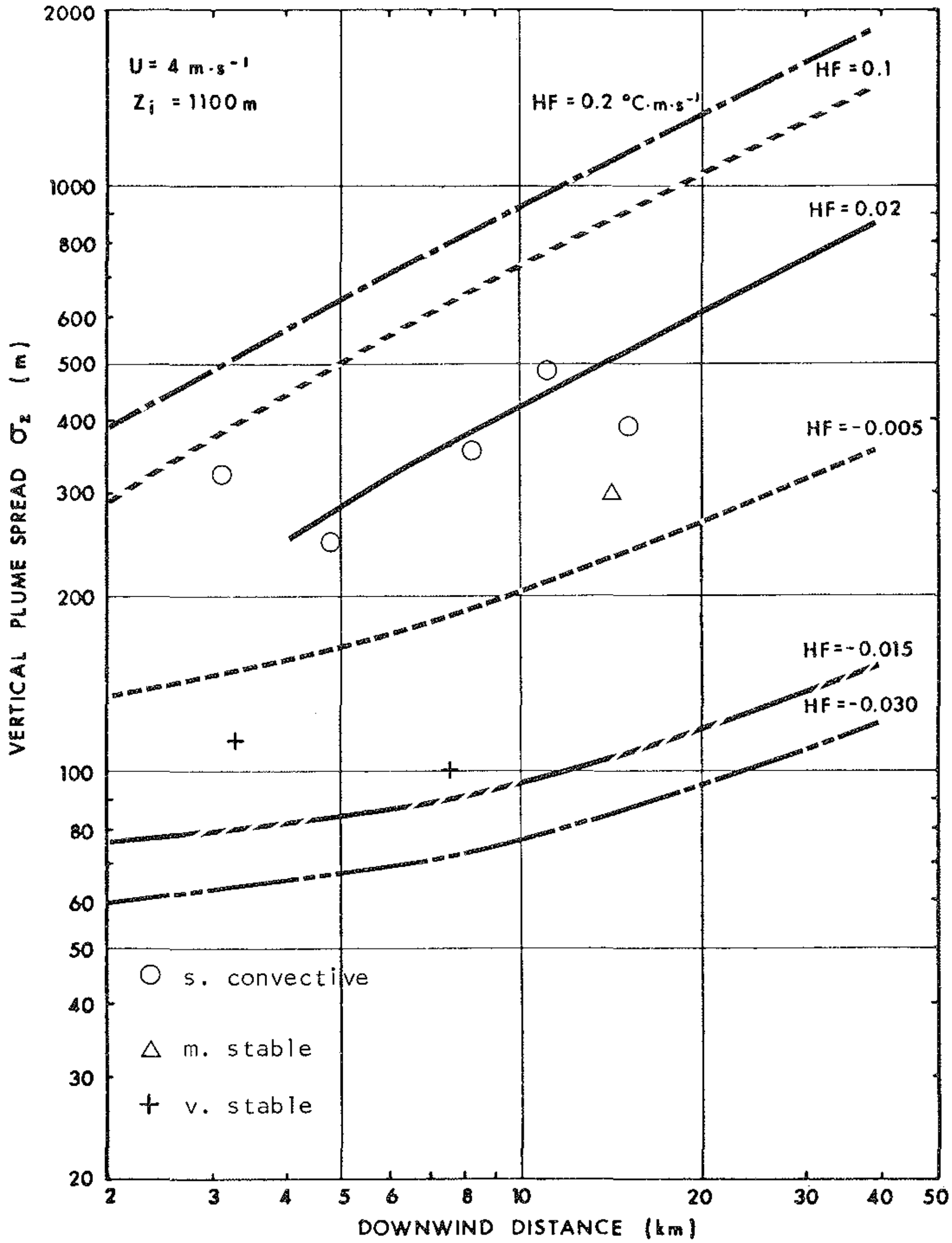

Figure 23. Comparison of observed σ_z values to σ_z curves predicted for a wind speed of 4 m/s and a mixing height of 1100 m. The effects of variations in mixing heights are not included.

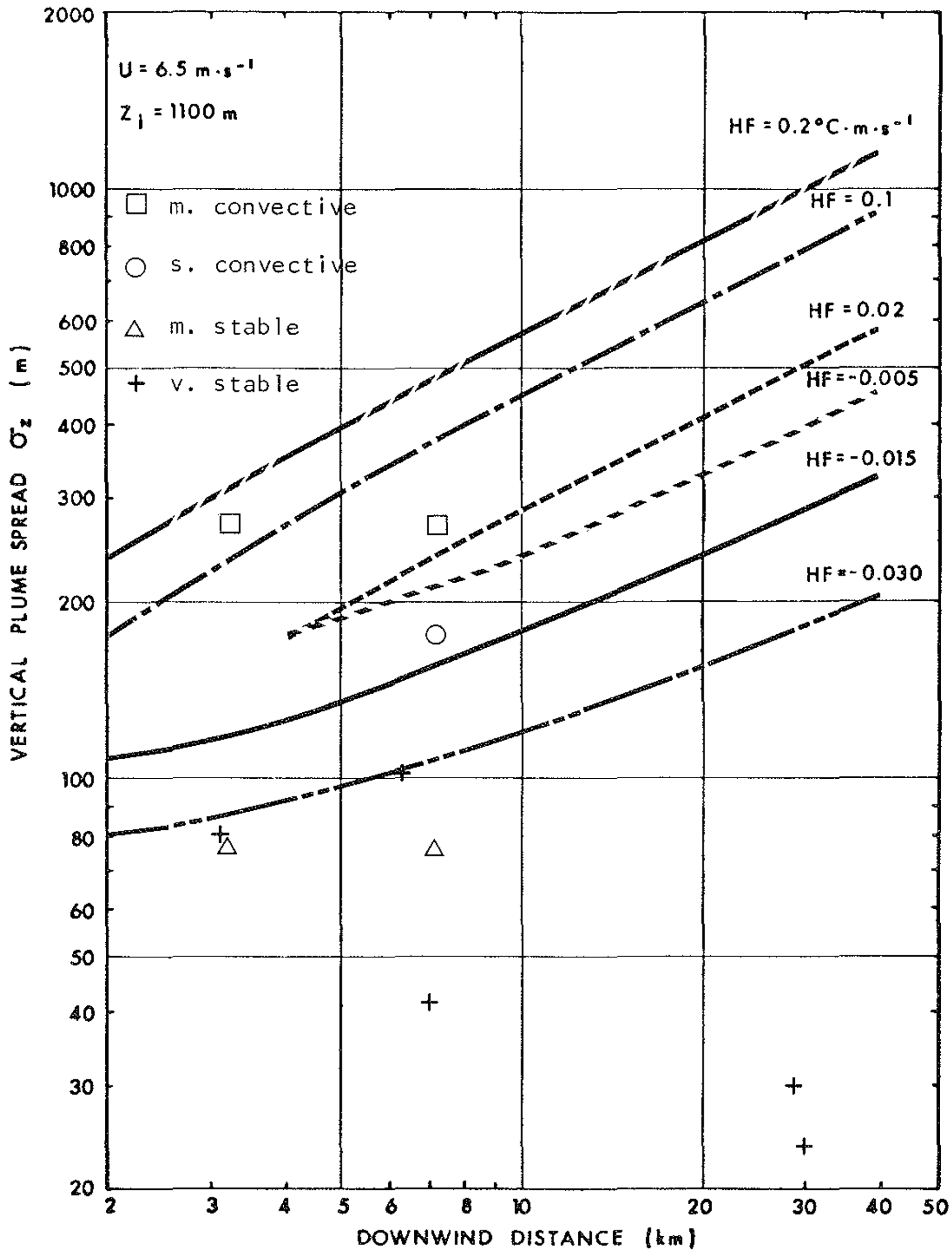

Figure 24. Comparison of observed σ_z values to σ_z curves predicted for a wind speed of 6.5 m/s and a mixing height of 1100 m. The effects of variations in mixing heights are not included.

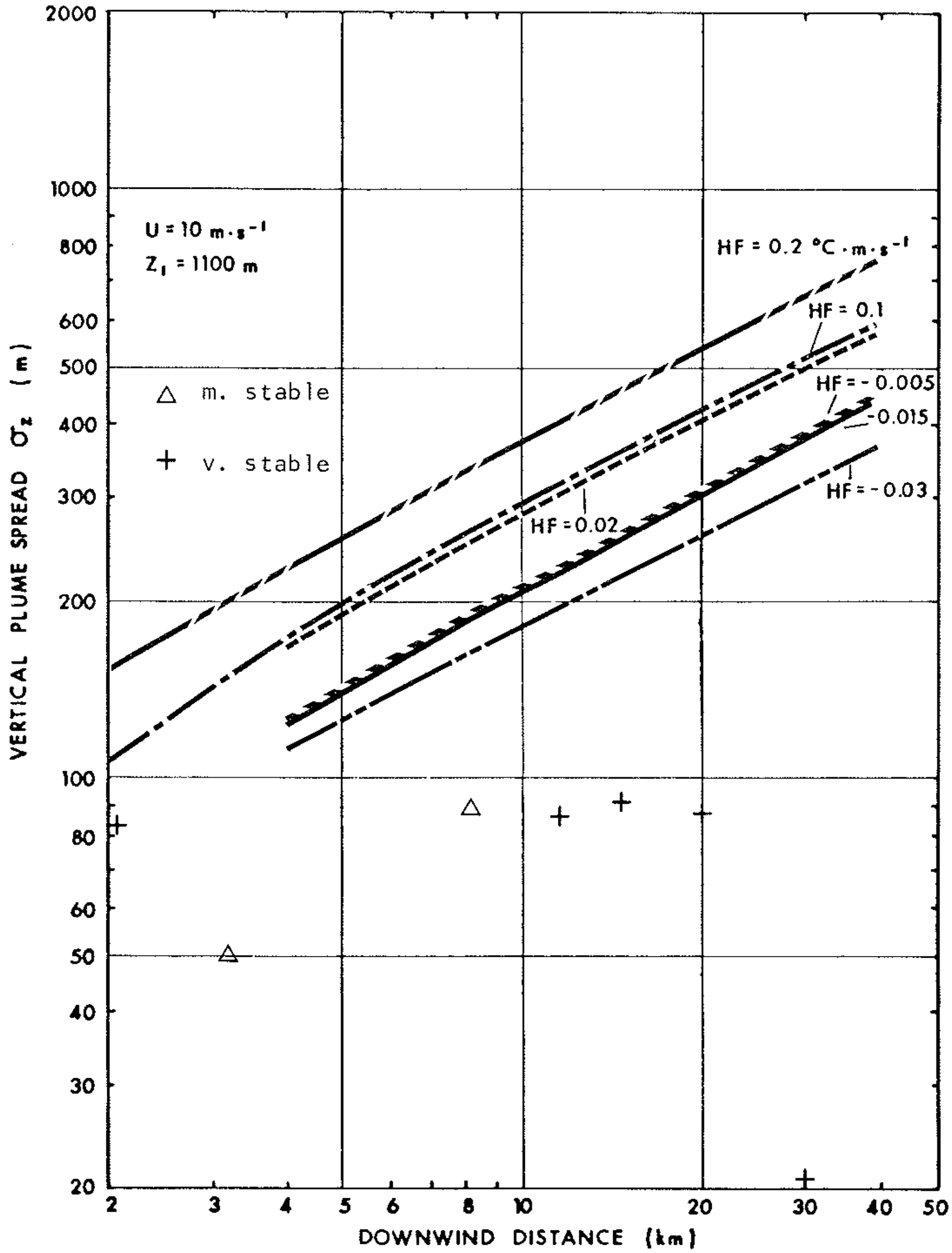

Figure 25. Comparison of observed σ_z values to σ_z curves predicted for a wind speed of 10 m/s and a mixing height of 1100 m. The effects of variations in mixing heights are not included.

