

# **Sub-Grid Analysis Technical Report**

**Sub-Grid Ambient Air Quality Technical Report  
for the  
Desolation Flats Natural Gas Exploration  
and Development Project**

Prepared for:

Bureau of Land Management

Rawlins Field Office  
1300 North Third Street  
Rawlins, Wyoming

and

Rock Springs Field Office  
280 Highway 191 North  
Rock Springs, Wyoming

Prepared by:

Buys & Associates, Inc.  
Environmental Consultants  
4720 South Santa Fe Circle, Suite #6  
Englewood, Colorado 80110  
303-781-8211

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## 1.0 INTRODUCTION

The Desolation Flats air quality impact assessment was conducted in accordance with a modeling protocol (Buys and Associates, 2000) methodology that was developed by Buys and Associates and the BLM. The modeling protocol was reviewed and accepted by interested parties prior to conducting the analysis. The protocol specified three analytical regimes: sub-grid, near-field, and far-field. The sub-grid analysis was for receptors less than 4 kilometers (km) from the source (as 4 km is the grid spacing for the near- and far-field analyses). Near-field is the region within 50 km of the Desolation Flats project area, and far-field is the full modeling domain (400 km north-south by 500 km east-west) and includes sensitive area receptors as much as 300 km from the Desolation Flats project area. This technical report addresses the Sub-grid ambient air quality analysis. A separate technical report (Buys and Associates, 2001) addresses the near- and far-field analyses (since both the near- and far-field analyses are based on the CALPUFF model). The sub-grid impact analysis is based on the Industrial Source Complex (ISCST3) model to assess point and area source impacts and the CALINE4 dispersion model to assess roadway traffic impacts.

The ISCST3 dispersion model (Version 00101) was utilized for the point and area source sub-grid impact analysis. ISCST3 is an EPA regulatory model designed to calculate downwind concentrations of air pollutants for various averaging times. The model includes specific controls to account for stack-tip downwash, buoyancy-induced dispersion, final plume rise, calm winds, and default values for wind profile exponents and the vertical potential temperature gradients. To account for possible building downwash affects on the plume, the Building Profile Input Program (BPIP) Model (Version 95086) was also used. The BPIP model creates an input file that is used in ISCST3 downwash calculations. ISCST3 uses actual meteorological data to calculate concentrations. The South Baggs meteorological data from the Continental Divide/Wamsutter II/South Baggs near-field air quality impact analysis (BLM, 1999) for December 1994 through November 1995 was used to represent calendar year 1995 in the ISCST3 model. CALINE4 is a line source model that uses hypothetical meteorological data to calculate a worst-case ambient concentration related to emissions from vehicles traveling on linear roadways.

The primary input variables in all of the models are the emission rates for the pollutants of interest. The emission inventory for the project is documented in a separate technical report (Buys and Associates, 2001). In general, the emissions fall into the following five categories, for which the resulting impacts are discussed separately in the following sections:

1. Individual well site emissions (along with the well site's short access road) of CO, NO/NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub>;
2. Combined emissions of CO, NO/NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub> from a central gathering station / gas plant and nearby wells;
3. Emissions of VOCs and NOx leading to photochemical reactions and potential increased ozone concentrations;
4. Hazardous air pollutant emissions, and
5. Traffic emissions of CO, NO/NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub> on the support roads leading to well site access roads.

Individual well site emissions are described in the Emissions Inventory Technical Report (Buys and Associates, 2001), and include the following:

1. Fugitive dust emissions that could occur during well pad and access road construction, drilling, and completion;
2. Heavy equipment and vehicle tailpipe emissions of CO, NO/NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub> during construction, drilling, completion and production;
3. Emissions of CO, NO/NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub> from diesel-fueled drill rig engines during drilling;
4. Emissions of CO, NO/NO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub>, from completion flares (during completion) and production heaters (during production);
5. VOC emissions from dehydrators and condensate storage tanks during well production;
6. Fugitive dust caused by wind erosion of exposed, un-reclaimed surface areas during construction, drilling, completion, and production.
7. Central gathering station / gas plant emissions that include emissions from nearby individual well sites (once the wells are in production) and emissions of CO, NO/NO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub> from natural gas-fueled compressor engines.

The purpose of the sub-grid modeling analysis is to identify the maximum predicted concentrations in the vicinity of project emission sources for the emitted pollutants. The predicted maximum concentrations are compared with the applicable ambient air quality standards and PSD Class II increments. The objective of the sub-grid modeling is to identify impacts at receptors very near (on the order of 100 meters) the sources that would not otherwise be evaluated in the 4-km grid CALPUFF model used for the near-field and far-field impact assessment. The ambient air quality standards (Wyoming, Colorado, and National) and PSD Class I and II increments are shown in Table 1-1, as well as the assumed background concentrations for the area. The PSD increments are shown for informational purposes only, as this impact analysis is not a regulatory increment consumption analysis. Such an analysis is conducted under separate regulatory authority by the Wyoming Department of Environmental Quality (WDEQ).

Table 1-1 Background Concentrations, Ambient Air Quality Standards, and PSD Increments (. g/m<sup>3</sup>)

Pollutant and Averaging Time	Background Concentration	Wyoming Ambient Air Quality Standards	Colorado Ambient Air Quality Standards	National Ambient Air Quality Standards	PSD Class I Increment	PSD Class II Increment
<b>Carbon Monoxide (CO)</b>						
CO 1-hr	2,299 <sup>a</sup>	40,000	40,000	40,000	None	None
CO 8-hr	1,148 <sup>a</sup>	10,000	10,000	10,000	None	None
<b>Nitrogen Dioxide (NO<sub>2</sub>)</b>						
NO <sub>2</sub> Annual	10 <sup>b</sup>	100	100	100	2.5	25
<b>Ozone (O<sub>3</sub>)</b>						
O <sub>3</sub> 1-hr	144 <sup>d</sup>	None	None	235	None	None
O <sub>3</sub> 8-hr	139 <sup>d</sup>	157	157	157	None	None
<b>Particulate Matter less than 10 microns (PM<sub>10</sub>)</b>						
PM <sub>10</sub> 24-hr	20 <sup>c</sup>	150	150	150	8	30
PM <sub>10</sub> Annual	12 <sup>c</sup>	50	50	50	4	17
<b>Particulate Matter less than 2.5 microns (PM<sub>2.5</sub>)</b>						
PM <sub>2.5</sub> 24-hr	10 <sup>e</sup>	None	None	65	None	None
PM <sub>2.5</sub> Annual	6 <sup>e</sup>	None	None	15	None	None
<b>Sulfur Dioxide (SO<sub>2</sub>)</b>						
SO <sub>2</sub> 3-hr	29 <sup>f</sup>	1,300	700	1,300	25	512
SO <sub>2</sub> 24-hr	18 <sup>f</sup>	260	365	365	5	91
SO <sub>2</sub> Annual	5 <sup>f</sup>	60	80	80	2	20

**Note:** Effective February 27, 2001 the U.S. Supreme Court upheld the EPA's position on the proposed national 8-hr ozone and PM2.5 standards. Implementation of these standards is pending.

