VALIDATION STUDIES OF THE CRSTER MODEL IN APPLICATION TO THE AOSERP STUDY AREA

BY

D. BAGG

Environment Canada

Atmospheric Environment Service

ALBERTA OIL SANDS
ENVIRONMENTAL RESEARCH PROGRAM

Project AS 4.2.3
March 1979

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ABSTRACT

Methods to improve air quality emission and meteorological model input data records and validation techniques used to verify calculated annual, monthly, and daily calculations at ground level for the CRSTER model are described. Due to the limited nature of verification data and unique polar co-ordinate receptor grid network, a point-spatial validation approach, involving calculations along the most important windrose axial directions relative to the GCOS source, is advanced in annual time studies covering 1975 and 1976.

Selected Syncrude, Shell Hartley Creek, and GCOS monitor site observations are also utilized in the two studies on an annual, monthly and daily basis for statistical comparison with model results on a point-spatial verification basis only. As in the axial validation, this statistical verification excluded objective analysis smoothing of calculated concentrations.

Results are related to similar studies in a discussion of CRSTER's modelling capabilities. Environmental impact analyses for both time studies, including levels of confidence assigned to concentration estimates are described. A guide for future use of current and future versions of the model in the Oil Sands study area is advanced.

ACKNOWLEDGEMENT

The author wishes to acknowledge the assistance of Mr. M. Webb, Central Services Directorate, Atmospheric Environment Service, in providing the necessary meteorological and rawinsonde data. Mr. M. Strosher, Air Quality, AOSERP, is thanked for information on the ambient monitoring stations. Dr. C. S. Matthias provided comments on discussions of plume rise modelling difficulties. Dr. A. Christie is thanked for his constructive advice in proof-reading the manuscript. Finally, thanks are due to Ms. B. Primus for typing the manuscript and Mr. John Rautenberg for drafting the diagrams.

1. INTRODUCTION AND REVIEW OF CURRENT STATE OF KNOWLEDGE

The primary aim of applying air quality simulation models to the Oil Sands study area is to determine ground-level SO_2 concentrations resulting from processing heavy oil deposits.

Realistic simulation would permit impact assessments of the Oil Sands refining activities' effects upon the Air System of AOSERP to be prepared. These assessments, in turn, can be utilized by remaining ASOERP systems to meet their own essential objectives.

The EPA Gaussian model CRSTER has been used to identify worst case situations from a subset of existing data files (Padro and Bagg, 1978).

The former report provided a summary description of source emissions, meteorological and radiational parametric data and preliminary calculations with CRSTER.

The purpose of this report, however, is to apply CRSTER to the Oil Sands study area to obtain information on model sensitivity to source variability and to carry out validation time studies. Model deficiencies giving rise to errors in estimated concentrations are thereby illustrated in spatial and temporal frameworks. The level of confidence to be assigned to subsequent estimates can be better appreciated (EPA, 1977).

We begin by describing techniques used to improve existing meteorological and air quality emission data. A brief description of spatial distribution patterns for annual and monthly concentrations will then be given. Next, we proceed to a comparison of results with those of the CDM model as reported by Walmsley and Bagg (1977) and supported by snowpack studies of Barrie and Walmsley (1978) on an annual basis. Finally, results are compared with Syncrude, Shell, and GCOS monitor observations on an annual and monthly basis. These results are used to interpret CRSTER's modelling capabilities and to provide a guide for future use. Recommendations based upon air quality monitor network and model unrepresentativeness are given.

2. STUDY AREA

The contribution of Syncrude and, implictly, the proposed Alysands Shell plant to total annual sulphur dioxide concentrations at ground level is expected to be of the order of 1 μgm^{-3} or less provided that stack design characteristics are met and that no breakdowns necessitate flaring in the study area used for CDM (Walmsley and Bagg 1977).

Consequently it was decided that the same study area (Figure 1) as used in CDM modelling should apply in these short-term CRSTER modelling studies and that only those study areal ground-level concentrations due to the GCOS pollutants sources (Table 1) need be included for representative application of CRSTER.

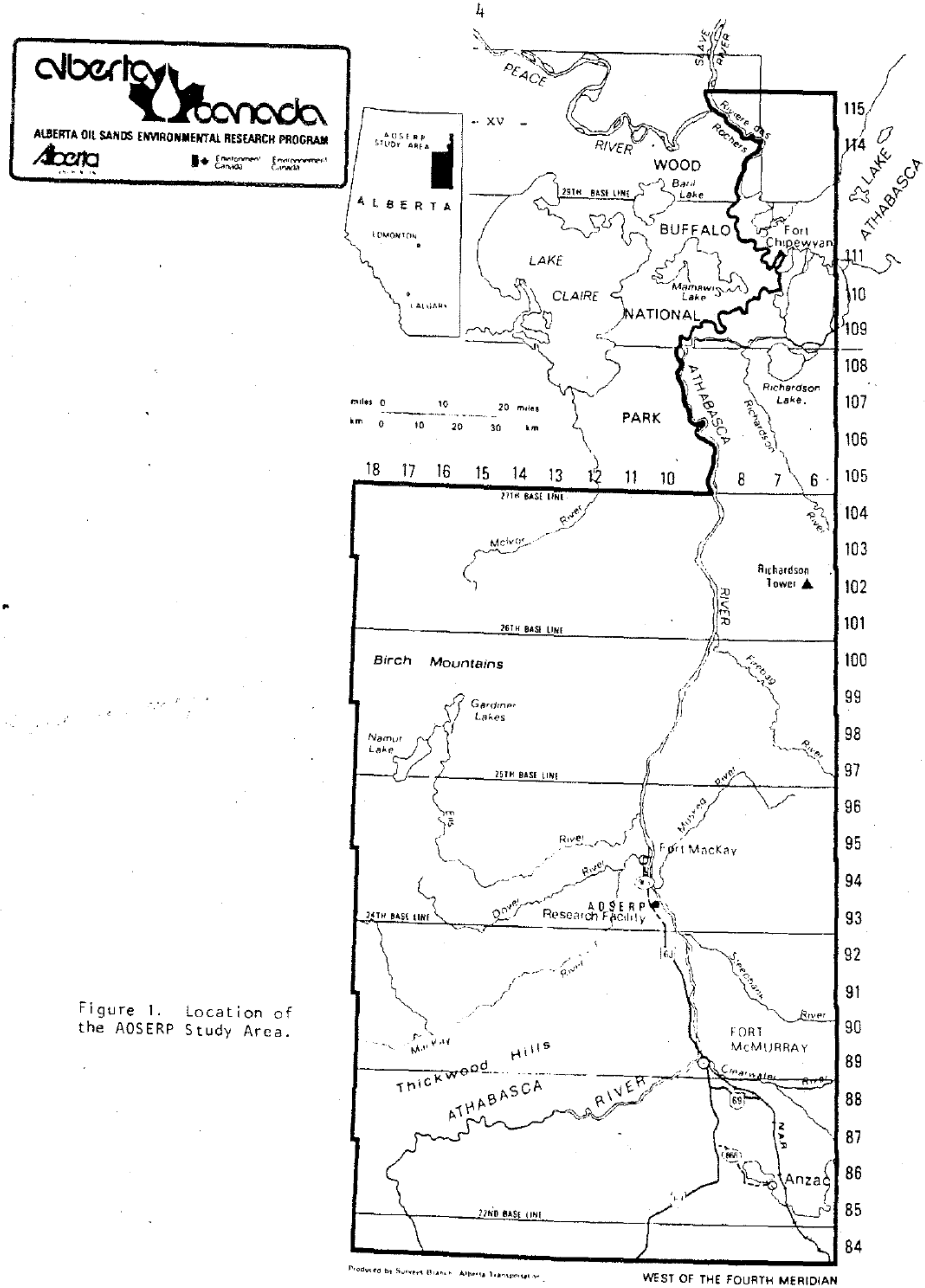

Figure 1. Location of the AOSERP Study Area.