and a magnitude that is consistent with the predicted σ_z curves. However, at U = 10 m/s the predicted values are much greater than observed, particularly at distances greater than 10 km. Note that all of the observed values at U = 10 m/s are for stable conditions.

The discrepancies at larger downwind distances in stable conditions at moderate and high wind speeds, may reflect a model limitation. The plume level winds may actually decouple from the surface layer in stable conditions. In such a situation, there may be minimal mixing at plume level, in spite of the presence of moderate and high winds. The model, however, assumes there is no decoupling and that the higher wind speed will generate significant mechanical turbulence. Matching the observed σ_z values in a decoupled stable situation is probably not worthwhile, since there will be minimal GLC values. It might be worthwhile for the model to parameterize the conditions leading to a decoupling so that no GLC values result. At present, the model will overestimate the GLC values under decoupled conditions.

The limitation on σ_z values, due to the present procedure for estimating surface winds, was outlined in a previous section. The adoption of a single power law exponent to estimate surface winds from 400-m level winds will tend to overestimate surface winds in stable conditions and, thus, tend to make the dispersion more similar to neutral conditions. In particular, the predicted dispersion for U = 10 m/s in stable conditions cannot be much different than that for near-neutral conditions. With a correct power law, the curve for U = m/s for the most negative heat flux level simulated in Figures 23, 24, and 25 would be close to that for U = 6 m/s.

In summary, the predicted σ_z values appear to be consistent with limited observations at lower wind speeds, but they probably overestimate the actual values in stable conditions. The formulation does not allow for a decoupled wind flow in stable conditions.

The σ_y values generated by the model are frequently a factor of two less than the field observed values of σ_y. A major exception is the Slawson neutral-to-slightly-stable data without significant wind direction shear. For this data set, which incorporates only regular and noise-free plume profiles, the agreement is very good. However, for any of the more typically irregular plume profiles that occur during convective mixing, and for stable conditions with wind direction shear, the model significantly underpredicts for all wind speeds.

Some comparisons between limited observations and the model formulation suggest that a major part of the problem lies with the determination of σ_A. The formulation for σ_A incorporated in the model was an empirical formulation based upon data primarily from relatively homogeneous terrain in stationary conditions. Major differences can result from terrain and roughness influences and can occur in disturbed weather due, for example, to the presence of convective clouds. The model contains essentially the same σ_y formulation as was tested by Davison and Leavitt (1979). When observed values of σ_A were utilized, most of the observed σ_y values were less than 40% larger than predicted. This strongly suggests that the PBL parameterization underestimates σ_A.

There probably exist sufficient data to begin to clarify the σ_A specification. The Doppler accoustic radar, operated by Syncrude, is generating a data base which should be very useful in developing a more accurate σ_A specification. For strongly convective conditions, the data from the Tall Tower should be applicable, since valley effects are presumably small.

For moderately stable conditions (or in the presence of a direction shear due to baroclinicity), the effects of wind direction shear in the source region can totally dominate σ_y for the first 10 or 15 km. Thus, a useful σ_y formualtion for these conditions may require an estimation of wind direction shear in the time series file. Such an improvement would be difficult with the existing data base.

The Lagrangian integral scale in the model was initially taken to be 500 m. Some of the discrepancies between the predicted and observed values of σ_y may be due to a systematic underestimate of the integral scale appropriate for the AOSERP study area. In addition, an allowance may be necessary for changes in the integral scale as a function of turbulent intensity and thermal stability.

In summary, the predicted σ_Y values are smaller than observed values in typical convective conditions and in stable conditions when a directional wind shear is present. The problem in convective conditions appears to be in the σ_A specification.

5.6.2 Summary of GLC Prediction Problems

The comparison of the time series of predicted and observed concentrations at Mannix and Fina for 1977 provided an assessment of the model and data base performance for various mixing processes.

The predictions in convective conditions appeared to be reasonable, with the exception of July. In January, there was little convective mixng predicted, matching observations. A careful selection of mixing height, calculational levels and boundaries is essential to produce proper results. In April, predictions were of the correct magnitude, except for a single hour when a value of 500 ppb was observed at Fina. In July, more frequent, lower-level concentrations were observed in convective conditions than predicted. The maximum observed GLC values were lower than observed values in April. In October, the magnitude of the predicted and observed values in convective conditions were consistent.

For mechanical mixing conditions, the model can predict GLC values consistent with observations. The specific timing of events at a given receptor is generally poor. This discrepancy is largely due to wind direction errors. The frequency of occurrence of GLC values at Mannix and Fina due to mechanical mixing is underestimated. The problem could be systematic wind speed underestimation, problems in the formulation or parameters adopted for mechanical mixing, or a possible low-level source.

The GLC predictions showed a 60% systematic underprediction when averaged over all the 12 months of the time series file for the five Suncor stations. There are several reasonable means by which to remove most of the systematic error; however, it is important to ensure that parameter manipulation does not lead to incorrect simulations of the various mixing processes.

5.6.3 The Prediction of an Extreme Value

The presence of an extreme value of 500 ppb in conditions that are predicted to be convective for a single hour in April at Fina has several possible explanations. The fact that it is much higher than any other observed value suggests that the problem is not a frequent systematic error in the model formulation; rather, it is probably a source specification error, or possibly a statistical sampling characteristic in the observed data.

Assuming the measured value is valid, then there may be a statistical sampling problem involved. The model is formulated for ensemble-averaged dispersion. The time averaging over 1 h at a given receptor represents one value of a large population of similarly measured values. The values comprising this ensemble population will have a standard deviation about the ensemble mean. The representativeness of a single measurement depends upon the size of the ensemble standard deviation and, hence, upon the amount of variation associated with time scales of the order of one hour. In convective conditions, it is possible to have large-scale features which may give significant variations at time scales of 1 h (Venkatram 1980). The prediction of extreme values for 1 h averaging times is difficult since the ensemble values and the standard deviation about the ensemble average must be known. Recent work (Djurfors 1980) has suggested that 1 h averages may have significant ensemble standard deviations.

A brief examination of the available meteorological parameters on 2 April indicate that a sampling problem relating to atmospheric non-stationarity may indeed have contributed to the extreme value. Predicted 400-m winds are northwesterly at about 4 m/s for the hours around 1100 on 2 April. Fort McMurray airport observations indicate clear skies with temperature of -10°C and warming. Temperatures from previous days suggest the beginning of a warming trend after several days of cooling temperatures. Radiation measurements suggest the atmosphere to be slightly unstable. In fact, this is what the model calculates for this case, accounting for the effect of snow cover on albedo. However, given these values, the model cannot predict a concentration of 500 ppb; non-stationary effects must be factors.

One of several factors may cause the extreme value. Advection effects are almost certainly present, due to the activity of air masses in the spring season and as evidenced by warming and cooling trends in the hours before and after the event. If warm air is present aloft, with positive heat flux near the surface, one can postulate a weakly mixed layer topped by warm air which may reduce both plume rise and mixing height, resulting in higher surface concentrations. Similar results could be produced by subsidence induced by lee waves, inflectional instability, or other secondary local circulations. None of these factors are accounted for by the Gaussian model. A detailed case study is required to determine which, if any, of these factors are involved.

5.6.4 Summertime Convective Conditions

The less frequent and larger GLC values predicted for convective conditions in July are probably due to the large σ_A values in strongly convectinve mixing, combined with the restrictions of sector averaging at downwind distances of 5 km. With a strong positive heat flux, the value of σ_A can be 15 to 20°; therefore, near the source, averaging withing 22.5° sectors may be restrictive. As a first approximation from Volume 1 of this report

$$\sigma_y = \sigma_A (2\ell_v X)^{1/2} \qquad (19)$$

At 5 km, where σ_A = 0.36 radians, corresponding to strong convection in light winds, σ_y = 800 m. The sector width for 22.5° sectors at 5 km is 1950 m. Thus, the sector is only about 2.3 σ_y, meaning that the calculated GLC value would be about one-third too large. Since the predicted σ_y values were often less than observed values in convective conditions, the discrepancy may be larger. If the wind also meanders through more than one section within the hour, then the effects of sector-averaging would be even more pronounced. Thus, the overprediction in summertime convection is probably due to the effects of sector-averaging. There should not be any systematic error in cumulative effects.

5.6.5 Application of Sensitivity Study Results

The sensitivity studies provide a basis for resolving model prediction errors. The range of possible parameter modifications are constrained by the requirements to maintain realistic predictions for the various mixing processes. The need for parameter changes is limited by uncertainties in both the input and observed data. The Suncor stations used for model comparisons were all about 5 km from the source, except for Supertest; thus, there remains some uncertainty as to the discrepancies at larger downwind distances.

The heat flux values have significant uncertainty due to the limited data utilized in the formulation. At 5 km, the change from a heat flux value of 0.02 to 0.10°C·m/s causes a major change in GLC values. Thus, it may be advisable to choose a smaller second value of positive heat flux rather than 0.10. However, the net effect of this discretization will be small. When the effects of sector-averaging are allowed for, the convective conditions appear to be reasonably well predicted. Thus, there is no strong evidence that the heat flux formulation should be altered, or that the radiation values have major systematic errors that impact on average GLC values.