The ozone 1-hour background concentration represents the 90<sup>th</sup> percentile of the annual maximum daily 1-hour concentrations for the months April through August.

The 8-hour ozone background concentration represents the average annual 4<sup>th</sup> highest daily maximum 8-hour average.

Other short-term background concentrations represent the second highest measured value.

**Sources:**

- a. CDPHE, 1996 - Data collected at Rifle and Mack, Colorado in conjunction with proposed oil shale development during early 1980s.
- b. BLM, 1996 - To supplement monitored NO<sub>2</sub> data, a separate NO<sub>2</sub> modeling analysis was performed which included many NO<sub>x</sub> emission sources.
- c. WDEQ-AQD, 1997 data collected for the Carbon County UCG Project, data collected 9 miles west of Rawlins, WY, June 1994-November, 1994
- d. Clean Air Status and Trends Network, n.d. - Data collected at Pinedale, Wyoming (1997 - 1999).
- e. Background PM<sub>2.5</sub> concentrations estimated at one-half of PM<sub>10</sub> values based upon EPA literature.
- f. CDPHE-APCD, 1996 - Data collected at the Craig Power Plant site and at Colorado Oil Shale areas from 1980 to 1984.

## 2.0 INDIVIDUAL WELL SITE EMISSIONS IMPACT ANALYSIS

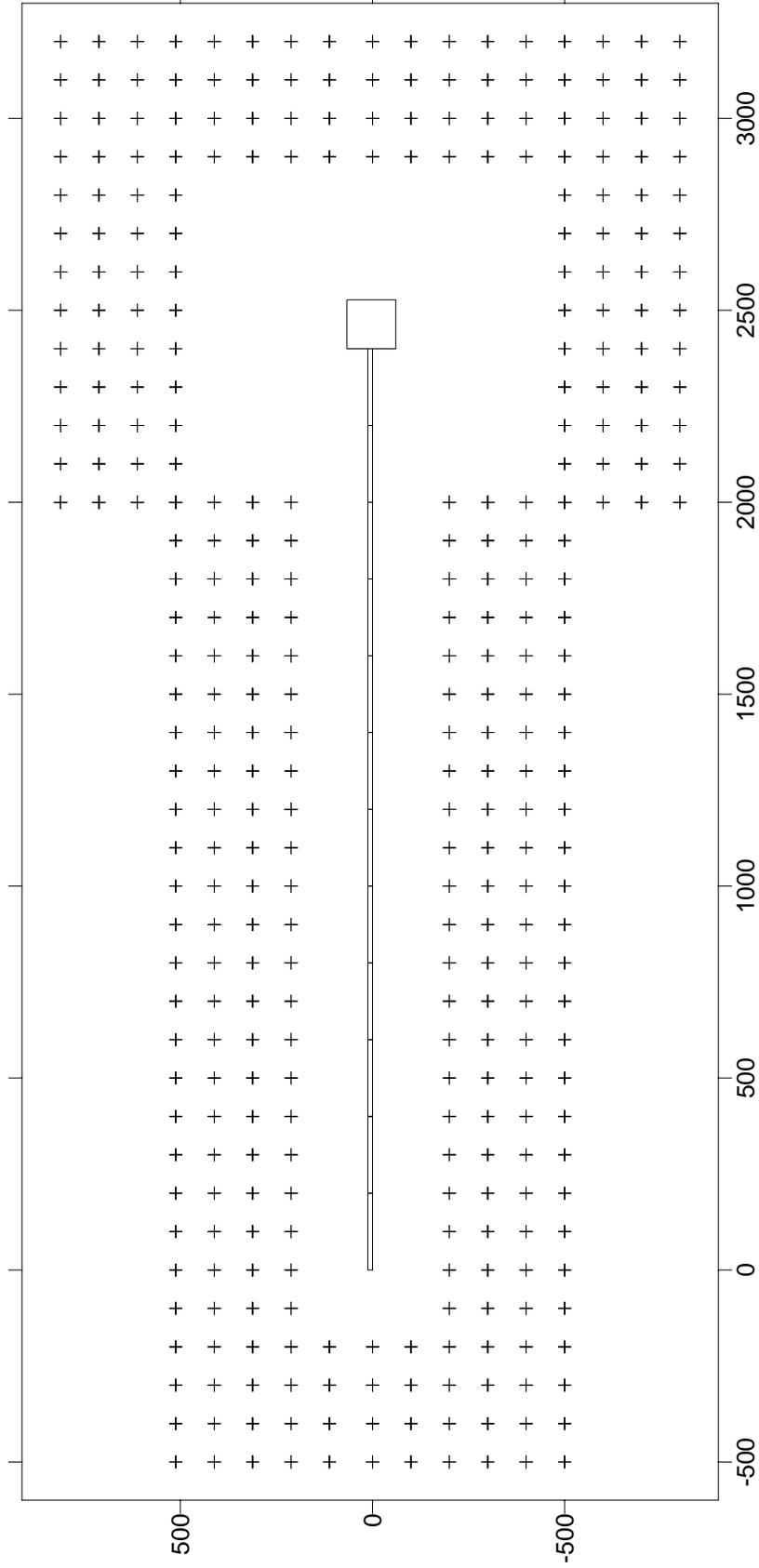
Individual well site emissions are related to the individual well pad (4 acres or 16,130 km<sup>2</sup> or 127 m by 127 m square) and the short (1.5 mile or 2.4 km by 40 feet or 12.2 m) access road. The layout of the well pad, access road, and receptor grid is presented in Figure 2-1.

Receptors were located 200 meters from the access road and 400 meters from the well pad at 100 meter spacing. Since the impacts are within a few hundred meters of the source, it was assumed that all receptors were at the same base elevation of the source. The 200 meter/400 meter minimum distance corresponds to a reasonable distance that heavy equipment operators would prevent the public from approaching during construction of the road and the minimum distance that wells are allowed to be sited from residences. Emissions of CO, NO/NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, and PM<sub>2.5</sub> were modeled as area sources, with the area of the well pad used for well site emissions and twelve 200 meter by 12.2 meter area sources representing the road. The 200 meter distance of the road area sources was chosen to correspond to the minimum receptor distance, which helps avoid unrealistic ISCST3 model results for area sources when receptor distances are much less than area dimensions.