TABLE 1 GCOS Emissions AND Stack Characteristics Inventory

Emission Rates:	Main Powerhouse	Incinerator	Main Flare		Acid Gas Flare ($g.s^{-1}$) 1975	1976
	2600. $g.s^{-1}$	270. $g.s^{-1}$	141.21. $g.s^{-1}$			
				Jan.	0.74	46.28
				Feb.	6.82	2.27
				Mar.	5.31	0.0
				Apr.	8.62	33.95
				Jun.	315.62	29.44
				Jul.	972.14	378.67
				Aug.	1762.45	0.0
				Sept.	1054.59	0.0
				Oct.	69.77	0.0[1]
				Nov.	10.62	0.0[1]
				Dec.	98.63	0.0[1]
VTM Locations, Block 12VVU						
East (km)	71.010	70.976	71.131		71.166	
North (km)	17.736	17.991	18.130		18.076	
Stack Height (m)	107.	107.	99.		76.	
Stack Diameter (m)	5.8	1.8	1.1		0.52	
Exist Velocity ($m.s^{-1}$)	17.5	17.0	5.0		5.0	
Gas Temperature (^{o}K)	545.	883.	873.		873.	

[1]Monthly Emission Rate Assumed to enable two annual time studies.

3. METHODS TO IMPROVE METEOROLOGICAL AND AIR QUALITY EMISSION DATA BASES

Within the 1975-76 study period no continuous record of mixing heights was available. A somewhat interrupted record was provided by the MEP contractors for the period February 6, 1975 to September 30, 1976 and bogus data, consistent with that record, was generated to complete the sequence. The procedure involved applying Holzworth's method (1967) to Ft. Smith Lower Rawinsonde charts using daily maximum temperatures interpolated from Ft. Smith, N.W.T., and Ft. McMurray, Alta., values as synoptic conditions dictated.

The representativeness of Ft. McMurray hourly surface meteorological data for the Oil Sands region was improved by replacing its wind data with Mildred Lake hourly wind data. Gaps in Mildred Lake wind data were partially filled using available hourly Shell/Hartley Creek winds.

Air quality source emission data was identical to data used in the Climatological Dispersion Model (Walmsley and Bagg, 1977) for GCOS powerhouse and incinerator stacks. The main flare stack used an annual emission rate based upon available emission data. The acid gas flare used exact monthly emission rates for the period.

4. VALIDATION OF APPLICATION OF CRSTER TO OIL SANDS STUDY AREA IN 1975 AND 1976 STUDIES

Due to heavy GCOS flaring activity in the summer of 1975 (Table 1) and high monitor concentrations at Mildred Lake in the spring of 1976, separate annual and monthly time studies for 1975 and 1976 were deemed necessary for accurate impact assessment.

These annual time studies for the GCOS study area showed almost identical spatial patterns of SO_2 concentrations (see Figures 2 and 3). Analysis of these patterns led to the decision to concentrate verification procedures upon three major areas: Northwest (or North-northwest), Northeast, and Southeast of the GCOS source. These directional areas will henceforth be delineated in this report by direction designation '1' (or in 1976 '1a'), '2', and '3', respectively.

Although objective analysis would normally give smoother concentration patterns, calculated plume spread via the "narrow plume hypothesis" assumed CRSTER's calculated concentrations were representative only along each wind direction sector's centerline. Hence, this "point"-spatial validation approach is acceptable as lower hourly concentrations off centerline are excluded by this "beaming" effect when time-averaged over longer periods.

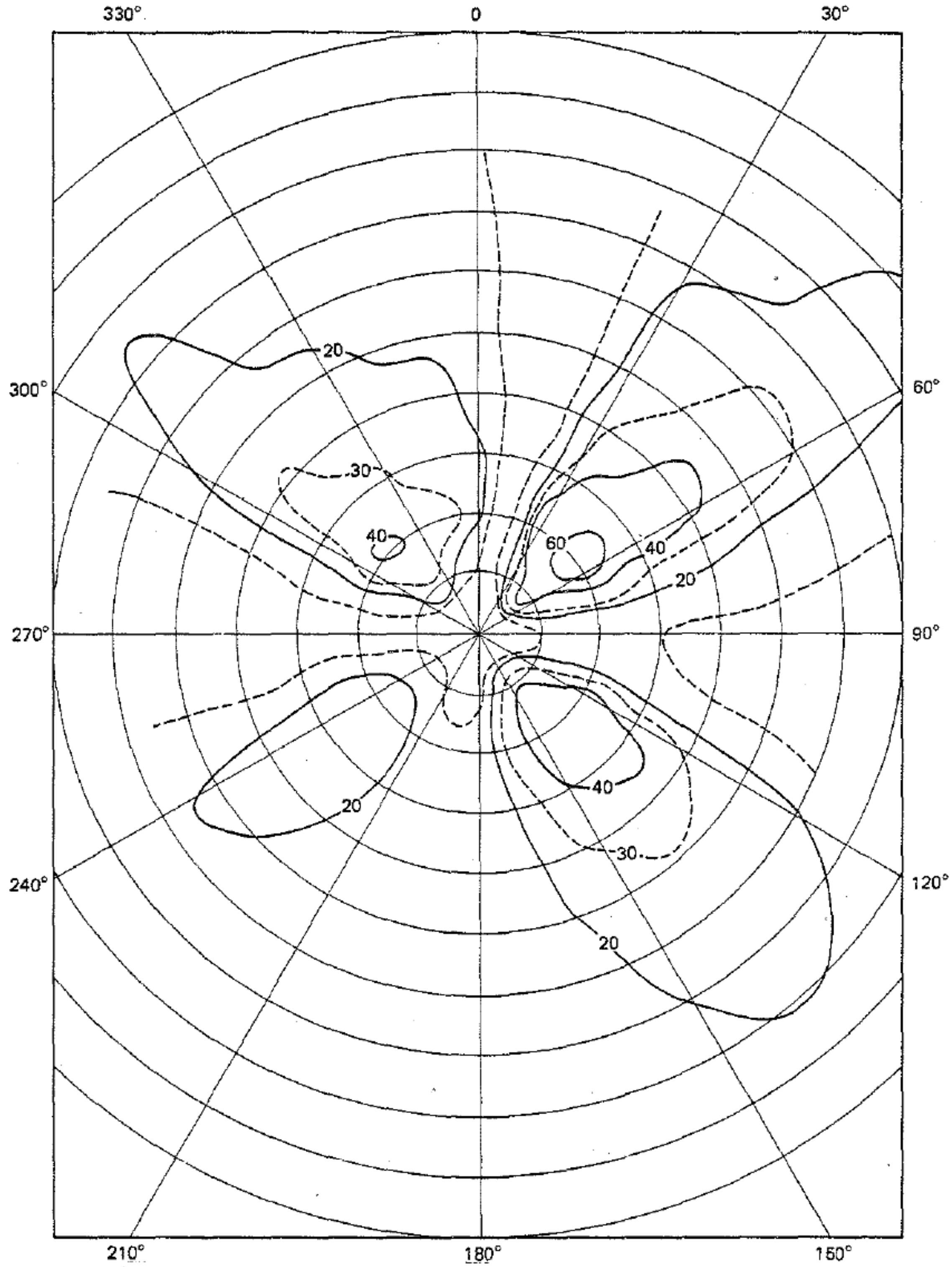

FIGURE 2: ANNUAL AVERAGE SO_2 CONCENTRATIONS AT GROUND-LEVEL IN 1975: FOUR GCOS SOURCES, NO POLLUTANT REMOVAL.