The mixing height has little effect at 5 km, except for inclusion or exclusion of plumes. The mixing height data in the present time series file are probably adequate for the purposes of the present model, and modification to this data set will not lead to the resolving of the discrepancies between predictions and observations.

The wind direction is a major source of errors for specific case studies and for monthly averages. However, the 60% systematic underprediction of GLC values, when averaged over all stations, is almost certainly not due to wind direction errors.

A systematic underprediction of wind speed could possibly account for the overall 60% underprediction. However, a change in wind speed of about 70% is necessary for a 60% change in GLC values at a downwind distance of 5 km. It is very unlikely that values in the time series have that large a systematic error.

The use of 60-m stacks at Suncor to attempt to simulate a possible terrain effect lead to better overall agreement. The same effect could be realized with a lower plume rise through the use of either a smaller value of C_1 or X_f. It is only in mechanically dominated or convective conditions that significant GLC values can occur at 5 km from the source; thus, C_2 variations should not affect the overall discrepancy. A change to $C_1 = 1.2$, or $X_f = 16\ 000$ m, could also generate changes in average GLC values of about 40%.

An increased roughness length, Z_o, could also remove the 60% discrepancy of the overall averages. From the sensitivity study presented earlier, a change in Z_o can produce changes of GLC values at 5 km downwind of up to a factor of 2. However, in convectively dominated mixing, the roughness length has no effect. In stable conditions, increasing Z_o results in more frequent mechanically dominated mixing, and higher GLC values. Thus, an increase in Z_o would tend to increase the magnitude and frequency of GLC values throughout the day, except in convectively dominated conditions.

6. COMPARISONS WITH OTHER FREQUENCY DISTRIBUTION MODELS

In the following sections, the present model is compared to the more familiar Climatological Dispersion Model (CDM). Both models are examined in terms of their structure, flexibility, data requirements, and dispersion formulations. A direct comparison of model predictions was not possible because equivalent data bases were not available for the two models. Nevertheless, a discussion of the residuals of observed to predicted values for different applications of the models provides some indication as to the limiting factors for each model at the present time. The scope of the present project precluded the development of a data base that would enable a more definitive model comparison.

6.1 GENERAL MODEL FEATURES

The present model provides users with a much more flexible airshed management tool than traditional frequency distribution models. The additional model capabilities are due to the way in which the calculated ground level concentrations are stored and utilized. As outlined in Volume I, the present model calculates the ground level concentration for each source-receptor pair for each dispersion class. To this extent, it is similar to normal frequency distribution models. The major change in model structure is that, in the present model, the GLC contributions are calculated directly for a time series of meteorological data. By calculating GLC values in this way, the exclusion or selected weighting of particular meteorological conditions can be varied from run to run without the need to redo the major dispersion calculations. A time series of calculated values may be listed for validation purposes, or for further time series or statistical analyses.

In a traditional frequency distribution model, the time series of meteorological data is reduced to a frequency distribution of dispersion classes; this frequency distribution is then used to calculate a frequency distribution of GLC values. No time series of GLC values is generated for validation or other analyses. In the CDM model, there is no way to selectively weight the GLC values occurring in certain conditions, nor is there the flexibility of source specification without re-running the dispersion calculations. In summary, one of the important feaures of the present model is its flexible usage of the calculated GLC values.

The present model incorporates a different disperion formulation from the CDM. It would be possible to use the identical dispersion calculation procedures that exist in CDM or other similar models. However, it was recognized that the CDM did not incorporate many of the advances in dispersion meteorology that have arisen over the last 20 years. The dispersion and meteorological characteristics of the Athabasca Oil Sands region, in particular, have been studied through a number of major programs, the results of which could be incorporated into a more modern dispersion framework.

The dispersion class specifications are somewhat similar in the broad physical concepts incorporated. In the Pasquill-Gifford approach used by the CDM, the dispersion class is a function of both solar radiation and wind speed; thus, it contains a ratio of thermal and mechanical mixing. In the present model, which incorporates a PBL parameterization to generate σ_A and σ_E, scaling velocities and length scales are calculated for both mechanically and convectively dominated planetary boundary layers, according to similarity theory. In this way, the extensive results of measurements and theoretical developments in boundary layer similarity theory can be utilized in a dispersion formulation. Although there remain uncertainties in the value of certain parameters and in some of the approximations used, the components can be separately evaluated and form a complete and consistent theoretical framework.

Direct measurements of wind direction and elevation fluctuation would be superior to either the Pasquill-Gifford classes or the PBL parameterization adopted in the present model. The present model will utilize these measurements, when they become available, with only minor coding changes.

The present model incorporates the mixing height, Z_i, in convective conditions directly into the plume sigmas through the scaling velocity, w_*. This dependence on Z_i means that the maximum concentration for a trapped plume will not be double that of a plume in a boundary layer with a large mixing height. The scaling of the dispersion with Z_i is not included in the CDM.

The present model has a physical basis for site-specific features. If the model is applied in another region, then the roughness length, Z_o, can be changed as necessary, in keeping with the new site characteristics. There is no clear physical basis for changing dispersion curves according to site characteristics in the CDM.

In summary, the present model incorporates a dispersion formulation that is more consistent with present understandings of the PBL than the CDM formulation. The parameters in the model can be subjected to separate tests, and sensitivity and error studies; thus, the model becomes open to continual improvement of its components.

A critical factor in the successful operation of a model as an airshed management tool is the development of a suitable data base to drive the model. The basic data requirements of climatological dispersion models are similar. Input data must include wind speed, wind direction, a measure of the thermal stability, and convective mixing heights. The necessary measure of thermal stability depends upon the dispersion algorithms being used and can include the incoming solar radiation, the net radiation, the surface heat flux, or the temperature profile. A comparison of models when different data sets are used to drive the models cannot differentiate the model formulation effects from the data effects.

6.2 DISPERSION FORMULATIONS

The present model has two basic differences in the dispersion formulation from the CDM. The same Gaussian formulation is the basis for both models; however, in the present model, the plume sigma specification and the dispersion class specification are different from the CDM.

The plume sigmas in the present model are related to the wind azimuth and elevation angle fluctuations through the statistical disperson theory. As discussed more thoroughly in Volume I of this report and in an earlier section of Volume 3, the model contains the concept of a source-dominated region and 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 if not directly measured. Site-specific characteristics enter the dispersion formulation by means of known physical parameters such as the roughness length. In comparison, the CDM utilizes plume sigma curves which have no theoretical basis and which are known to be poor predictors in the AOSERP study region (Davison and Leavitt 1979).

6.3 DATA BASE

Normally, the CDM operates on a data bank generated by a "STAR" analysis. This analysis normally examines surface data from a standard observing facility, such as an airport, over a period of typically 25 years and calculates the frequency distribution of the Pasquill-Gifford dispersion classes, wind speed, and wind direction. Walmsley and Bagg (1977) developed a correlation technique to generate a longer time-based wind field at Mildred Lake using the longer time series at Fort McMurray Airport.

The present data bank is different in that other data sources are used. The Fort McMurray Airport observations are used to generate many of the meteorological parameters on the time series data file. The mixing height is based upon a climatology of over 2000 minisonde releases in the Athabasca Oil Sands area. The wind speed and direction time series were estimated from the 850 mb analysis.

Another major difference in the data bank is that the present data bank consists of 12 months spread over three years. It would be clearly advantageous to expand the data base to be more climatologically representative; however, the optimum data source or generation procedure, particularly for the winds, needs to be established first.

The wind data represent a major source of uncertainty. The surface winds at Mildred Lake, and even the winds at the top of the 152-m tower at Lower Syncrude, were shown in Volume 2 to be very poor predictors of the wind at typical plume heights, as measured by minisondes. This finding was the rationale for estimating plume level winds from the 850 mb analyses.

6.4 DISCUSSION OF MODEL PREDICTIONS

Walmsley and Bagg (1977) applied the CDM to the Athabasca Oil Sands area in order to predict average SO_2 concentrations. The CDM predictions were compared with available observed data; the results are shown in Table 16. A direct comparison could not be made with the present model because data to drive the model for the same period were not available. However, GLC predictions from the present model for the same stations used in the CDM study were used for a preliminary comparison and are shown in Table 17. The values for Syncrude 3 may be suspect, because of the major change in the discretization of monthly values beginning in July 1977, as discussed earlier. Because of this uncertainty, the residual calculations included a case where Syncrude 3 was omitted and also a case when Lower Camp was substituted, so that a station towards the north or northwest was included in the comparisons.

The CDM predictions in Table 16 have a striking feature in the value of the residuals, with repsect to wind direction. The concentrations for Fina, to the east of the Suncor plant, are underpredicted; the concentrations for Syncrude 3 (Mildred Lake) to the northwest are overpredicted; and the values for Supertest and Mannix to the south are overpredicted. Walmsley and Bagg used winds based upon Mildred Lake winds, which are now known to be strongly influenced by the river valley. Some of the residuals from the CDM predictions of annual concentrations may be explainable in terms of a systematic wind direction error in the data base used to drive the model.

For the present model, there appears to be a systematic underprediction. Areal averaging is approximated by averaging over the Suncor stations. This procedure tends to diminish the effects of wind direction errors. The possible sources of the overall discrepancy in

Table 16. A comparison of observed annual average SO_2 concentrations and values predicted by the CDM dispersion model (based on Walmsely and Bagg 1977).

Station	Observed (ppb) 1974	1975	1976	Average	Predicted (ppb)	Residuals
Mannix	-	-	3.1	3.1	5.5	2.4
Ruth Lake	-	-	2.7	2.7	2.9	0.2
Fina	-	-	6.5	6.5	4.0	-2.5
Supertest	3.3	1.1	1.9	2.1	2.8	0.7
Syncrude 3	2.0	1.4	3.7	2.4	4.5	2.1

1. Average of residuals = 0.6
2. Average absolute value of residuals = 1.6.
3. Linear correlation coefficient R = 0.17
4. Rank correlation coefficient P = 0.50

Table 17. Residuals of the predicted and observed GLC values for the present model.