Two sets of emission rates were used in the model corresponding to the ambient air quality standards and increments of interest; short-term and long term. The short-term emission rates are the maximum hourly emission rates that are used to assess one to 24-hour average standards and increments. The long-term emission rates are the annual average emission rates used to assess annual average standards and increments. Short-term emissions were assumed to occur eight hours per day and annual emissions assumed to occur 24 hours per day.

Initially, the construction-related emissions were run, with one set of runs for short-term emission rates and one set of runs for long-term emission rates. The ISCST3 model was then run 36 times for each set of construction related emissions, with the orientation of the access road/well pad combination incrementally rotated 10 degrees for each run (a total of 72 runs). This allows for the worst-case wind angle to be determined, and it was found that the worst-case wind angle was different for short-term versus long-term emissions. The short-term worst-case wind angle was then used for all additional short-term impact analyses, and the long-term worst-case wind angle was used for all additional annual average impact analyses.

**Figure 2-1**  
**Individual Well Site Recpetor Grid**  
**(distances in meters)**



The emission characteristics for each source analyzed in the model are as follows:

- Release height of heavy equipment and vehicle emissions: 2 m
- Release height of wind erosion: 2 m
- Stack Height of drill rig engines: 7.62 m
- Stack height of the flare: 0.305 m
- Stack height of the heater: 3.66 m
- Stack height of the dehydrator: 3.66 m
- Stack height of the condensate storage tank vent: 6.86 m
- Exit temperature and velocity of drill rig engines: 800 degrees K, 50 m/s, 0.1 m diameter
- Exit temperature and velocity of the flare: 800 degrees K, 33 m/s, 0.116 m diameter
- Exit temperature and velocity of the heater: 700 degrees K, 10 m/s, 0.153 m diameter
- Exit temperature and velocity of the dehydrator: 377 degrees K, 0.5 m/s, 0.051 m diameter
- Exit temperature and velocity of the condensate storage tank vent: 282 degrees K, 10 m/s, 0.051 m diameter

Table 2-1 presents the potential ambient air quality impacts for each development phase of an individual well. The maximum impact for each individual phase of operation was added to the monitored background concentrations and compared to the applicable ambient air quality standards. As presented in Table 2-2, potential impacts for a single well will not cause an exceedance of the state or federal ambient air quality standards.

Table 2-1 Ambient Air Quality Impacts Adjacent to a Single Well

Pollutant	Averaging Period	Construction Impact (. g/m <sup>3</sup> )	Drilling Impact (. g/m <sup>3</sup> )	Completion Impact (. g/m <sup>3</sup> )	Production Impact (. g/m <sup>3</sup> )	Maximum Impact (. g/m <sup>3</sup> )
NO <sub>2</sub>	Annual	0.0026	1.92	0.014	0.02	1.92
CO	1-hour	22.83	123.61	438.83	0.22	438.83
CO	8-hour	4.00	59.79	191.64	0.09	191.64
SO <sub>2</sub>	3-hour	0.83	5.93	0.012	0	5.93
SO <sub>2</sub>	24-hour	0.17	2.29	0.0027	0	2.29
SO <sub>2</sub>	Annual	0.00005	0.032	0.00001	0	0.032
PM <sub>10</sub>	24-hour	23.69	3.48	4.99	0.03	23.69
PM <sub>10</sub>	Annual	0.0015	0.047	0.012	0.001	0.047
PM <sub>2.5</sub>	24-hour	3.29	2.72	2.05	0.02	3.29
PM <sub>2.5</sub>	Annual	0.00037	0.038	0.002	0.001	0.038

Table 2-2 Maximum Ambient Air Quality Impacts for an Individual Well

Pollutant	Averaging Period	Maximum Single Well Impact (. g/m <sup>3</sup> )	Monitored Back-ground Level (. g/m <sup>3</sup> )	Maximum Impact Plus Back-ground (. g/m <sup>3</sup> )	National Ambient Air Quality Standard (. g/m <sup>3</sup> )	Wyoming Ambient Air Quality Standard (. g/m <sup>3</sup> )	Colorado Ambient Air Quality Standard (. g/m <sup>3</sup> )	Percentage of Most Stringent Ambient Air Quality Standard
NO <sub>2</sub>	Annual	1.92	10	11.92	100	100	100	12%
CO	1-hour	438.83	2,299	2,738	40,000	40,000	40,000	7%
CO	8-hour	191.64	1,148	1,340	10,000	10,000	10,000	13%
SO <sub>2</sub>	3-hour	5.93	29	34.93	1,300	1,300	700	5%
SO <sub>2</sub>	24-hour	2.29	18	20.29	365	260	365	8%
SO <sub>2</sub>	Annual	0.032	5	5.032	80	60	80	8%
PM <sub>10</sub>	24-hour	23.69	20	43.69	150	150	150	29%
PM <sub>10</sub>	Annual	0.047	12	12.047	50	50	50	24%
PM <sub>2.5</sub>	24-hour	3.29	10	13.29	65	NA	NA	20%
PM <sub>2.5</sub>	Annual	0.038	6	6.038	15	NA	NA	40%

Note: PM<sub>2.5</sub> background assumed to be one-half of PM<sub>10</sub> background.

By adding the maximum modeled concentrations at the model receptors to representative background concentrations, it was demonstrated that both short- and long-term total predicted criteria pollutant impacts are less than applicable WAAQS, CAAQS, and NAAQS, with the maximum impact being less than 40% of the PM<sub>2.5</sub> NAAQS. Note that adding the modeled maximum to the background results in an overestimate of actual impacts because these two events would occur under very different meteorological conditions, which are not expected to coincide. Furthermore, since no background PM<sub>2.5</sub> data are available, it was assumed that background PM<sub>2.5</sub> concentrations were one-half of the PM<sub>10</sub> background concentrations. This is most likely a considerable overestimate as well since the primary source of background particulate in Wyoming and Colorado is dust generated by processes other than chemical reactions (e.g., vehicle traffic on dirt roads, wind blown dust, etc.) within which the fraction of PM<sub>2.5</sub> tends to be much lower than one-half of the PM<sub>10</sub> level.

Although presented in Table 2-2, it should be noted that particular matter emissions associated with temporary construction activity do not consume PSD Class II increments. At the Federal level, all temporary emissions of any pollutant are excluded from increment consumption:

The EPA allows for the exclusion of temporary emissions (e.g., emissions occurring during the construction phase of a project) when establishing the impact area and conducting the subsequent air quality analysis (EPA 1990).

In Wyoming, particulate matter emissions are excluded according to Chapter 6, Section 4 (b)(iii):

Temporary particulate matter emissions such as those associated with the construction phase of the source shall not be included in the determination on the issuance or denial of a required permit and shall not be taken into account when determining compliance with the maximum allowable increments... (WDEQ-AQD 1999).

“Temporary” is defined as less than 2 years in both the EPA and Wyoming regulations. Clearly, the road and pad construction emissions, drilling, and completion activities are construction-related, and each well site requires far less than 2 years to construct. Consequently, the particulate matter PSD Class II increment regulations do not apply.