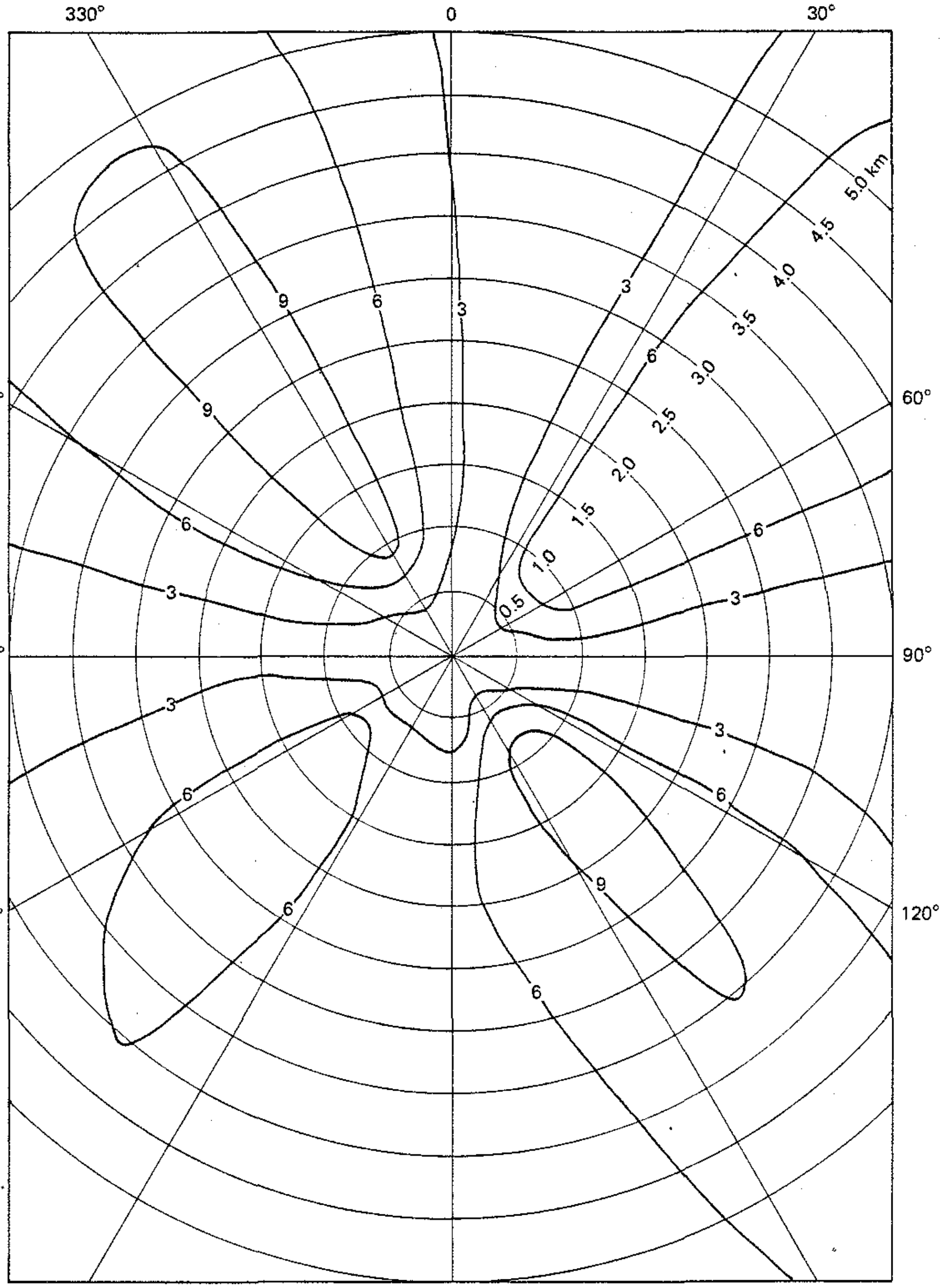

FIGURE 3: ANNUAL AVERAGED SO_2 CONCENTRATIONS AT GROUND-LEVEL IN 1976: FOUR GCOS SOURCES, NO POLLUTANT REMOVAL.

5. NUMERICAL EXPERIMENTS

5.1. Annual Time Studies

5.1.1. Experiment No. 1: 1975 Annual Study

5.1.1.1. Comparison with CDM modelled results

Annual calculated maximums of 55.9 $\mu g.m.^{-3}$ at a radial distance 0.8 km. along axis '3' and 42.1 and 68.5 $\mu g.m.^{-3}$ at 0.9 and 1.0 km. downrange along axes '1' and '2' respectively (see Figures 4-6) compare well with CDM peaks 2.3 km. south-southeast and 2.0 km. northwest-to-northeast of GCOS (Walmsley and Bagg, 1977). The fractional contributions of the two flare stacks to totals along all three axes are very high. Spatially, CRSTER's two peaks north of GCOS were separate and distinct in contrast to the CDM's single northerly peak concentration. Maximums along the above axes averaged two-to-three times as high as CDM contour map values. As CDM results were consistent with snowpack measurement data, CRSTER peak values are suspected of being too high as discussed in Appendix 1.

5.1.1.2. Comparison with GCOS, Syncrude and Shell Monitor Network Observations:

Annual observations made over portions of the period 1974-76 at four GCOS network sites were time averaged as were data from the Syncrude and Shell refinery sites and are compared with CRSTER results in Table 2. Calculated 1975 values representative of the monitor site agreed with measured values very well except at the GCOS monitors '3' and '4'. Statistical parameters based on modelled and observed values were generally poor in all cases. Linear regression and rank correlation coefficients improved when Syncrude and Shell monitors were included.

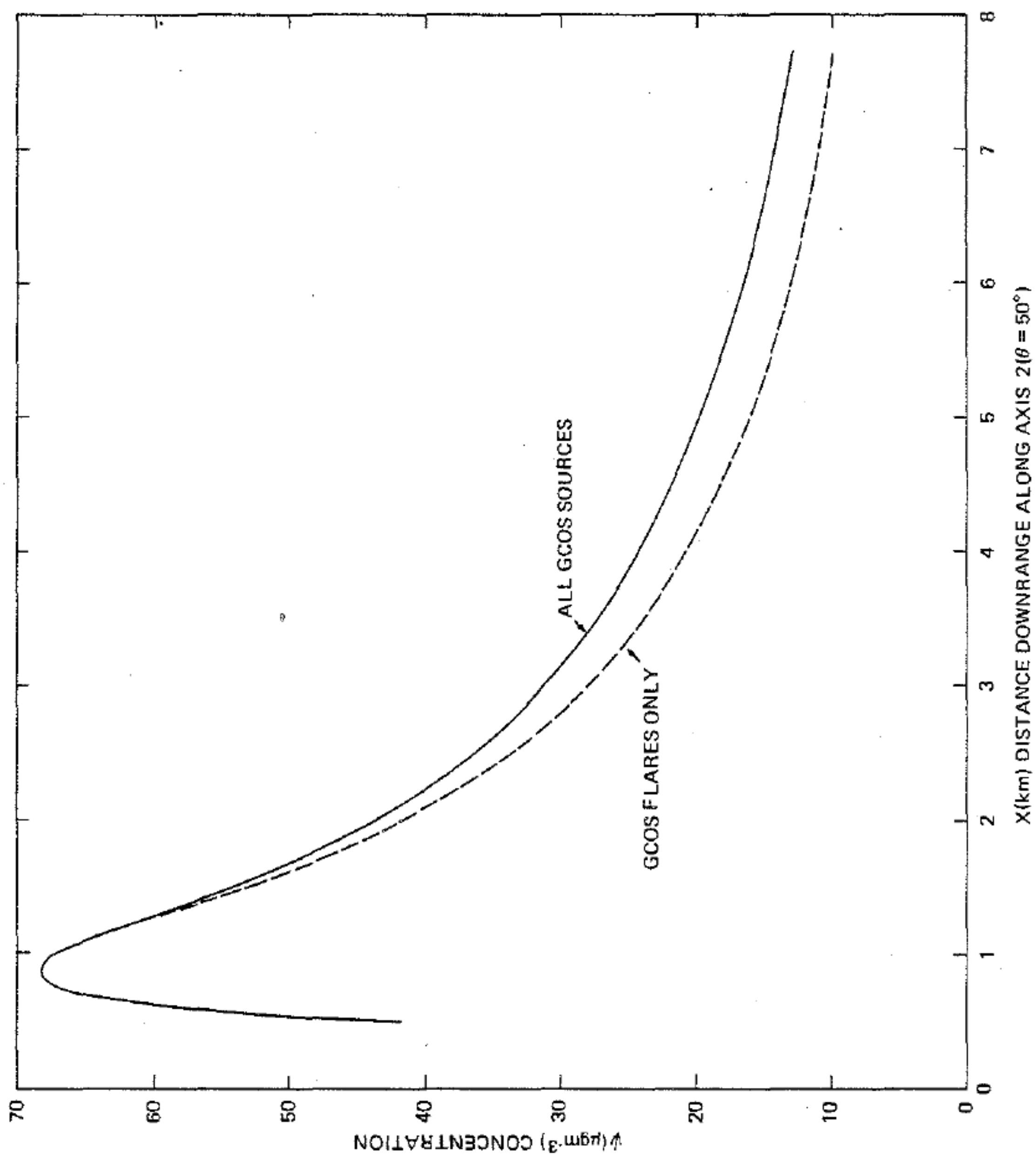

FIGURE 4: PLOT OF 1975 ANNUAL AVERAGED SO_2 CONCENTRATION VERSUS DISTANCE DOWNRANGE OF GCOS SOURCES ALONG AXIS 2 (θ=50°).