Station	No. of Months	Obs.	107m [a] stack Pred.	107 m stack Residuals [b]	84 m [c] stack Residuals	Mod.[d] Dir. Residual
Mannix	12	2.8	1.6	-1.2	-0.1	1.6
Ruth Lake	12	1.8	0.3	-1.5	-1.4	-0.6
Fina	11	4.4	3.2	-1.2	0.8	0.0
Supertest	11	1.8	1.7	-0.1	0.4	-0.7
Syncrude 3	11	3.9	0.6	-3.3	-3.1	-2.1
Average		2.9	1.5	-1.5	-0.7	-0.4
Average absolute value of residuals				1.5	1.2	1.0
Omitting Syncrude 3:						
Average		2.7	1.7	-1.0	-0.1	0.1
Average absolute value of residuals				1.0	0.7	0.7
Substituting Lower Camp for Syncrude 3:						
Average		2.6	1.6	-1.0	-0.3	-0.1
Average absolute value of residuals				1.0	0.8	0.7

[a] For the 107 m stack predictions involving Syncrude 3, the linear correlation R and rank correlation p values are:
R = 0.5, p = 0.5.

[b] Residuals are defined as Predicted less Observed.

[c] The 84-m stack values represent the average of simulations using the actual 107-m height and a test height of 60 m for the Suncor stack; the lower height was adopted to test for possible effects due to the lower elevation of the Suncor plant compared to most of the monitors.

[d] The "Mod Dir" values are values generated by multiplying the 84-m stack values by a factor which corrects, for the systematic frequency distribution, errors in wind directions.

predictions were discussed in the previous section. Adopting a lower physical stack height would give good time- and space-averaged GLC predictions; however, changes in the adopted values of several other parameters could have a similar effect. Adjusting the adopted value of the roughness parameter, Z_O, to a value of about 0.9, rather than the present value of 0.3, would also remove the underprediction and is reasonable from a physical viewpoint. Increasing the value of the roughness length has the advantage of leaving the predicted GLC values in convective conditions unaffected. Adjustment of parameters, however, should be based upon the examination of GLC values at downwind distances different from those for the Suncor stations. In addition, an estimate of the appropriate value for the roughness length, Z_O, could be made through an analysis of existing data to remove that significant uncertainty.

A direct comparison of the CDM and the present model is difficult. If better wind data were used, the CDM predictions would almost certainly be improved. Better wind direction data would also improve the present model's predictions, as shown by the improvements, due to a gross correction factor based upon frequency distribution errors in the wind direction. There is a systematic underprediction in the present model which can be easily overcome for annual predictions by adjustment of one or more physical parameters in the model subject to constraints on the time series GLC predictions, and on improvements in physically measureable parameters.

In summary, the present model appears to be at least comparable to the CDM in long-term accuracy. However, uncertainties in the data base are critical for both models and this precludes a more definitive statement. The present model, however, is more suited for evaluating the reasons for discrepancies and for component validation than the CDM, because of the model structure and because of the use of definable and measureable physical parameters. Specific analyses or measurements can be undertaken to clarify the value of such parameters as the roughness length.

7. CONCLUSIONS

The accuracy of model predictions is a function of at least four components:

1. the model formulation and the dispersion formulation parameters;
2. the meteorological data base used to drive the model;
3. the source specification; and
4. the air quality data used to determine the prediction accuracies.

Each of these components was discussed in previous sections; a summary of each follows.

7.1 MODEL AND DISPERSION FORMULATION

The model formulation is a steady-state Gaussian dispersion model with sector-averaging. The use of a Gaussian formulation means that a single dispersion class is used, regardless of vertical variations. A steady-state formulation means that changes in dispersion during transit time are not simulated, nor are processes such as fumigation. Sector-averaging removes artifacts of concentration fluctuations across a sector, due to the use of a short meteorological data time series to represent a long-term average. These characteristics of the model formulation are adequate for a frequency distribution type of model where accuracy is desired for averages, or frequency distributions in certain desired meteorological or seasonal conditions. However, these same characteristics mean that the use of the existing version of the model for an episodal case study is inappropriate and would lead to significant errors.

The dispersion formulation is based upon statistical theory in both the horizontal and vertical, together with a PBL parameterization for σ_A and σ_E. In addition, the formulation includes an effective downwind distance formulation for the effects of source-dominated dispersion. The plume sigma formulation underestimates σ_y for typical convective conditions; the problem appears to be in the underestimation of σ_A. However, for sector-averaged GLC values, the σ_y value is of little concern. The plume σ_z values appear to be reasonably well predicted for light winds, based on a limited validation. In stronger winds, σ_z is overpredicted for stable conditions. This overprediction is partly due to the power law exponent used to estimate surface winds from the 400-m level winds for the calculation of the friction velocity. The size of the error, in very stable conditions, is equivalent to the use of a lower wind speed (about one typical wind class). The σ_z values in a situation of a decoupled surface and upper layer are not predicted. A comprehensive validation of σ_z values has not yet been undertaken.

The dispersion formulation parameters may be site-specific or of more general applicability. In the present model, efforts were made to formulate the dispersion process in terms of parameters that had clear physical meaning and that could be estimated independently of the GLC values. Sensitivity studies were undertaken to estimate the effects of their uncertainties.

Uncertainties in the plume rise coefficients, and in the duration of plume rise in neutral or convective conditions, can have a significant impact upon GLC values, depending upon atmospheric stability and downwind distance from the source. Changing C_1 from 1.4 to 1.6 decreases the maximum GLC by about 25% and moves the maximum about 1.5 km farther from the source. That change in C_1 is the same as changing X_f from 2000 to about 2400 m. Generally, changing a typical wind speed or heat flux class has a more important effect, especially for uncertainty levels of the stable plume rise coefficient, C_2.

The roughness length, Z_o, can have a major impact on GLC values. The roughness length is a site-specific parameter which affects the amount of mechanical turbulence generated for a given wind speed and thermal stability. In convectively dominated situations, the roughness length has no effect. At a distance of 5 km from the source, the change in Z_o from 0.3 to 0.9 m in mechanically dominated mixing increases sector-averaged GLC values by over 40%. The effect is greater than changing the wind speed from 10 to 15 m/s, but less than changing the wind speed from 10 to 6.5 m/s. In stable conditions, the effect of a Z_o change from 0.3 to 0.9 m is to change the GLC value by several factors, and to change the location of the maximum by many kilometres.

The free convective scaling constant linearly scales the fluctuations of the vertical wind, σ_E. A decrease in the constant results in a lower maximum GLC value farther from the source; however, the magnitude of the estimated uncertainty suggests that there is not a significant error.

7.2 METEOROLOGICAL DATA BASE

The frequency distribution model requires a time series file of selected meteorological parameters. Any uncertainties in the time series file parameters can have an effect on the results generated by the model. Parameters of particular concern are those that can enter directly into the model formulation and include hourly values of wind speed and direction in the plume layer and convective mixing heights.

Limited scatter in these parameters is acceptable due to the discretization of plume dispersion classes. The application of the model results can also determine the level of accuracy required in the data. For example, an evaluation of a case study would require more accurate data than an evaluation of a long-term annual average concentration. However, even if a user is only interested in long-term averages, a reasonably accurate time series data base is still required, because monthly average concentrations in the Athabasca Oil Sands area are dominated by infrequent events during which relatively large concentrations are observed. If the data base precludes the possibility of predicting the occurrence of these events then there may be some question as to the validity of the monthly average values. An evaluation of the wind speed, wind direction, and mixing height data indicated that the scatter or uncertainty in the time series value can cause a shift from one dispersion class to another. The comparison of predicted and observed concentrations at Fina and Mannix indicated that the data base has significant limitations, with respect to predicting case studies and monthly events.

On a number of occasions, the wind direction could not account for observed concentrations at either of the receptors. For example, during January, only 25% of the non-zero concentrations observed at Fina were associated with a westerly wind. A westerly wind is required to bring a plume from the Suncor plant to Fina. The mixing height is most important when it is similar to the plume height. This can result in either an elevated plume embedded in a stable layer, or a trapped plume that can be mixed down to the ground. Limited mixing situations are important to estimate GLC values during the winter months.

Hourly time series mixing height values are seasonal averages; that is, the same diurnal variation is assumed for each season. The use of seasonal averages is of limited use for the purposes of evaluating case studies.

7.3 SOURCE SPECIFICATION

The GLC values predicted by a model can be accurate only if there is an accurate source specification. If there are significant variations about the average emissions, then additional noise is introduced into the comparison of observed and predicted values.

The treatment of flare stacks may present problems. The emissions from flare stacks may vary significantly and may introduce some significant perturbations on the actual GLC values. Since the emissions of the flare stacks represented only about 1% of total sulphur emissions at Suncor, flare stacks were ignored for the validation runs.

Fugitive or other non-specified, low-level emissions may have a major effect on a nearby air quality monitor. The apparent accuracy of model predictions can be very low if there are any low-level emissions close to a monitor.

7.4 AIR QUALITY DATA

The accuracy of a model is usually defined by how well it compares with observed data; however, the observed data may have significant uncertainties which may generate an apparent model accuracy problem. In the Athabasca Oil Sands area, there are major uncertainties in the observed data. Perhaps the most serious problem is the specification of a lower truncation level. The monthly averages from the Syncrude stations are subject to a 10 ppb discretization; monthly averages were never greater than 10 ppb. A proper evaluation of model performance should be based upon the predicted and observed hourly time series of concentrations which exceed a truncation level beyond the level of observer bias. The actual monthly averages of observed data may, indeed, warrant the 10 ppb discretization because of the near-zero uncertainties, but these data should not then be used as accurate observations for model comparisons.

7.5 SUMMARY OF MODEL ACCURACY

Based upon the comparisons with measured GLC values some conclusions can be drawn as to the overall accuracy of the present model. The model with present parameters appears to underpredict the time and directionally averaged GLC values at approximately 5 km by about 60% (for the five Suncor monitors). A change in the Suncor physical stack heights used in the model run from 107 m to about 85 m to account for terrain effects would reduce the discrepancy to 25% and a further correction for the wind direction frequency distribution would reduce the discrepancy to about 7%. An increase of Z_o to about 0.9 m from the adopted value of 0.3 m could also largely remove the discrepancy. The model appears to be predicting GLC values in convective situations in a reasonable way. At 5 km, the 16-point sector-averaging leads to an overestimation of GLC values during strong summertime convection, due to the large σ_y values; however, during the weaker convection in spring, when sector-averaging has no significant effect, the predictions are very good.

The model appears to underpredict the frequency of GLC values during mechanical mixing events in non-convective or weakly convective hours. An increase in Z_o could probably remove this problem and lead to better overall agreement without affecting the more strongly convective cases.