### 3.0 COMBINED IMPACTS OF CENTRAL GATHERING STATION AND NEARBY WELLS

In order to assess the combined impacts of a central gathering station (with compressor engine emissions) and nearby wells, two sets of ISCST3 model runs were completed. The first set was to identify the significant impact area of the central gathering station emissions alone in order to determine how many nearby wells could significantly contribute to a combined impact.

The significant impact level (SIL) runs for the central gathering station alone were made assuming that there would be a total of four 1,250 horsepower and one 1,000 horsepower compressor engines located at the gathering station / gas plant. The modeled stack emission characteristics for the compressor engines are as follows:

- Stack height: 9.3 m, vertical orientation
- Exit Temperature: 800 degrees K
- Stack Diameter: 0.305 m
- Exit Velocity: 13.7 m/s
- Compressor Building Horizontal Dimension: 10.97 m by 8.13 m
- Compressor Building Height: 6.09 m
- Stack Location: Short side of compressor building, about 1 m away from building

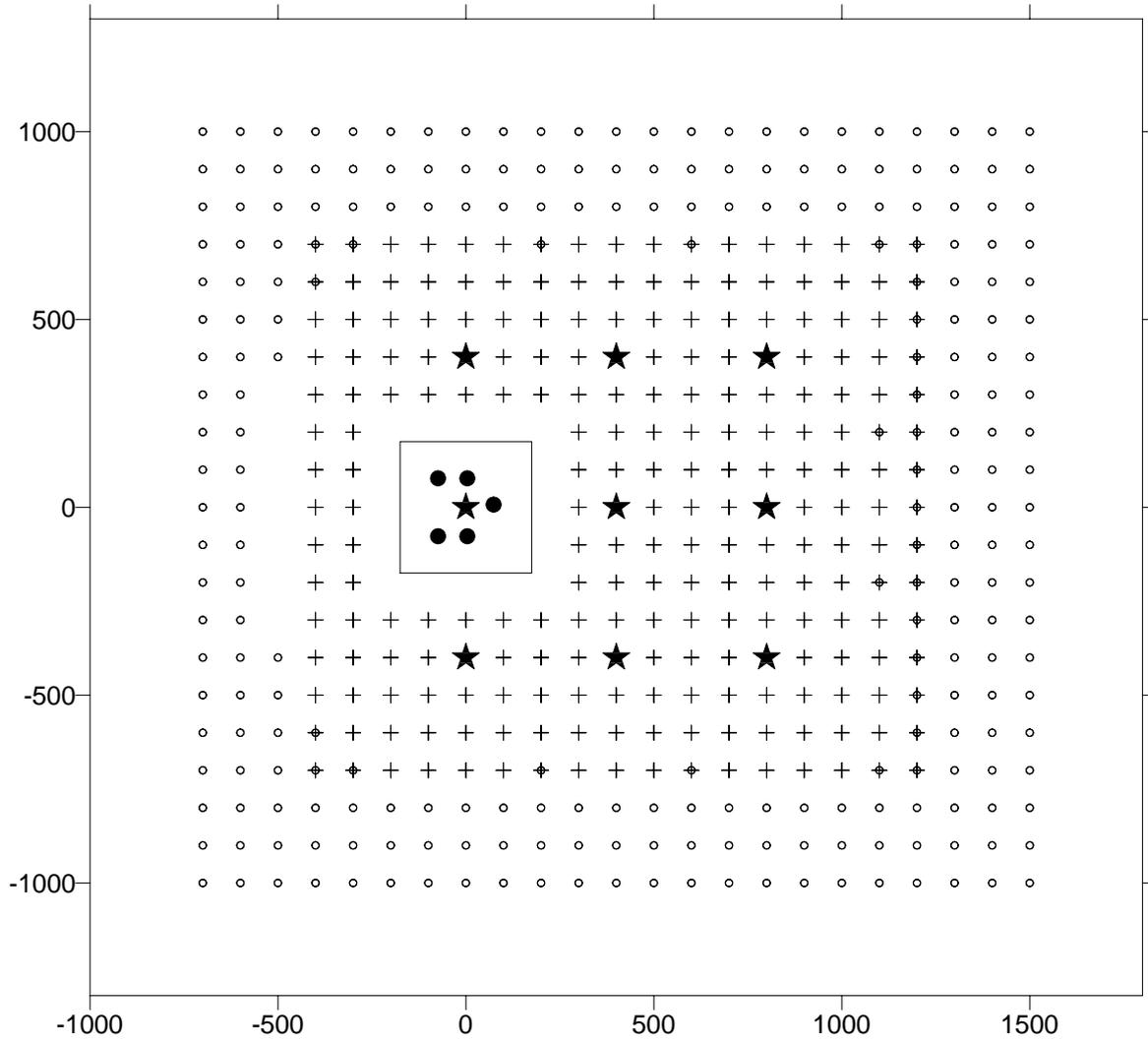
Emissions of both NO<sub>x</sub> and PM<sub>10</sub> were modeled to evaluate the SIL since these are the largest emissions from compressor engines. The USEPA definition of SIL was used, i.e., 1 . g/m<sup>3</sup> annual average concentration. It was found that the SIL for NO<sub>x</sub> was much greater than PM<sub>10</sub>. Again, just as in the individual well site analysis, the worst-case wind angle was used for the SIL modeling. The results are shown in Figure 3-1. Note from Figure 3-1, that for the SIL analysis, standard Wyoming DEQ procedures of a 100 meter spacing receptor grid was used from 100 meters away from the boundary to the site to 1 km, and a 500 meters spacing receptor grid beyond 1 km from the boundary. The gathering station site dimensions were conservatively chosen as 350 meters by 350 meters.

Figure 3-1 shows that the maximum SIL area is less than about 1.5 km from the gathering station, however, the largest concentrations (2 . g/m<sup>3</sup> and greater) are well within 1 km from the gathering station. Therefore, in order to determine maximum combined impact concentrations of the gathering station and nearby wells, a set of 9 wells was assumed to be located at the same location as the maximum gathering station impacts. This configuration is shown in Figure 3-2. Note that one well was assumed to be located in the center of the gathering station, and the remaining 8 wells assumed to be located at the minimum well spacing that could be encountered of one well every 400 meters.

The results of the combined impact modeling are shown in Table 3-1. Note that for the combined impacts modeling, it was assumed that wind erosion could occur from the gathering station site as well as the well pads, even though after construction, the gathering station and well pad site surfaces would rapidly become stabilized, and wind erosion minimized. In addition, the worst-case wind angle for short-term and long-term concentrations was used in the assessment. The maximum combined impacts, including background, are 45% of the PM<sub>2.5</sub> standard, but just as in the case of the individual well pad impacts, this value conservatively assumed that the background PM<sub>2.5</sub> concentration was one-half the PM<sub>10</sub> background.