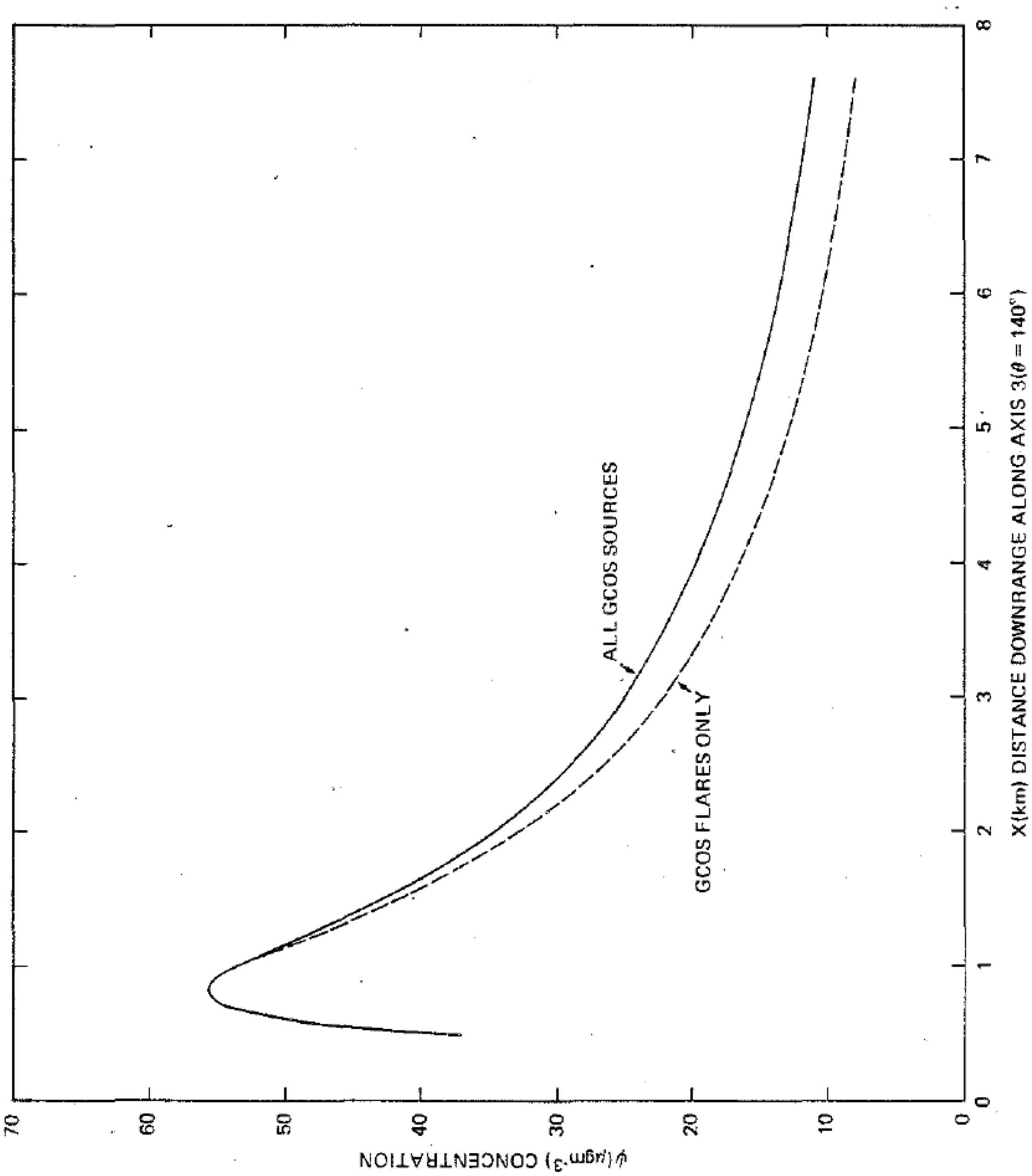

FIGURE 5: PLOT OF 1976 ANNUAL AVERAGED SO_2 CONCENTRATION VERSUS DISTANCE DOWNRANGE OF GCOS SOURCES ALONG AXIS 3 (θ=140°).

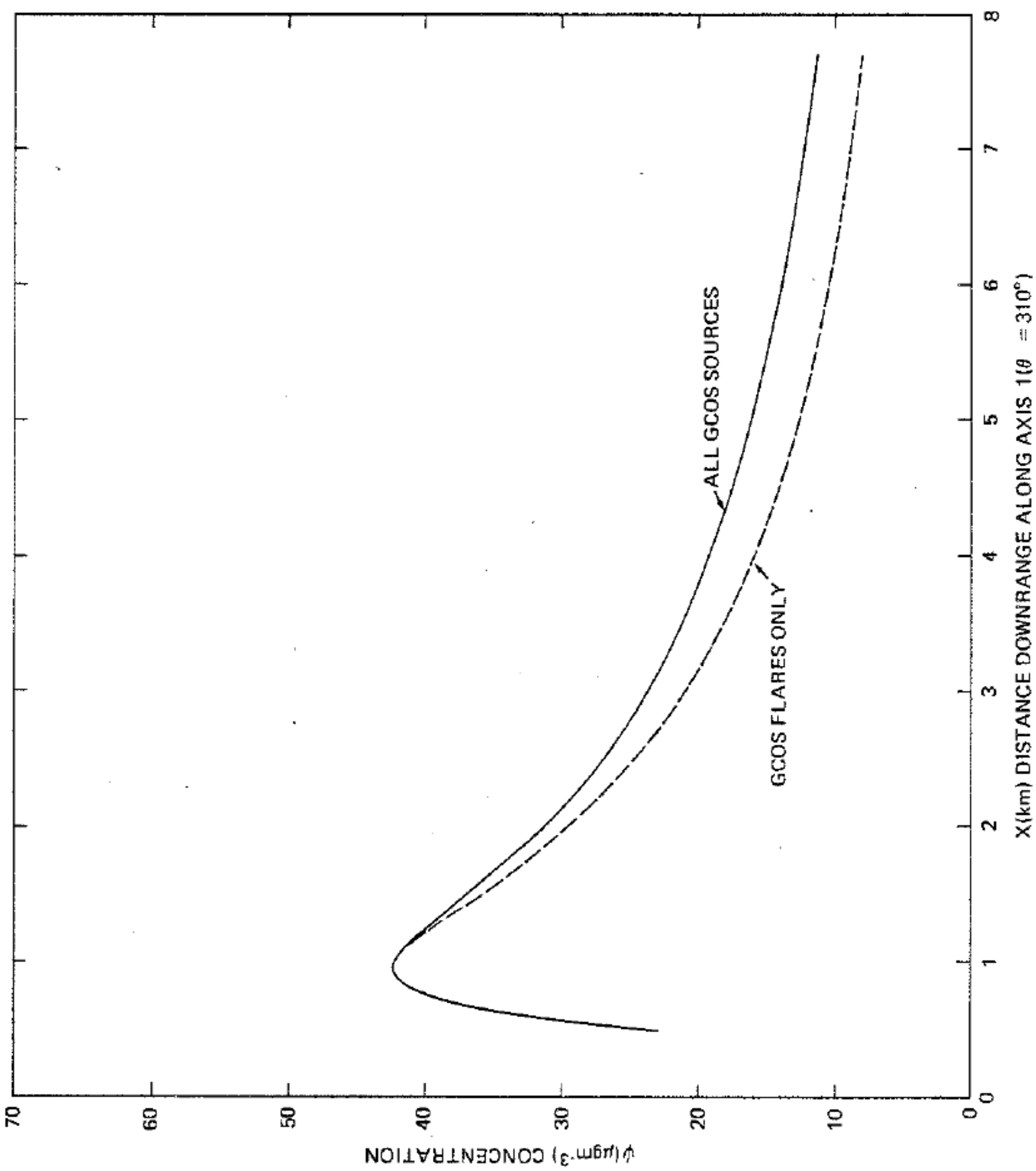

FIGURE 6: PLOT OF 1975 ANNUAL AVERAGED SO_2 CONCENTRATION VERSUS DISTANCE DOWNRANGE OF GCOS SOURCES ALONG AXIS 1 (θ=310°).