The timing of specific events is not well predicted. Wind direction errors are sufficiently large that the model cannot be used to reliably predict concentrations at a given receptor at a given hour.

Monthly averages at a given receptor are usually dominated by a very small number of events. This feature of the observed (and predicted) data means that reliable averages at a single receptor generally require a longer averaging time than one month.

There are systematic errors in the wind direction frequencies which appear to impact significantly (factor of two) upon long-term averages at a given receptor. Until an improved directional data set is available, some form of directional averaging is highly advisable.

8. RECOMMENDATIONS

The validation and sensitivity studies provided a basis for evaluating the existing uncertainties in the model predictions. The magnitude of uncertainties in various components of the model and data system could be compared, leading to the following recommendations:

1. The air quality data from all the monitors should be put into a computer-compatible format so that a standard analysis of the observed data can be undertaken. The standard analysis should include the adoption of a realistic truncation limit to remove observer bias.
2. The validation of the model should be extended to include the Syncrude monitors, to ensure that model evaluation and tuning is consistent with observations at several downwind distances. For testing purposes, the same truncation limit applied to the data should be applied to the model predictions.
3. The value of the roughness length, Z_o, appropriate for the Athabasca Oil Sands area, should be estimated from existing data. The minisonde data, which are in the process of being digitized, should provide a basis for the calculation if care is used in the selection of profiles for analysis, to remove cases with significant advection or transient effects.
4. The magnitude of terrain effects should be estimated using existing numerical models to assess whether the terrain effects are a likely cause of the apparent model underpredictions of GLC values. Specifically, it should be determined whether the terrain effects on the Suncor plume can be approximated by a lower physical stack height.
5. The calculation of the friction velocity, u_* , should include an allowance for a stability dependent power law exponent to estimate near surface winds from the 400-m level winds on the time series.

6. The plume rise formulation should be reviewed, due to the impact that minor variations in plume rise coefficients have on the final GLC values. The results of the extensive work undertaken by Syncrude Canada Ltd. should be parameterized for inclusion into the model, if significant systematic discrepancies exist with the present formulation.
7. The wind speed and direction data base should be re-examined to attempt to find a better way to estimate plume level winds. The use of surface level winds at one or more well-exposed surface sites, such as Stoney Mountains, should be considered, possibly in an interative mode such that the appropriate station is chosen depending upon the overall wind field from several stations. The data base being generated by Syncrude with their accoustic doppler radar should be utilized, if possible, as another major data set for the generation of the wind algorithms.

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10. APPENDIX

Figures 26 through 35 compare observed and predicted monthly average SO_2 concentrations for 10 air quality monitoring sites: Manix, Ruth Lake, Fina, Lower Camp, Supertest, and Syncrude 1 through Syncrude 5. The effects of 107 m and 60 m stacks at Suncor are shown.

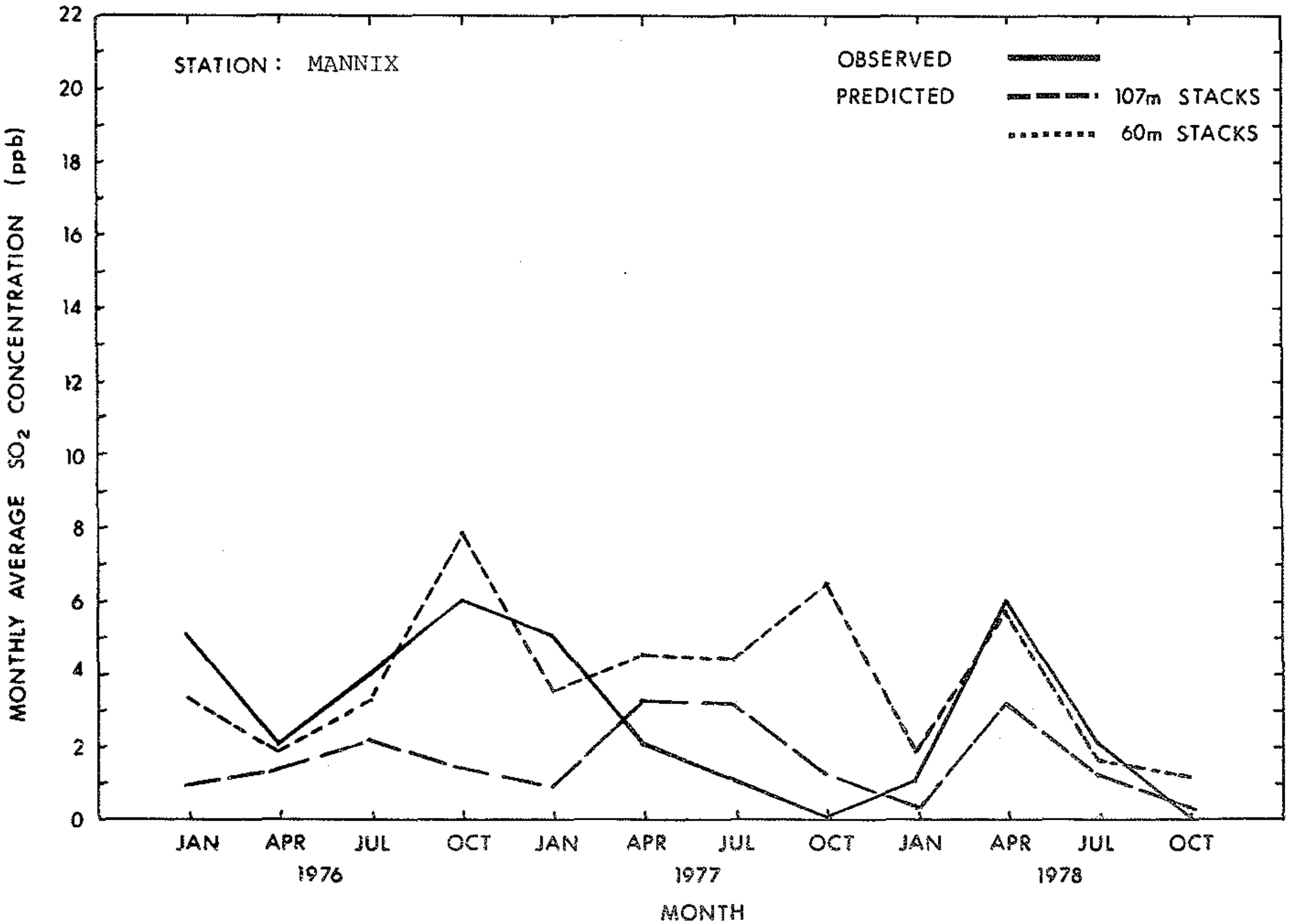

Figure 26. Mannix Station.

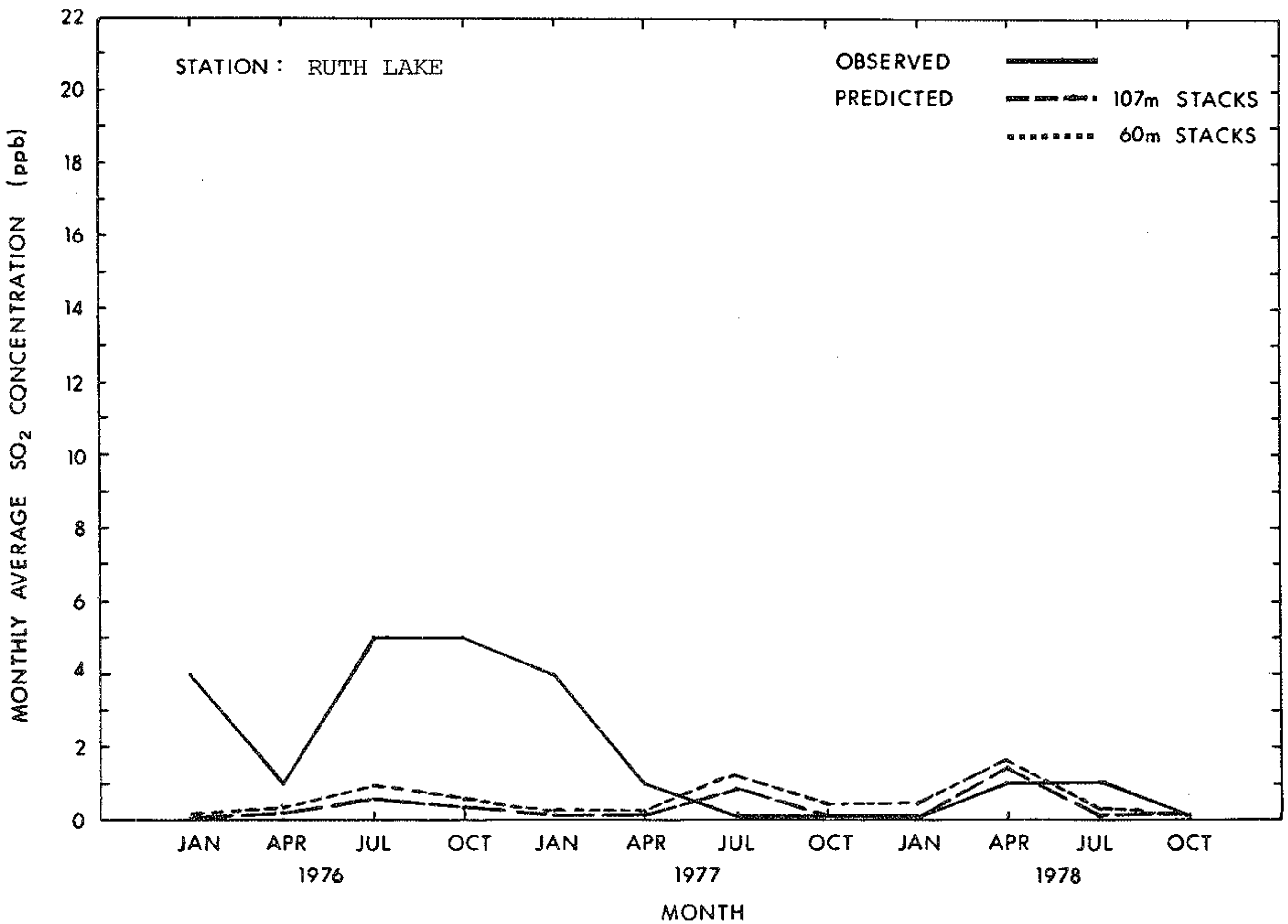

Figure 27. Ruth Lake Station.