**Figure 3-2**  
**Receptor Grid For Combined Impacts**  
**Of Central Gathering Station and**  
**Nearby Wells**



- ★ Well Sites
- Compressor Engines
- Long Term HAP Receptors
- + Short Term HAP Receptors and Criteria Pollutant Receptors

Table 3-1 Gas Plant and Well Field Impact

Pollutant	Averaging Period	Gas Plant and Well Field Impact (. g/m <sup>3</sup> )	Monitored Back-ground Level (. g/m <sup>3</sup> )	Maximum Impact Plus Back-ground (. g/m <sup>3</sup> )	National Ambient Air Quality Standard (. g/m <sup>3</sup> )	Wyoming Ambient Air Quality Standard (. g/m <sup>3</sup> )	Colorado Ambient Air Quality Standard (. g/m <sup>3</sup> )	Percentage of Most Stringent Ambient Air Quality Standard
NO <sub>2</sub>	Annual	4.17	10	14.17	100	100	100	14%
CO	1-hour	168.39	2,299	2,467	40,000	40,000	40,000	6%
CO	8-hour	83.69	1,148	1,232	10,000	10,000	10,000	12%
SO <sub>2</sub>	3-hour	0	29	29	1,300	1,300	700	4%
SO <sub>2</sub>	24-hour	0	18	18	365	260	365	7%
SO <sub>2</sub>	Annual	0	5	5	80	60	80	8%
PM <sub>10</sub>	24-hour	7.31	20	27.31	150	150	150	18%
PM <sub>10</sub>	Annual	1.69	12	13.69	50	50	50	27%
PM <sub>2.5</sub>	24-hour	2.58	10	12.58	65	NA	NA	19%
PM <sub>2.5</sub>	Annual	0.71	6	6.71	15	NA	NA	45%

Note: PM<sub>2.5</sub> background assumed to be one-half of PM<sub>10</sub> background.

#### 4.0 POTENTIAL OZONE IMPACTS

Excess ozone may be formed in the lower atmosphere from photochemical reactions involving ambient concentrations of  $\text{NO}_x$  and VOC. Because of the complex photochemical reactions necessary to form ozone, compliance with the NAAQS cannot be determined with a conventional Gaussian dispersion model. Instead, a nomograph developed from the Reactive Plume Model (Scheffe 1988) was used to predict maximum potential ozone impacts. The screening method, based on the referenced nomograph for ozone, involves computing the  $\text{NO}_x$  to VOC emission ratio, and then using this ratio (along with VOC emissions), to obtain incremental ozone concentration values.

Since ozone formation is a regional issue (as it takes time for the VOC and  $\text{NO}_x$  to react), to evaluate the incremental ozone concentrations that could be caused by the Desolation Flats project, the entire project area production emissions were used in the ozone impact assessment as well as the "point source" emissions of a gathering station plus nine nearby wells. (The project total emissions were used to determine the VOC to  $\text{NO}_x$  ratio, while the point source emissions were used to assess the impact on ambient 1-hour and 8-hour ozone concentrations.) Since well construction, drilling, completion, and development would occur serially at a maximum rate of 45 wells per year, but once developed, there could be as many as 385 wells operating continuously each year, the well construction, drilling, completion, and development emissions are considerably less than the ultimate production emissions. Therefore, production emissions (assuming a fully developed well field of 385 wells and associated compression) were evaluated for the VOC to  $\text{NO}_x$  ratio.

At ultimate production, there are 4,358 tons per year (tpy) of VOC from the dehydrators, 10,031.2 tpy from flashing the condensate storage tanks, 365.5 tpy from working and breathing losses in the condensate storage tanks, 54.5 tpy from compressors, and 0.3 tpy from the heaters; for a total of 14,909.5 tpy of VOC emissions.  $\text{NO}_x$  emissions occur only from the compressor engines (309 tpy) and heaters (41,525 tpy); for a total of 350.5 tpy  $\text{NO}_x$ . This is a VOC to  $\text{NO}_x$  ratio of 359.1.

The combined emission rate of VOCs from the gathering station and nine wells is 101.9 tpy from the dehydrators, 234.5 tpy from flashing, 8.5 tpy from condensate tank working and breathing losses, and 28.97 tpy from compression, for a total of 373.87 tpy. At this VOC emission rate and a VOC to  $\text{NO}_x$  ratio greater than 20.7, the nomograph (Appendix A, Table 1), yields an incremental ozone concentration of 0.009 parts per million (ppm). This is equivalent to  $18 \text{ g/m}^3$ . The results of the ozone impact analysis are shown in Table 4-1

Table 4-1 Maximum Modeled Ozone Concentration

Pollutant	Ave. Time	Direct Modeled ( $\mu\text{g}/\text{m}^3$ )	Back-ground ( $\mu\text{g}/\text{m}^3$ )	Total ( $\mu\text{g}/\text{m}^3$ )	WAAQS ( $\mu\text{g}/\text{m}^3$ )	CAAQS ( $\mu\text{g}/\text{m}^3$ )	NAAQS ( $\mu\text{g}/\text{m}^3$ )
Ozone	1-hour	18	144	162	None	None	235
Ozone	8-Hour	18	139	157	157	157	157

Note: The 1-hour background concentration is the 90<sup>th</sup> percentile of the maximum daily 1-hour concentrations for the months of April through August.

The 8-hour background concentration is the average annual 4<sup>th</sup> highest daily maximum 8-hour average.

Table 4-1 appears to indicate that the project could cause a maximum 8-hour ozone concentration equal to the AAQS. However, it must be kept in mind that the screening nomograph is a highly conservative methodology that intentionally over-estimates the impacts. In addition, the emissions used in the assessment are conservatively large values. Therefore, an ozone exceedance is not expected.

## 5.0 HAZARDOUS AIR POLLUTANT IMPACTS

During production, there are potential emissions of six hazardous air pollutants (HAPs): benzene, toluene, ethylbenzene, xylene (BTEX), n-hexane, and formaldehyde. These emissions can occur from the compressor engines in addition to producing wells. Therefore, to assess potential HAPs impacts, the same combined impact scenario of a central gathering station plus nine nearby wells that was used to assess maximum criteria pollutant impacts (Section 3.0 of this report) was used to assess HAP impacts. However, two different receptor grids were used, depending upon the potential health effect to be evaluated.

For potential short-term (i.e., 8-hour exposure) health effects, the HAPs receptor grid was the same that was used for criteria pollutant impacts: receptors located as near as 100 meters from the site boundaries out to 1 km, at 100 meter spacing. Short-term health effects were evaluated for all six HAPs. For long-term health effects (i.e., annual exposure related to possible carcinogenesis), the nearest receptors were 400 meters from a well pad or gathering station boundary. This corresponds to the minimum distance that wells are allowed to be built next to a residence. (It is possible for a worker to be exposed 8-hours within 100 meters of a well, but not continuously for 365 days, 24 hours per day, as might a resident).