TABLE 2 1975 MODEL VERIFICATION STATISTICS: ANNUAL BASIS

Monitor Number	Identifier	Polar Co-ords in CRSTER: R (km)	Polar Co-ords in CRSTER: θ (degrees)	Observations ($\mu g.m.^{-3}$)	Calculations ($\mu g.m.^{-3}$)
1	GCOS	9.230	176°	5.6	4.7
2	GCOS	4.119	187°	8.2	7.9
3	GCOS	4.751	236°	7.2	13.6
4	GCOS	7.218	313°	6.4	11.2
5	SYNCRUDE	8.500	295°	3.4	5.9
6	SHELL	27.200	351°	4.5	2.2
			MONITORS INCLUDED:	1-4	1-6

STATISTICS

	Observations	Calculations
Standard Error ($\mu g.m.^{-3}$)	4.0	3.6
Modified Standard Error ($\mu g.m.^{-3}$)	5.7	4.4
Linear Regression, Slope, a_1	1.22	1.48
Linear Regression, Intercept, a_o	1.02	-1.12
Linear Correlation Coefficient r^1	0.35	0.62
Rank Difference Correlation Coefficient	0.40	0.66

5.1.2 Experiment No. 2: 1976 Annual Study:

5.1.2.1 Comparison with CDM modelled results:

Calculated maximums were 11.2 $\mu g.m.^{-3}$ at a range 1.2 km. from source along axis '3', 10.6 $\mu g.m.^{-3}$ at 1.6 km. from source along '1a', and 7.7 and 7.6 $\mu g.m.^{-3}$ at 1.3 and 3.0 km. respectively, from source along axis '2' (see Figures 7-9). The fractional contributions of the two flare stacks to these totals were not quite as pronounced as in experiment 1. Spatially, agreement with CDM peaks had improved slightly as the peak along axis '1' in 1975 had shifted to axis '1a'. In contrast to experiment 1, 1976 CRSTER peaks are within the defined acceptable accuracy range relative to CDM contour map values (Walmsley and Bagg, 1977). Regions where CRSTER values slightly exceed that accuracy range occurred midway between axes '1a' and '1' and due south of the source at all radial distances.

5.1.2.2 Comparison with GCOS, Syncrude and Shell Monitor Network Observations:

Comparison CRSTER's 1976 calculated values with all available monitor data averaged over portions of the period 1974-76 produced results shown in Table 3. This study showed better standard error and modified standard error values than in 1975. Linear regression slopes, intercepts and correlation coefficients with all GCOS monitor are slightly worse than in 1975. Significant improvement in linear regression slope, intercept, and correlation coefficient values occurred when Syncrude and Shell comparison data was included in both studies. This pattern was also true with the rank difference correlation coefficient (see Appendix 2).

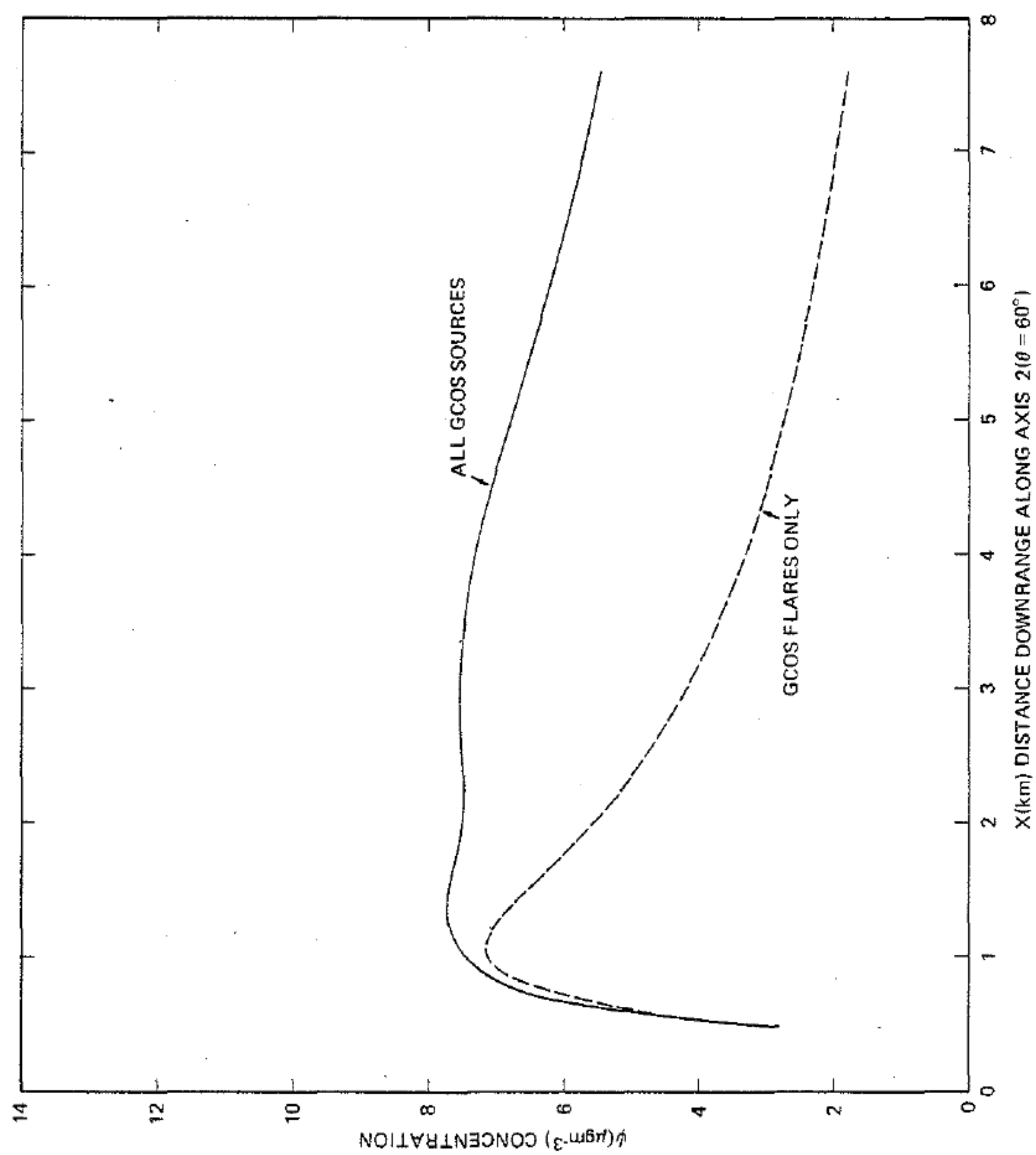

FIGURE 7: PLOT OF 1976 ANNUAL AVERAGED SO_2 CONCENTRATION VERSUS DISTANCE DOWNRANGE OF SOURCES ALONG AXIS 2 (θ=60°).