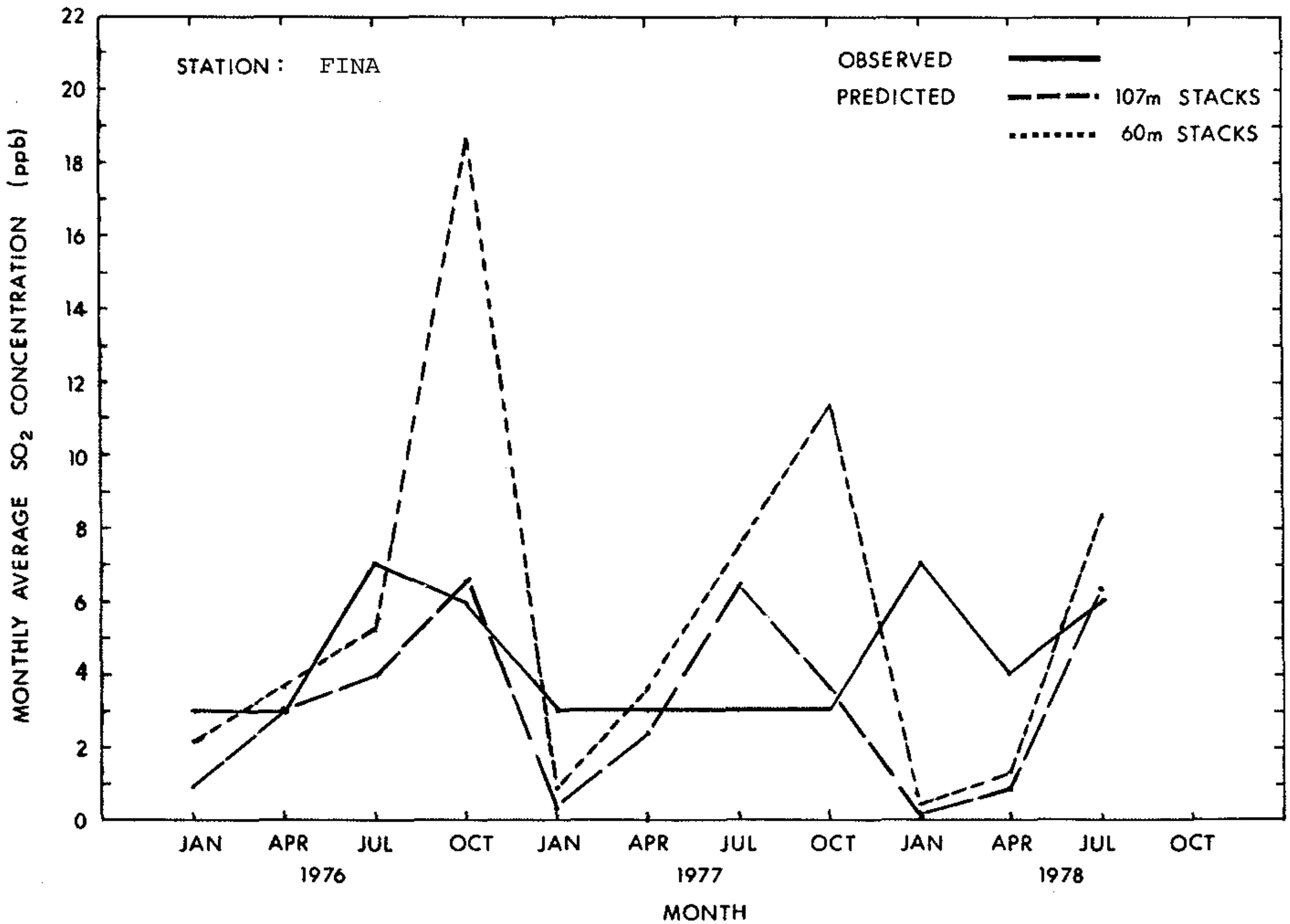

Figure 28. Fina Station.

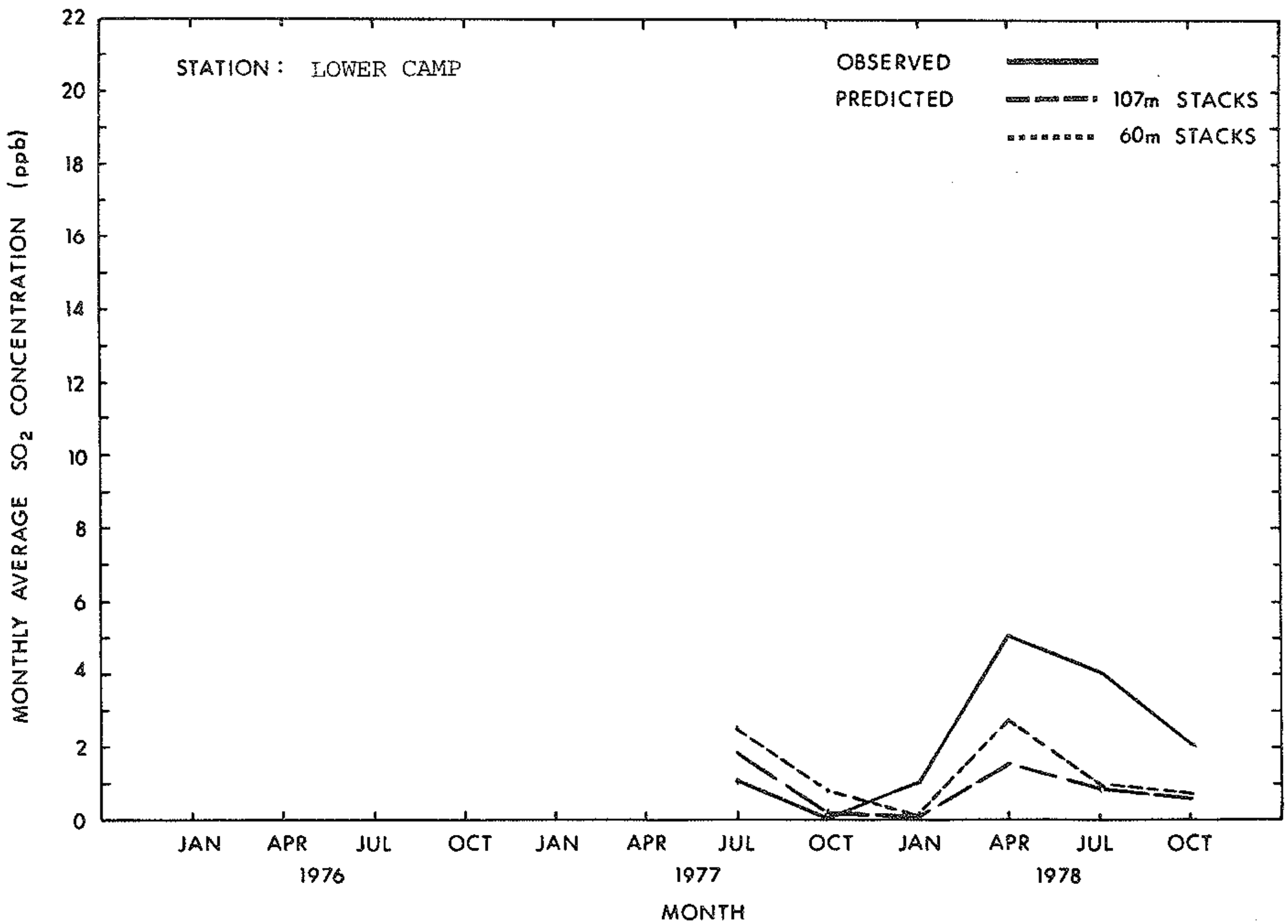

Figure 29. Lower Camp Station.

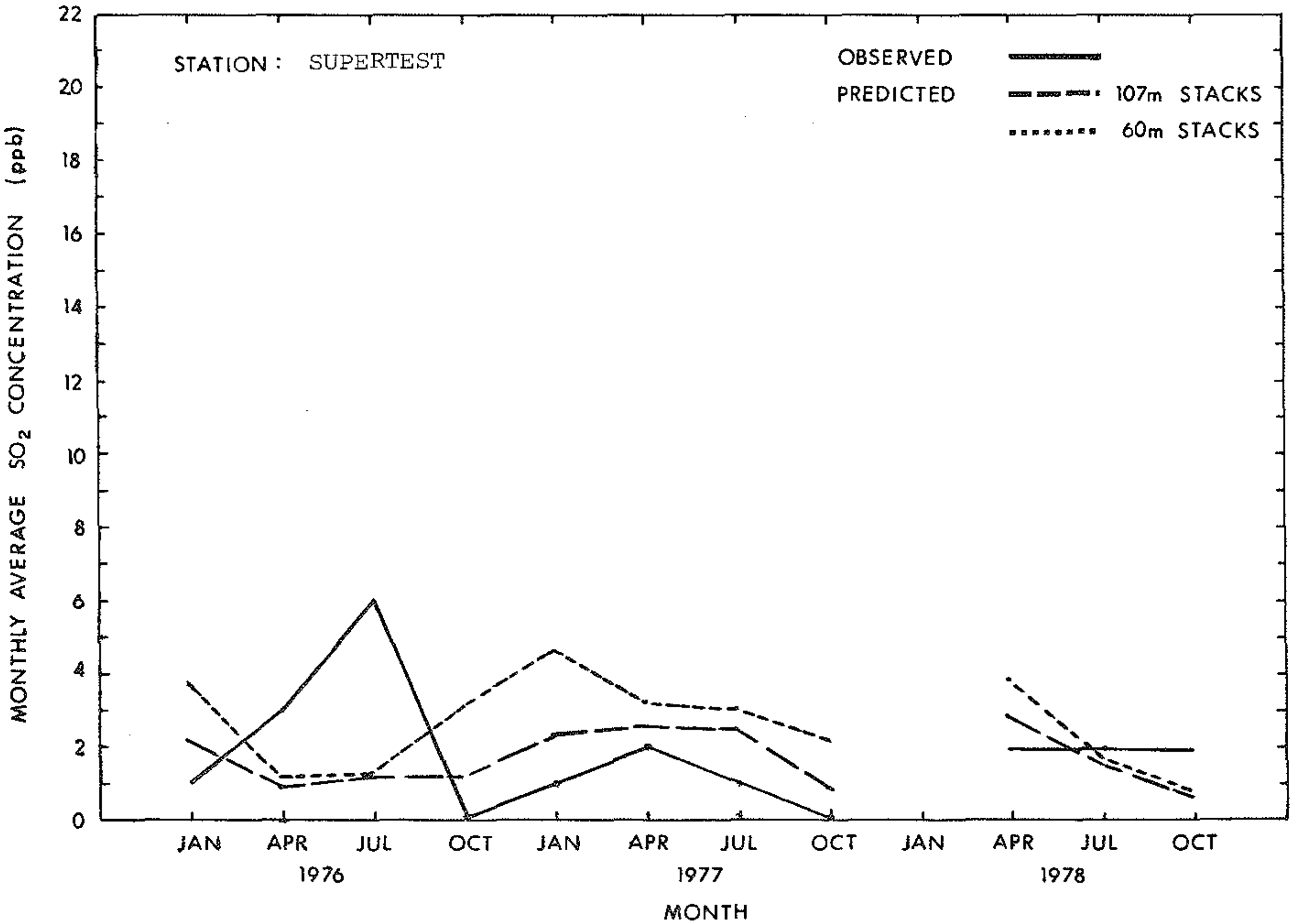

Figure 30. Supertest Station.