To evaluate the significance of HAP emissions, short-term Acceptable Ambient Concentration Levels (AACL) were developed and presented in the Modeling Protocol (Buys and Associates, 2000). The short-term AACLs are shown in Table 5-1.

Table 5-1 AACLs for Short-term HAP Exposure

Pollutant	Range of State 8-hour AACL ( $\mu\text{g}/\text{m}^3$ )
Benzene	30 <sub>FL07</sub> - 714 <sub>NV01</sub>
Toluene	1,870 <sub>IN03</sub> - 8,930 <sub>NV01</sub>
Ethylbenzene	4,340 <sub>ND01</sub> - 43,500 <sub>VT01</sub>
Xylene	2,170 <sub>IN01</sub> - 10,000 <sub>NV01</sub>
n-Hexane	1,800 <sub>FL07</sub> - 36,000 <sub>CT01</sub>
Formaldehyde	4.5 <sub>FL07</sub> - 71 <sub>NV01</sub>

Source: EPA (1997a).

CT01	Connecticut Department of Environmental Protection, Air Compliance Unit
FL07	Florida, Pinellas County Air Pollution Control Board
IN01	Indiana Department of Environmental Management
IN03	Indiana, Indianapolis Air Pollution Control Division
ND01	North Dakota Department of Health, Division of Environmental Engineering
NV01	Nevada Division of Environmental Protection, Air Quality Control
VT01	Vermont Department of Environmental Conservation, Air Pollution Control Division.

Comparison of short-term (8-hour) exposure and modeled HAP concentrations to the AACLs is straight-forward, simply comparing the modeled 8-hour concentration to the AACL. On the other hand, long-term exposure (annual average concentrations) is more difficult, since the AACLs are based on an incremental cancer risk of one additional cancer per million persons exposed (“one in a million”). The one in a million criterion is the most stringent normally used in practice, and the USEPA considers a range of one in a million to 100 in a million as acceptable. However, for this analysis, only the one in a million criterion will be used.

Incremental cancer risk is calculated from a Unit Risk Factor (URF) which is the probability of one additional cancer occurring if a person was exposed continuously for a lifetime of 70 years to an ambient concentration of 1  $\mu\text{g}/\text{m}^3$ . URFs are expressed in units of inverse  $\mu\text{g}/\text{m}^3$ . Of the six HAPs evaluated, only benzene and formaldehyde are suspected carcinogens. The URF for benzene is  $7.8 \times 10^{-6} (\mu\text{g}/\text{m}^3)^{-1}$  and the URF for formaldehyde is  $1.3 \times 10^{-5} (\mu\text{g}/\text{m}^3)^{-1}$ , assuming continuous outdoor exposure for a 70-year lifetime. These URFs are based on WDEQ policy for formaldehyde and USEPA unit risk factors for carcinogenic constituents (EPA 1997b) for benzene.

However, the Desolation Flats project lifetime is estimated at 20 years. Therefore, for comparison to the Most Stringent AACL, it was assumed that a person could be exposed continuously outdoors to the maximum modeled annual concentration, for 20 years. For comparison to the “Greatest AACL”, it was assumed that a person would be exposed outdoors 64% of the time, and indoors the remaining 36% of the time indoors. The indoor concentration was assumed to equal one-fourth the outdoor concentration. In addition, it was assumed that the duration of exposure was 9 years, corresponding to a reasonable maximum duration at a single residence. The maximum modeled annual concentration was that found using the worst-case long-term wind angle. The maximum modeled concentrations occurred at the closest receptor, and decrease rapidly with small incremental distances. The results of the HAPs impact analysis are presented in Table 5-2.

Table 5-2 Short-Term Hazardous Air Pollutant Impacts

Hazardous Air Pollutant	Combined Potential Impact from Gas Plant and Wells (8-hour Average) ( $\mu\text{g}/\text{m}^3$ )	Range of State Acceptable Ambient Concentration Limits ( $\mu\text{g}/\text{m}^3$ )	Percentage of Most Stringent Acceptable Ambient Concentration Limit	Percentage of Greatest Acceptable Ambient Concentration Limit
Benzene	31.21	30 to 714	104.0%	4.4%
Toluene	79.73	1,870 to 8,930	4.3%	0.9%
Ethylbenzene	42.81	4,340 to 43,500	1.0%	0.1%
Xylenes	55.9	2,170 to 10,000	2.6%	0.6%
n-Hexane	41.47	1,800 to 36,000	2.3%	0.1%
Formaldehyde	4.13	4.5 to 71	91.8%	5.8%

As Table 5-2 indicates, the short and long-term impacts for all HAPs except benzene and formaldehyde are much less than even the most stringent AACL. Short-term and long-term impacts for benzene and formaldehyde are near or slightly over the Most Stringent AACL, but much less than the Greatest AACL. Table 5-3 presents the benzene and formaldehyde long-term impacts in terms of incremental cancer risks. Considering the conservatism built into the modeling procedure, the emissions estimates, and the AACLs themselves, even though the modeled concentrations may exceed the Most Stringent AACL, HAPs emissions are not expected to cause an adverse environmental impact.

Table 5-3 Potential Incremental Carcinogenic Risk

Hazardous Air Pollutant	Incremental Carcinogenic Risk Resulting From The Maximum Exposure Scenario	Incremental Carcinogenic Risk Resulting From The Most Likely Exposure Scenario
Benzene	1.6 in one million	0.5 in one million
Formaldehyde	0.9 in one million	0.3 in one million

## 6.0 TRAFFIC EMISSION IMPACTS

The Desolation Flats project may generate additional vehicular traffic on support roads that lead from the normally traveled roads to the well site access roads. These support roads were assumed to be unpaved and 15 miles (24 km) long. Emissions from these roads include fugitive dust generated by construction equipment, light trucks (e.g., half-ton pickup trucks) used by construction employees, and light trucks used by well field employees; as well as tailpipe emissions from those vehicles.