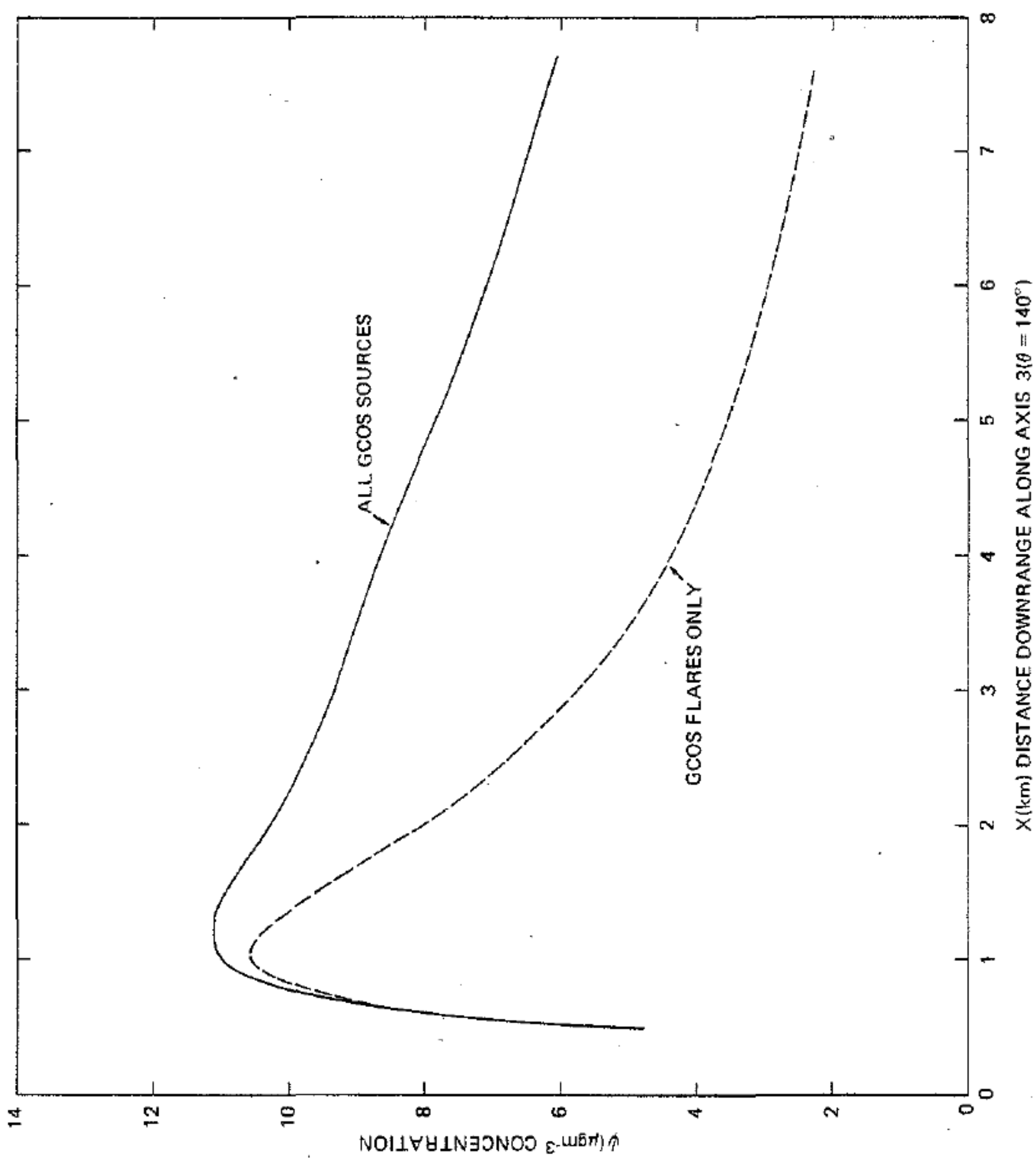

FIGURE 8: PLOT OF 1976 ANNUAL AVERAGED SO_2 CONCENTRATION VERSUS DISTANCE DOWNRANGE OF GCOS SOURCES ALONG AXIS 3 (θ=140°).

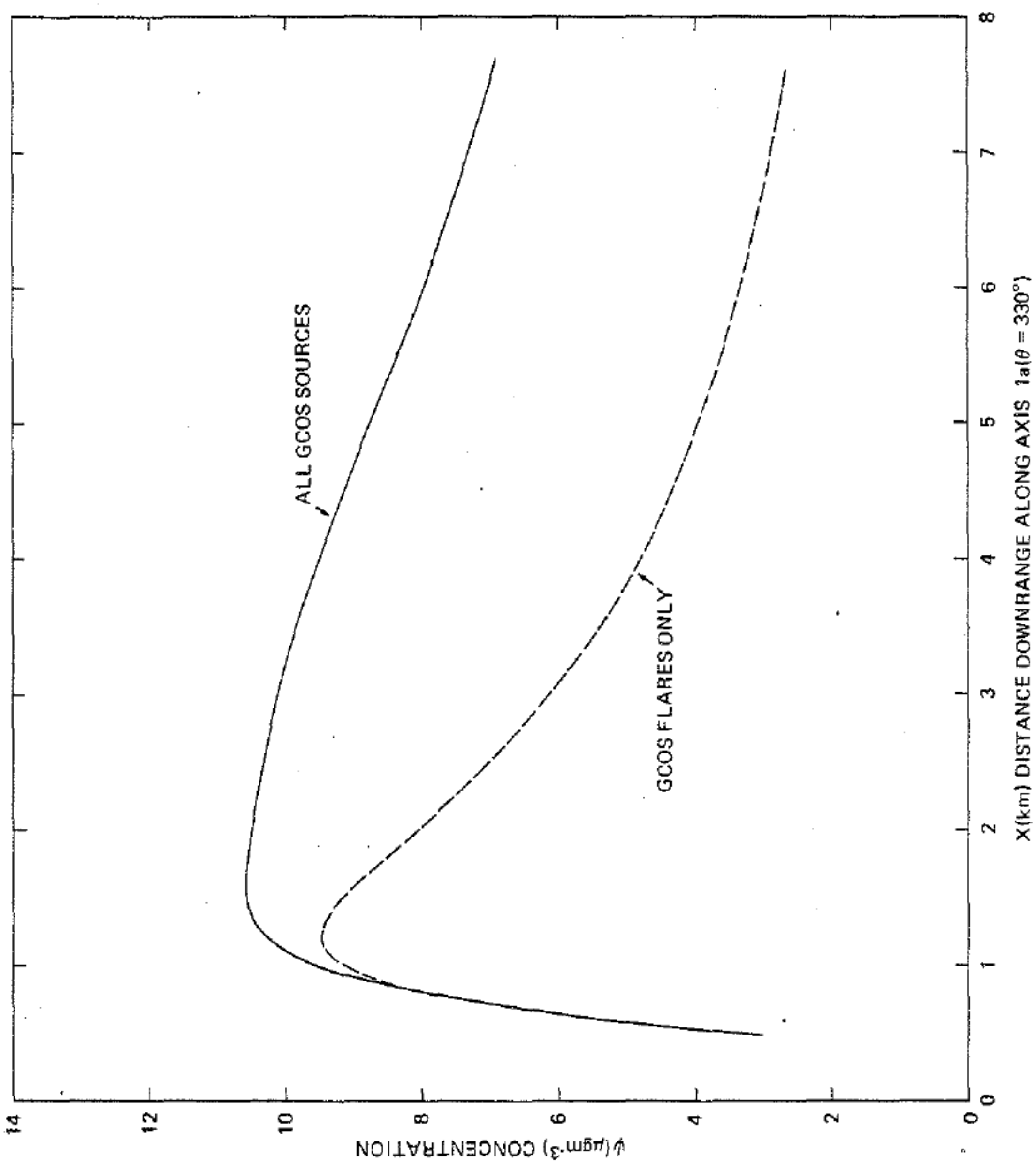

FIGURE 9: PLOT OF 1976 ANNUAL AVERAGED SO_2 CONCENTRATION VERSUS DISTANCE DOWNRANGE OF GCOS SOURCES ALONG AXIS 1A (θ=330°).

TABLE 3 1976 MODEL VERIFICATION STATISTICS: ANNUAL BASIS

Monitor Number	Identifier	Polar Co-ords in CRSTER R (km)	Polar Co-ords in CRSTER θ (degrees)	Observations (μg.m.$^{-3}$)	Calculations (μg.m.$^{-3}$)
1	GCOS	9.230	176°	5.6	3.0
2	GCOS	4.119	187°	8.2	4.7
3	GCOS	4.751	236°	7.2	5.1
4	GCOS	7.218	313°	6.4	6.5
5	SYNCRUDE	8.500	295°	3.4	3.1
6	SHELL	27.200	351°	4.5	1.4
		MONITORS INCLUDED		1-4	1-6

STATISTICS	Observations	Calculations
Standard Error (μg.m.$^{-3}$)	2.4	2.3
Modified Standard Error (μg.m.$^{-3}$)	3.4	2.8
Linear Regression, Slope	0.39	0.67
Linear Regression, Intercept	2.14	0.00
Linear Correlation Coefficient	0.30	0.65
Rank Difference Correlation Coefficient	0.20	0.60

5.2. Monthly Time Studies

5.2.1 Experiment No. 1: 1975 Monthly Study:

5.2.1.1 Comparison with Syncrude and Shell Monitor Sites Observations

Consistency between model results and observations within acceptable limits as defined in Appendix 1 held, with only three exceptions throughout the period April to October, 1975, at both Syncrude and Shell sites as shown in Table 4. The most glaring irregularity, a very low observation at Syncrude for July, contrasted sharply with a much higher July observation at the distant Shell site. Examination of average windspeeds and frequencies of windrose directions east, southeast, and south for both the Syncrude site and Mildred Lake observation site suggests that local bias in the Syncrude monitor for this month may be present. This phenomenon appears to be due to differences in topographical effects of the regional plateau upon east, south and especially southeast windrose directions at the two sites as described in Appendix 2.

Less representative results were obtained from CRSTER in late fall and winter months. This appears to be mainly due to low flare emission rates which precluded high flare concentration over-estimates in these months.

5.2.2 Experiment No. 2: 1976 Monthly Study:

5.2.2.1. Comparison with Mildred Lake and Supertest Hill GCOS Monitor Network Sites

In the 1976 study, the GCOS monitor network data for Mildred Lake and Supertest Hill was substituted for the inadequate monthly data record for Shell and Syncrude. Underestimation errors in the GCOS data record are possible in the first three months because monitor calibration tolerance was only valid to hourly concentrations of 0.50 $\mu g.m.^{-3}$.