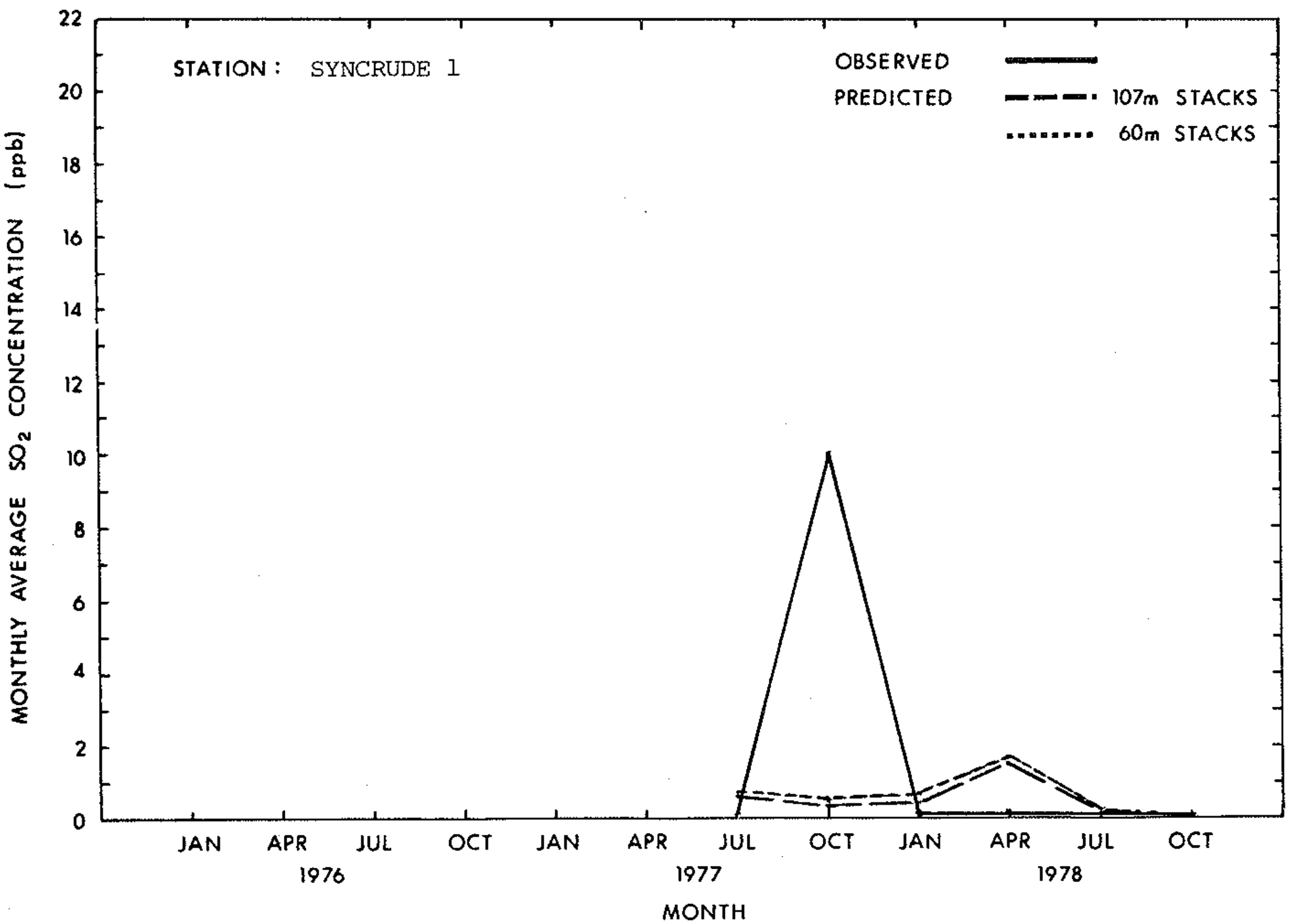

Figure 31. Syncrude 1 Station.

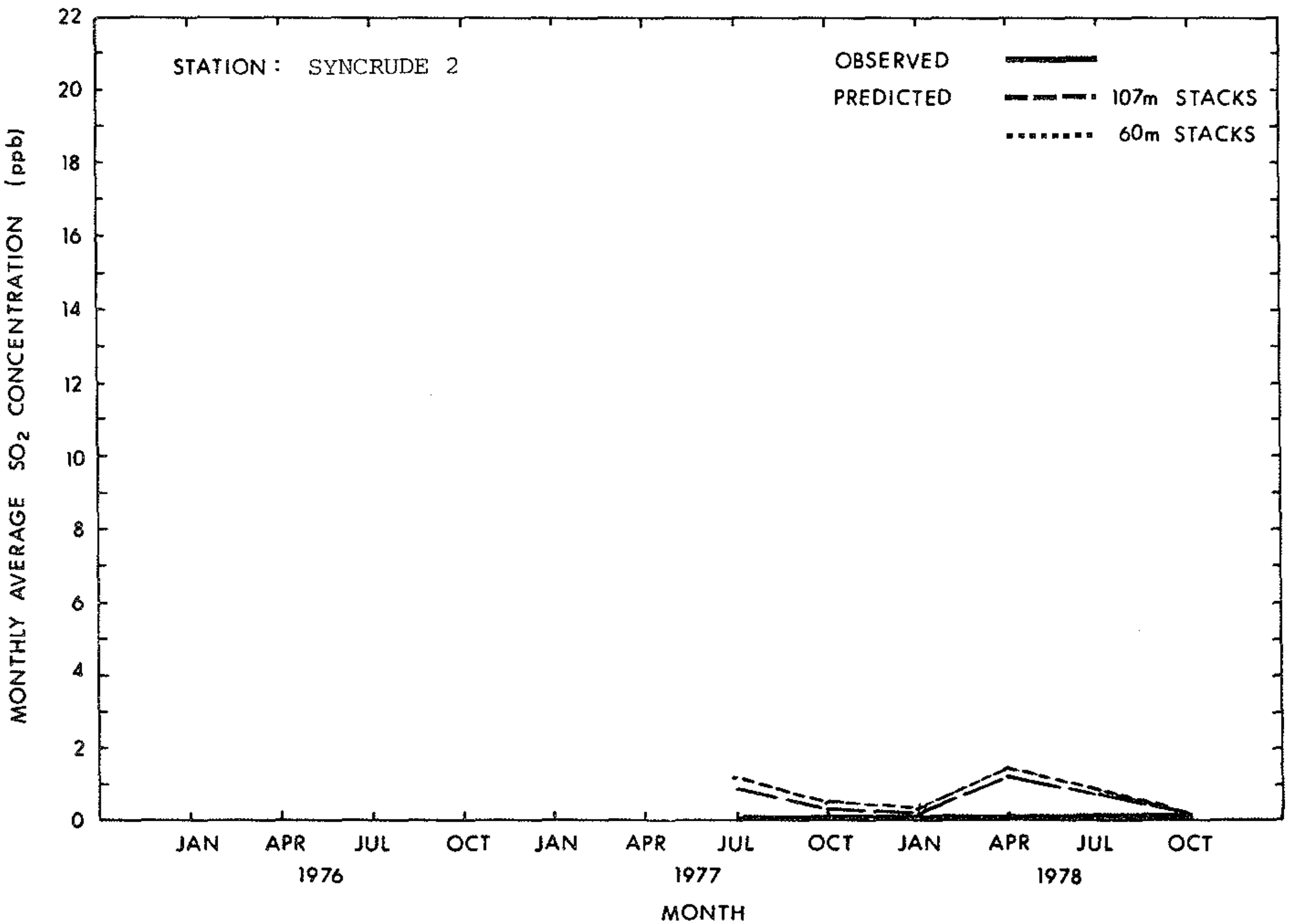

Figure 32. Syncrude 2 Station.