In order to assess the impacts, the CALINE4 Model (Version dated June, 1989) was used. CALINE4 uses hypothetical worst-case meteorology and emission rates to calculate worst-case hourly concentrations. These hourly concentrations can then be adjusted using USEPA default averaging time parameters to represent worst-case concentrations for 8-hour, 24-hour and annual averages. The emission rates used in the modeling are those reported in the Emission Inventory Report. Four combinations of receptor configuration and meteorology were run:

- F stability, 1 m/s wind speed, 50 meter receptor distance
- F stability, 1 m/s wind speed, 200 meter receptor distance
- D stability, 3 m/s wind speed, 50 meter receptor distance
- D stability, 3 m/s wind speed, 200 meter receptor distance

The remaining input parameters used in the CALINE4 modeling are as follows:

- Wind angle: worst-case
- Mixing height: 1000 meters
- Sigma theta: 20 degrees
- Surface roughness ( $z_0$ ): 100 cm
- Deposition velocity: zero
- Ambient temperature: 10 degree C
- Roadway width: 18 meters
- Base elevation of roadway: 2000 meters

The results of the CALINE4 modeling are shown in Table 6-1. As shown in the table, additional project-related vehicular traffic on support roads is not expected to cause an adverse ambient air quality impact.

Table 6-1 Vehicle Traffic Impacts

Pollutant	Averaging Period	Vehicle Traffic Impact (. g/m <sup>3</sup> )	Monitored Back-ground Level (. g/m <sup>3</sup> )	Maximum Impact Plus Back-ground (. g/m <sup>3</sup> )	National Ambient Air Quality Standard (. g/m <sup>3</sup> )	Wyoming Ambient Air Quality Standard (. g/m <sup>3</sup> )	Colorado Ambient Air Quality Standard (. g/m <sup>3</sup> )	Percentage of Most Stringent Ambient Air Quality Standard
NO <sub>2</sub>	Annual	0.0	10	10	100	100	100	10%
CO	1-hour	0.8	2,299	2,300	40,000	40,000	40,000	5.8%
CO	8-hour	0.6	1,148	1,149	10,000	10,000	10,000	12%
SO <sub>2</sub>	3-hour	0.0	29	29	1,300	1,300	700	4.1%
SO <sub>2</sub>	24-hour	0.0	18	18	365	260	365	6.9%
SO <sub>2</sub>	Annual	0.0	5	5	80	60	80	8.3%
PM <sub>10</sub>	24-hour	23.9	20	44	150	150	150	29%
PM <sub>10</sub>	Annual	6.0	12	18	50	50	50	36%
PM <sub>2.5</sub>	24-hour	3.5	10	13.5	65	NA	NA	21%
PM <sub>2.5</sub>	Annual	0.9	6	6.9	15	NA	NA	46%

Note: PM<sub>2.5</sub> background assumed to be one-half of PM<sub>10</sub> background.

## 7.0 SUMMARY

Five emissions scenarios were modeled to assess sub-grid (i.e., 4 km or less) impacts of Desolation Flats project sources: vehicular traffic on access and support roads, well sites, and gathering stations. Potential impacts of criteria pollutant (CO, NO/NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, PM<sub>2.5</sub> and VOC) emissions and hazardous air pollutant (benzene, toluene, ethylbenzene, xylene, n-hexane, and formaldehyde) were evaluated. The modeled impacts were compared to various criteria, including the state (Wyoming and Colorado) and federal ambient air quality standards and Acceptable Ambient Concentration Levels (AACLS) used by various states for the assessment of hazardous air pollutant (HAP) impacts.

It was found that the combined impact of a central gathering station and nearby well sites produces the maximum concentrations of both criteria pollutants and HAPs. Vehicular traffic impacts are less than the point source impacts of the gathering station and nearby wells. Maximum criteria pollutant impacts ranged from 4% to 45% of the most stringent ambient air quality standard (3-hour SO<sub>2</sub> and annual PM<sub>2.5</sub>, respectively). Short-term (8-hour) HAPs impacts ranged from 0.1% to 6% of the most stringent AACL and long-term potential carcinogenic impacts ranged from 0.3 to 1.6 incremental cancers per million persons exposed.

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## **APPENDIX A**

### **Scheffe Ozone Screening Methodology**

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VOC/NOX POINT SOURCE SCREENING TABLES

by Richard D. Scheffe

August 1988

United States Environmental Protection Agency  
Office of Air Quality Planning and Standards  
Technical Support Division  
Source Receptor Analysis Branch

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## 1.0 INTRODUCTION

This document provides a simple screening procedure presented in tabular form to calculate the ozone increment due to a VOC dominated (i.e., VOC mass emissions greater than NOx emissions) point source. [Throughout this document, ozone increment refers to a calculated increase in ozone above an assumed ambient value due to the effect of a single point source.] The tables are based on a series of applications of the Reactive Plume Model-II (RPM-II), a Lagrangian based photochemical model. Anticipated applications would include evaluation of the impact on ambient ozone due to new or modified point sources emitting more than 25 tons/year NMOC (nonmethane hydrocarbons). The screening technique is presented as two separate tables intended for application in urban and rural areas, respectively.

The user is directed to section 3 of this report for application procedures needed to conduct an ozone increment screening analysis. Required inputs for determining an ozone increment are limited to estimates of NMOC and NOx mass emissions rates. As a screening technique the procedure has been designed to be both robust and simple to use, while maintaining several inherent assumptions which lead to conservative (high ozone) ozone increment predictions. The user is not required to characterize ambient meteorology or source emissions and ambient speciation profiles. This technique is not intended to be substituted for a realistic photochemical modeling analysis; rather it is to be used only in the context of a first-step procedure which potentially can preclude further resource intensive analyses. The ozone increment estimates produced from this analysis should be interpreted as conservative predictions which would exceed ozone formation produced by actual episodic events.

A description of the protocol and assumptions used in developing the screening tables is given in Appendix A.

## 2.0 BACKGROUND

Estimations of impacts of point sources emitting ozone precursors (NOx and/or VOC emissions) on ambient ozone provide regulatory agencies with data to address air quality issues involving proposed new or modified sources. In theory many issues can be resolved by applying a photochemical air quality model. However, two questions regarding model application must be resolved: (1) what is the most appropriate model for a particular application, and (2) how should that model be applied (i.e., how are model inputs developed and output interpreted)?

The Guideline on Air Quality Models (1986) recommends application of two photochemical models for addressing ozone air quality issues, the Urban Airshed Model (UAM) or EXMA. The EXMA model is not designed to handle point sources, as point source emissions are immediately spread into a broadly based urban mix and the individual contribution of a single point source is quenched by such broad spatial dilution. Although the UAM explicitly handles spatial resolution of point sources through spatially gridded cells, the degree of resolution typically offered by such gridding (4-5 km) is still insufficient to account for near-source behavior. Also, the resources and input data required by the UAM are very extensive; consequently, it is an inefficient means for evaluating effects of individual sources.

The Reactive Plume Model-II (RPM-II) is an alternative air quality model which was developed in the late 1970's to address photochemically reactive plumes. The model's inherent flexibility accommodates recently developed chemical mechanisms; this work was based on use of the Carbon Bond Mechanism-Version IV (CBM-IV), which is consistent with other, current EPA photochemical models (ROM, EXMA).