TABLE 4: 1975 AND 1976 MODEL VERIFICATION DATA: MONTHLY BASIS

1975-76

		JAN.		FEB.		MAR.		APR.		MAY		JUN.		JUL.		AUG.		SEP.		OCT.		NOV.		DEC.	
Observed MONITOR SITE SO_2 Concentration (μgm^{-3})		SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL	SYN	SHL
	1975	5.3	4.5	3.7	3.7	11.1	4.0	4.8	4.8	1.9	0.5	5.3	4.2	0.5	8.5	5.0	2.9	1.3	1.6	3.4	1.6	1.3	6.1	1.3	11.9
	1976	0.5	6.1	3.7	N/A	9.3	N/A	4.2	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
SYN= Syncrude; SHL=Shell/Hartley Creek																									
1975 CRSTER Modelled SO_2 Concentrations (μgm^{-3})		1.4	1.4	0.4	0.2	1.9	0.6	3.4	1.2	3.6	2.3	6.9	3.8	11.2	6.8	7.9	5.3	4.4	2.2	1.9	1.1	0.4	0.4	0.0	0.1
1976 Observed MONITOR SITE SO_2 Concentrations[1] (μgm^{-3})		MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP	MLD	SUP
		N/A	N/A	0.1	1.1	13.0	9.8	34.5	8.0	29.2	8.0	5.3	15.9	8.0	5.3	4.3	4.5	6.6	2.7	10.6	0.0	1.3	1.3	0.0	3.2
MLD= Mildred Lake; SUP= Supertest Hill																									
1976 CRSTER Modelled SO_2 Concentrations (μgm^{-3})		2.0	2.0	2.0	2.9	2.3	3.5	12.7	1.7	15.1	2.3	16.3	10.1	8.5	3.4	9.0	3.9	6.3	2.3	5.5	1.1	5.3	1.3	2.1	2.4

1 Underestimation errors in the GCOS Monitor Network Mildred Lake and Supertest Hill site data are possible in the first three months of 1976 due below normal monitor calibration tolerance.

As acid gas flare emissions were not known in the final three months of 1976, values of 0.0 $g.s.^{-1}$ were assumed. This assumption - mdade to allow for monthly 1975 and 1976 time studies - appears not unreasonable as this rate held for this stack during the previous two months.

Calculations in the acceptable accuracy range (Appendix 1) for Mildred Lake occurred in May, and July to September inclusive, with November and December being borderline cases. Poorest simulations occurred in March and April where CRSTER values were much less than should have been the case. This poor March simulation occurred despite excellent agreement of calculated mixing heights using rawinsonde data with heights extracted from the March, 1976, AOSERP field experiment. A large Mildred Lake April observed concentration is considered statistically suspect because of the very low Syncrude value (Appendix 4). Conversely, December, February, and June Mildred Lake values are unusually low relative to the Supertest Hill values, suggesting possible plume re-penetration of the unstable layer from the stable layer at greater downrange distances. This observed phenomenon is impossible to simulate with CRSTER.

At Supertest Hill, calculations were in the acceptable range in the June through December period, except for October when a zero monitored value appears questionable. The poor simulation in early spring noted at Mildred Lake was much worse for Supertest Hill.

5.2.3. Statistical Analyses of Monthly Experiments:

Statistical analysis of the two sets of monthly experiments results, shown in Table 5, consistent with methods described by Walmsley and Bagg (1977), reveals that modified standard errors were reduced from 5.0 $\mu g.m.^{-3}$ at both sites in 1975 to 4.2 $\mu g.m.^{-3}$ in 1976 at Supertest Hill. The Mildred Lake

TABLE 5

STATISTICAL ANALYSIS OF MONTHLY RESULTS

Statistical Comparison Terms	EXPERIMENT #1: 1975 SYN	EXPERIMENT #1: 1975 SHELL	EXPERIMENT #2: 1976 MLD	EXPERIMENT #2: 1976 SUP
Number of Months, N	(N=12)	(N=12)	(N=11)	(N=11)
Standard Error, S ($\mu g.m^{-3}$)	4.6	4.4	9.5	3.8
Modified Standard Error, $\hat{s}$ ($\mu g.m^{-3}$)	5.0	4.8	10.5	4.2
Linear Regression, Slope a_1	-0.16	0.00	+0.27	+0.41
Linear Regression, Intercept, a_o	4.2	2.1	4.7	0.9
Linear Correlation Coefficient, r^1	0.13	0.01	0.60	0.79
Rank Difference Correlation Coefficient r_s	+0.12	-0.22	+0.60	+0.61
Test for Null Hypothesis that obs. vs. Exp't Data Independent Z ($Z=r_s \sqrt{n-1}$)	+0.39	-0.74	+1.90	+1.93

modified standard error values were large due to the spring concentration analomies mentioned above. Compared with ideal values of m = 1, b = o, the slopes and intercepts of the linear regression curves are poor for all cases.

Linear correlation coefficients with monthly flare emission sites at Syncrude and Shell sites in 1975 are poor. However, some CRSTER modelling skill with 1976 Mildred Lake and Supertest Hill data is indicated by the values of 0.60 and 0.79 respectively.

The rank correlation coefficient, another measure of the relationship between calculated and observed concentrations (Appendix 2) improved from 0.13 to 0.60 in switching from Syncrude in 1975 to Mildred Lake in 1976. The value of 0.61 for the Supertest Hill site in 1976 is an apparent improvement on the equivalent weakly negative value obtained with the Shell site data for 1975.

Calculated and observed monthly concentrations at all four sites were examined to see whether the X (observed concentration) and Y (calculated concentration) random variables from which they were derived are independent data sets (Appendix 2). Results for standardized normal variable Z (Table 5) indicate the null hypothesis of independence cannot be rejected at any of the sites at the 0.05 level of significance.

6. SUMMARY

1. The 1975 CRSTER simulations produced maximum concentrations that agreed well spatially with CDM modelling results. The latter CDM patterns (Walmsley and Bagg, 1977) were consistent with snowpack studies in the GCOS study area. The maximum to the north-northwest in the CDM simulation appeared as two distinct maximums on areas '1' and '2' using the CRSTER model. Due to a flow field randomization factor 4.5 times greater than in the original CRSTER model because of the eight-point windrose, the peak along '2' was re-distributed along areas $\theta = 40^{\circ}$ and $\theta = 60^{\circ}$ under the exaggerated influence of north and east winds. Peak values were validated indirectly against CDM peak values to be slightly above the acceptable accuracy range but there was insufficient data to validate the fine structure of the pattern.

2. The 1976 CRSTER peak concentrations showed greater consistency with CDM peak locations than the 1975 study. The peak along axis '1' at $\theta = 310^{\circ}$ in 1975 had shifted to axis '1a' at $\theta = 330^{\circ}$ and the peak along axis '2' in 1975 was more uniformly distributed from 1 to 6 km. downrange to the northeast in 1976. Comparison of these peak values with peaks at the same locations in CDM patterns showed that CRSTER peaks fell in the lower portion of the acceptable accuracy range (Appendix 1).

3. Analysis of concentration variations along axes '1' (or '1a'), '2' and '3' revealed that all 1975 peaks were less distinctive, occurring 1.6, 1.3 and 1.2 km from source along axes '1a', '2', and '3', respectively, and diminished in concentration much less rapidly with distance from the source.

4. Inclusion of Syncrude and Shell monitor data with GCOS observations in annual comparison statistics made standard errors worse, but improved linear regression slopes, intercepts

and correlation coefficients and rank correlation coefficients in 1975 and 1976 (Appendix 2).

5. Calculations with CRSTER were within the required accuracy range most frequently in summer and fall months of 1975 and 1976 using monthly acid gas flare emission rates. Model results for spring months were within such accuracy for the 1975 study only.

6. Although CRSTER was also intended for evaluation of daily-average concentrations, simulation of 'worst days' monitor values produced standard error and modified standard error daily values as high as 70 $\mu g.m.^{-3}$ in some months.

7. DISCUSSION

1. The CRSTER model systematically underestimates most fall, winter, and spring monthly concentrations due to model constraints on input data and poor simulation of physical phenomena. The GCOS powerhouse and incinerator stack plume rises appear to be over-estimated by as much as a factor of two. This leads to limited mixing for both stacks only when maximum afternoon mixing heights exceed 1500 meters. Even under these conditions, vertical dispersion dilutes their role in total contributions. Apparently, wind profile power-law coefficients, and horizontal and vertical sigma coefficients used in Brigg's plume-rise equations are poorly representative of the Oil Sands study area under less-than-ideal lapse conditions in these months. Additional sources of simulation error are the fixed GCOS flare emissions rates on a monthly basis and adaptation of CRSTER's interpolated diurnal variation of mixing height scheme for our study in the above months so overnight mixing heights went to zero overnight under stable lapse conditions.