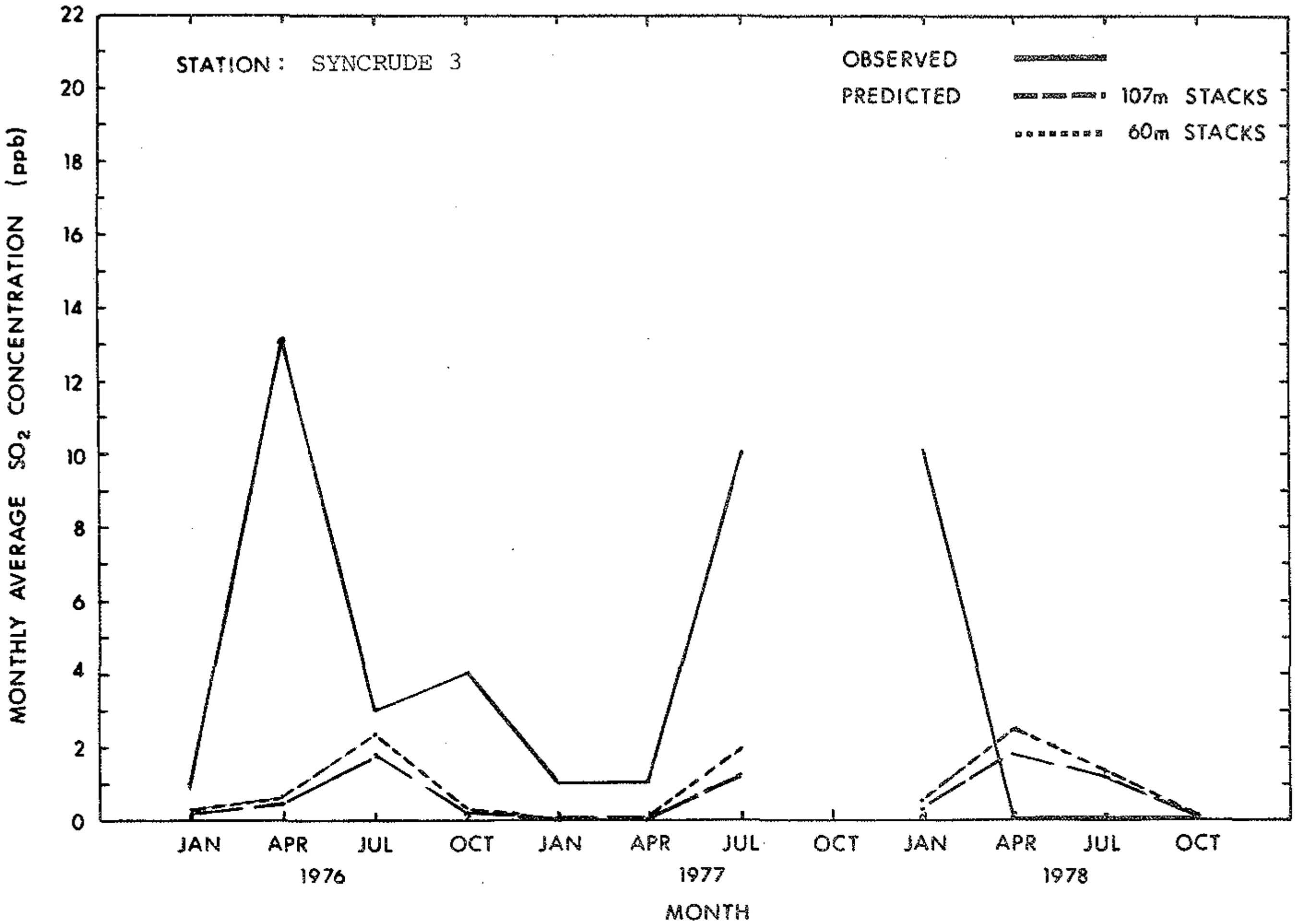

Figure 33. Syncrude 3 Station.

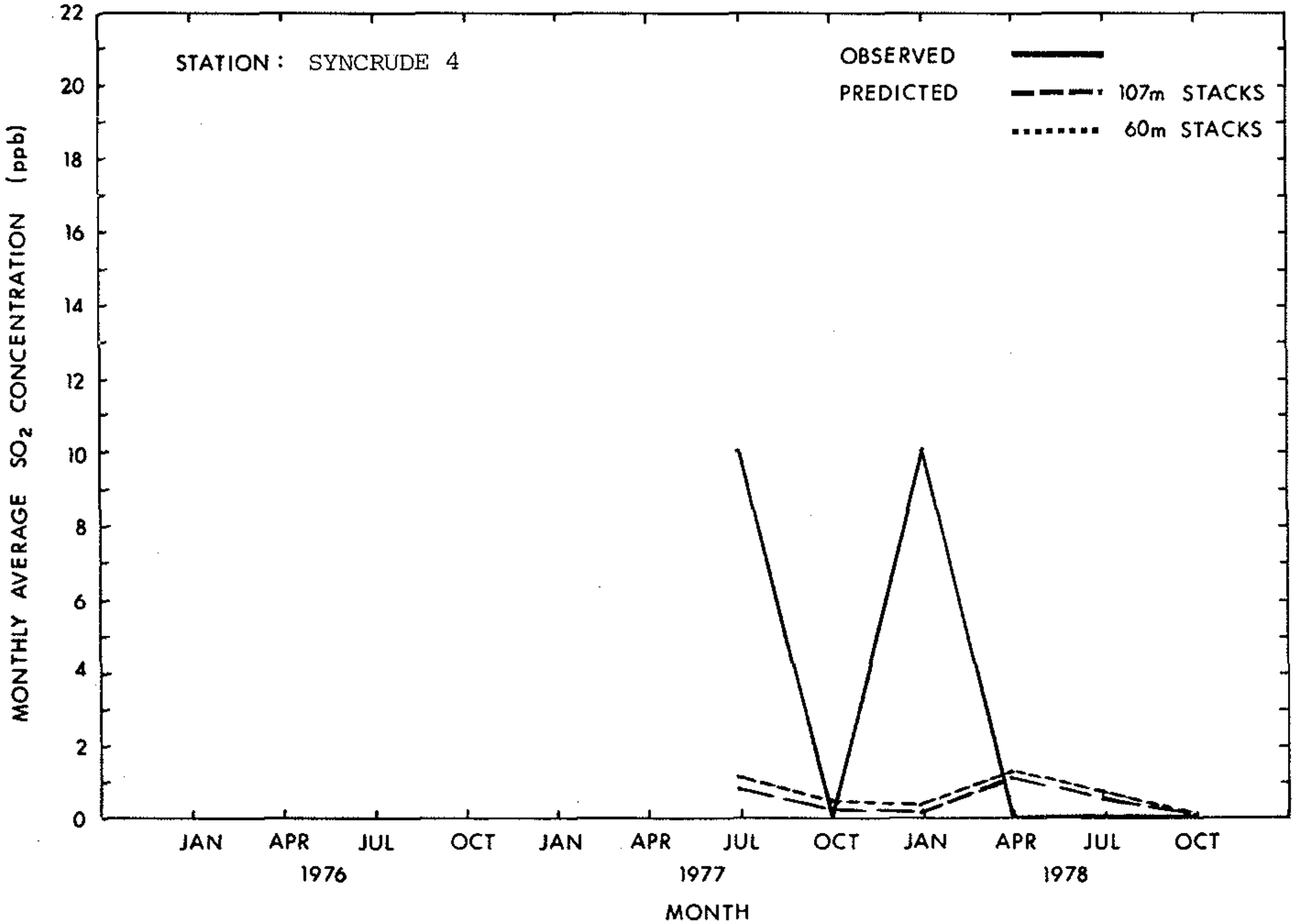

Figure 34. Syncrude 4 Station.

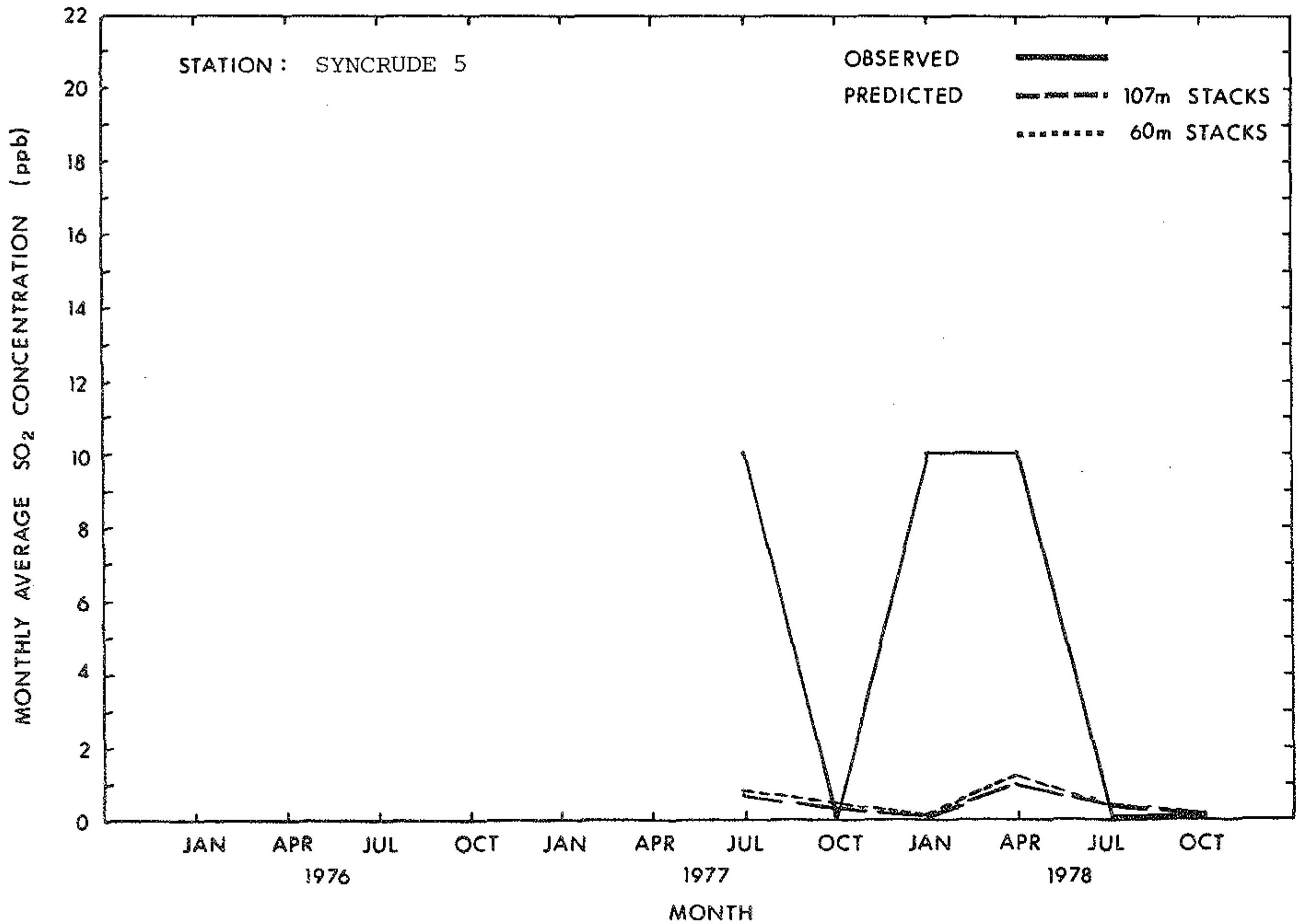

Figure 35. Syncrude 5 Station.

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3. Structure of a traditional baseline data system. 1976.
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5. The evaluation of wastewaters from an oil sand extraction plant. 1976.
6. Housing for the north--the stackwall system; construction report--Mildred Lake tank and pump house. 1976.
7. A synopsis of the physical and biological limnology and fishery programs within the Alberta oil sands area. 1977.
8. The impact of saline waters upon freshwater biota (a literature review and bibliography). 1977.
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10. Development of a research design related to archaeological studies in the Athabasca oil sands area. 1977.
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41. Acute and chronic toxicity of vanadium to fish. 1978.

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