2. Randomization of the flow field in CRSTER with respect to the eight-point compass in the study area appears to be inadequate as shown by splitting of the CDM annual peak north-west through north-east of GCOS into two separate peaks along axes '1' ('1a') and '2' in both years. More specifically, <u>north</u> and <u>east</u> winds figured unrealistically in the partial re-distribution of 1975's peak along '2' to directional axes $\theta = 40^{\circ}$ and $\theta = 60^{\circ}$ in 1976.

3. Because of the small amount of monthly monitor data at each site and due to poor correlation between Syncrude and Mildred Lake monitor results in three of the first four months of 1976 causing uncertainities in observations, linear regression coefficients were very sensitive to a shift in validation site. This is illustrated by the increase in this coefficient (+.47) in

switching from the 1975 monthly study at Syncrude to the 1976 study at Mildred Lake. This increase, however, may be partly accounted for by much higher mean monthly temperatures and mixing heights in most spring and summer months of 1976 relative to 1975.

4. Maximum monthly calculations at Syncrude and Shell in 1975 are well below the Federal Maximum Desirable Level, National Air Quality Objective Standard of 30 $\mu gm.^{-3}$. Annual 1975 peaks along axes '1', '2', and '3' slightly above acceptable accuracy coupled with the absence of monthly GCOS monitor network data signal that monthly statements concerning violations of air quality standards for the GCOS network in 1975 must be interpreted with extreme caution.

5. Although 1976 annual peaks were within the acceptable range, such accuracy on a monthly basis fails at Mildred Lake in some of the highest monthly observations (i.e April) or calculations (i.e. June). The fact that the Mildred Lake monitor April value is greater than the nearby Syncrude value by a factor of eight indicates the possibility of 'local bias' at Mildred Lake. Thus statements concerning violations of air quality standards during 1976 months also must be interpreted with extreme caution.

6. If GCOS acid gas flare emission data is available on a daily basis, and if the growth of the thermal or convective mixing layer is better simulated, analysis of 'worst cases' 24-hourly concentrations will be able to show whether CRSTER reproduces at least qualitatively the daily and diurnal variation of SO_2 concentrations needed to satisfy minimum validation requirements.

8. CONCLUSIONS AND RECOMMENDATIONS

1. In order to validate annual, monthly and episoidal calculations more accurately, it is recommended that the present GCOS monitor network be augmented by additional stations in the region between GCOS and Mildred Lake, Mannix, and Ruth Lake monitor sites. This new network should cover a period of at least two years to account for monthly concentration analomies due to abnormal seasonal weather. Additionally, a scheme to evaluate each monitor station's effectiveness as a measure of the GCOS source's impact similar to modelling methods described by Munn (1978) would aid in the above network design.

2. Over-estimated GCOS powerhouse and incinerator stack plume rise and usually slight flare stacks' plume rise apparently show that CRSTER's handling of plume rise in the Oil Sands area is adequate. This is in spite of CRSTER's use of the same wind profile exponents and horizontal and vertical dispersion coefficients algorithms as found in the CDM model. As plume exit gas temperatures and exit velocities are representative and within normal limits for Brigg's plume rises range of values for GCOS powerhouse and incinerator stacks, plume rise parametric sensitivity testing may be useful. It is recommended that a new method of flare plume rise computation similar to one devised by Trinity Consultants (1978) replace present methods of modelling flare plume rise in future sensitivity tests due to their high relative contributions to total concentrations

3. Other significant sources of CRSTER modelling error are:

(1) interpolated diurnal mixing height variations from nocturnal inversions to high daytime mixing depths on an hourly basis.

(2) poorly randomized wind flow field over an eight-point compass;

(3) fixed annual and monthly emission rates for the highest contributors - main and acid gas flare stacks respectively;

(4) inability to model GCOS powerhouse and incinerator plumes' re-entry through an elevated stable layer's "lid" into the mixing layer which apparently accounts for numerous observed worst cases in the Oil Sands. This latter phenomenon may also apply to Syncrude's main stack plume's similar behaviour.

It is therefore recommended that a multiple source revision of CRSTER presently being developed by EPA be examined to see if any changes in simulation of diurnal variation of the mixing depth on an hourly basis may help alleviate model errors due to this important factor. Our adaptation allowing nocturnal mixing heights to return to observed minimums under stable conditions should be maintained in future validation modelling.

With regard to the other three drawbacks, only the fixed flares emissions problem can be easily remedied. It is recommended, therefore, that episoidal field studies involving frequent monitoring of flaring activity be undertaken during periods of 'worst cases' data gathering.

4. In view of discrepancies between Syncrude and Mildred Lake monitor monthly concentrations for February and April, 1976, it is recommended that quality control tests of the Mildred Lake monitor be made from time to time.

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10. APPENDICES

10.1 APPENDIX 1: Accuracy Criteria for Validation Procedures:

Accuracy within the frequently quoted "factor of two" standards is the criteria used in all verification procedures in this report. This validation measurement involves a test to see if the model's calculated value is within the range represented by lower bound 50% below the observed value and upper bound 100% above this observation. This range covers calculated values occurring a "factor of two" below and above the observed value.

10.2 APPENDIX 2:

Comparison of Syncrude and Mildred Lake Air Quality and Meteorological Data for July, 1975:

Average windspeed at the Syncrude monitor in July, 1975 was 10.2 m.p.h. which was significantly higher than the average of 6.3 m.p.h. obtained at the Mildred Lake weather station a few kilometers away. The three windrose directions East, Southeast, and South - crucial in CRSTER calculations at Syncrude using GCOS emissions - had a combined frequency of 22.3% at Syncrude versus 29.0% at Mildred Lake. The most frequent contributor - the Southeast direction - occurred only 6.8% of the time at Syncrude versus 12.0% at Mildred Lake. The presence of a wind shelter represented by the regional plateau between GCOS and Syncrude may account for the less frequent southeast winds at Syncrude.

In the four days of predominantly light Southeast winds and two days with light south winds at both sites, Syncrude ambient air, SO_2 concentrations were all zero. Although lower Syncrude south, southeast, and east frequencies on these and other July days may be partly accounted for by the significant amount of missing data, its zero concentrations must remain suspect in some of these days.

10.3 **APPENDIX 3:**

Test for Null Hypothesis using Spearman's Rank Correlation Coefficient r_s in Standardized Normal Variable $Z = r_s \sqrt{n-1}$

Define Spearman's Rank Correlation Coefficients, r_s by:

$$r_s = 1 - \frac{6\Sigma D_i^2}{n(n-1)}$$, where

n = number of paired observations (x_i, y_i)

x_i = observed monthly SO_2 concentration

y_i = modelled monthly SO_2 concentration and

D_i = rank (x_i)-rank(y_i)

If the n pair of observed and calculated monthly concentrations (x_i, y_i) $i = 1, n$ [n =11,or 12 here] for all monitors in each experiment have independent random variables X and Y respectively, then r_s has a zero mean and variance $\left(\frac{1}{n-1}\right)$. A test for the null hypothesis

H_o X and Y are independent is made using

$Z = r_s \sqrt{n-1}$

which is approximately a standardized normal variable for large n, say $n \geq 10$, for all experiments.

Note: $-1 \leq r_s \leq +1$

$r_s = 1$ indicates complete agreement in order of ranks and

$r_s = -1$ indicates complete agreement in the opposite order of the ranks.

10.4 APPENDIX 4:

Comments on Meteorological and Air Quality Monitor Local Bias for Mildred Lake and Syncrude in April, 1976

An unusually large monitor value at Mildred Lake in April contributing to loss of required accuracy is suspect on two counts. First, April southeast hourly frequencies were 4.8% higher than 1975 values. Slightly less important south and east directions, although much more infrequent, showed only negligible increases in 1976. Secondly, 1976 Syncrude monitor site concentrations a few kilometers away agreed well with Mildred Lake monitor values in March (9.3 $\mu gm.^{-3}$), but were well below in February (3.7 $\mu gm.^{-3}$) and April (4.2 $\mu gm.^{-3}$). On the other hand, April cases of prevailing southeast winds and large SO_2 concentrations at both sites had light windspeeds in the 5-7 m.p.h range most days. Thus the higher Mildred Lake April concentration appears to be more reliable than the much lower Syncrude value. In view of similar statistics, the May Mildred Lake concentration also appears to be acceptable despite its high value.