The RPM-II is an appropriate choice for case by case refined (i.e., not as an initial screening estimate) modeling applications. However, the prospective model user faces the possibility of conducting an exhaustive compilation of meteorological and emissions source data. Consequently, use of photochemical models to assess individual point sources has been limited. The development of a screening analysis may eliminate, in certain applications, the need for a more intensive refined modeling analysis. Current modeling guidelines do not offer recommendations for screening of individual source impacts on ozone. The tables presented herein are intended to serve as a means for screening effects on ozone from individual point sources so that subsequent, more refined analyses can be focused on sources where it is warranted.

## 2.0 SCREENING TABLES

The interpretation or definition of a "rural" or "urban" area within the framework of this technique is intended to be rather broad and flexible. The rationale for having rural and urban tables stems from the need to account for the coupled effect of point source emissions and background chemistry on ozone formation. Background chemistry in the context of this procedure refers to a characterization of the ambient atmospheric chemistry into which a point source emits. The underlying model runs used to develop the rural table (Table 1) were performed with spatially invariant background chemistry representative of "clean" continental U.S. areas. Model runs used to develop the urban table (Table 2) were based on background chemistry incorporating daily temporal fluctuations of NOx and hydrocarbons associated with a typical urban atmosphere (refer to Appendix A for details regarding background chemistry). Background chemistry is an important factor in estimating ozone formation; however, characterization of background chemistry is perhaps the most difficult aspect of reactive plume modeling because of data scarcity and the level of resources required to measure or model (temporally and spatially) the components necessary to characterize the ambient atmosphere along the trajectory of a point source plume.

Recognizing the conflicting needs of using simple characterizations of background chemistries and applying this screening technique in situations where sources are located in or impact on areas which can not be simply categorized, the following steps should be used to choose an appropriate table:

- (1) If the source location and downwind impact area can be described as rural and where ozone exceedances have never been reported, choose the rural area table.
- (2) If the source location and downwind impact area are of urban character, choose the urban area table.
- (3) If an urban based source potentially can impact a downwind rural area, or a rural based source can potentially impact a downwind urban area, use the highest value obtained from applying both tables.

The VOC point source screening tables (Tables 1 and 2) provide ozone increments as a function of NMOC (nonmethane organic carbon) mass emissions rates and NMOC/NOx emissions ratios. To determine an ozone impact the user is required to apply best estimates of maximum daily NMOC emissions rate, and estimated annual mass emissions rates of NMOC and NOx which are used to determine NMOC/NOx ratio for ascribing the applicable column in Table 1 or 2. The reasons for basing application on daily maximum NMOC emissions rates are (1) to avoid

underestimates resulting from discontinuous operations and (2) the underlying modeling simulations are based on single day episodes. The NMOC emissions rates in Tables 1 and 2 are given on an annual basis; consequently the user must project daily maximum to annual emissions rates, as illustrated in the example application given below. One purpose of this technique is to provide a simple, non-resource intensive tool; therefore, annual NMOC/NOx emissions ratios are used because consideration of daily fluctuations would require a screening application applied to each day.

Parameters describing background chemistry, episodic meteorology, and source emissions speciation affect actual ozone impact produced by a point source. However, as a screening methodology the application should be simple, robust and yield conservative (high ozone) values. Thus, only NMOC and NOx emissions rates are required as input to Tables 1 and 2.

### Rural Example Application

A manufacturing company intends to construct a facility in an isolated rural location where ozone exceedances have never been observed. The pollution control agency requires that the company submit an analysis showing that operation of the proposed facility will not result in an ozone increment greater than X ppm in order to permit operation. The estimated daily maximum NMOC emissions rate is 9000 lbs/day. The annual estimated emissions rates for NMOC and NOx are 1000 tons/yr and 80 tons/yr, respectively. The company's strategy is to provide a screening analysis using the rural area table to prove future compliance. If the screening result exceeds X ppm, the company will initiate a detailed modeling analysis requiring characterization of source emissions speciation, ambient chemistry, and episodic meteorology.

#### Screening Estimate:

- 1 - Determine which column of Table (1) is applicable:

The NMOC/NOx ratio is based on annual estimates; thus,  $1000/80 = 12.5$  and middle column values are applied.

- 2 - Calculate annual NMOC emissions rates in tons/yr from maximum daily rate:

$$(9000 \text{ lbs/day}) (1 \text{ ton}/2000 \text{ lbs}) (365 \text{ days/yr}) = 1643 \text{ tons/yr}$$

- 3 - Interpolate linearly between 1500 tons/yr and 2000 tons/yr to produce an interpolated column 2 ozone increment:

$$(1643-1500)(3.84-3.05)/(2000-1500) + 3.04 = 3.27 \text{ pphm}$$

$$3.27\text{pphm}(1 \text{ ppm}/100 \text{ pphm}) = \underline{0.0327 \text{ ppm}}$$

If 0.0327 ppm is below the criterion value (X ppm), no further modeling analysis is required and operation may be permitted. Otherwise, the company will proceed with an additional case-specific modeling analysis.

Table 1. Rural based ozone increment (pphm) as a function of NMOC emissions and NMOC/NOx ratios.

NMOC EMISSIONS (TONS/YR)	NMOC/NOx		
	TONS NMOC/TONS NOx (PPMC/PPM)		
	> 20.7 (> 20)	5.2-20.7 (5-20)	< 5.2 (< 5)
50	0.36	0.38	1.05
75	0.38	0.44	1.24
100	0.42	0.51	1.38
300	0.80	1.03	1.71
500	1.14	1.44	1.88
750	1.58	1.94	2.33
1000	2.00	2.35	2.70
1500	2.73	3.05	3.30
2000	3.36	3.84	3.66
3000	4.80	5.19	4.31
5000	6.98	7.50	4.83
7500	9.78	10.10	5.10
10000	12.15	12.86	5.43

\* multiply pphm by 0.01 to obtain ppm

Table 2. Urban based ozone increment (pphm) as a function of NMOC emissions and NMOC/NOx ratios.

NMOC EMISSIONS (TONS/YR)	NMOC/NOx TONS NMOC/TONS NOx (PPMC/PPM)
50 75 100 300 500 750 1000 1500 2000 3000 5000 7500 10000	TO BE AVAILABLE BY OCTOBER 1, 1988

#### 4.0 REFERENCES

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## APPENDIX A

### DEVELOPMENT OF SCREENING TABLES

#### RPM-II DESCRIPTION

Screening tables presented in this report were derived using the Reactive Plume Model-II (RPM-II). RPM-II was originally developed by Systems Applications, Incorporated (SAI) under contract to EPA in the late 1970's. RPM-II is a Lagrangian based model which describes the downwind transport and chemical behaviour of a plume emitted from a point source. Plume concentrations are a function of meteorological, source emission and ambient air quality inputs. Downwind plume dimensions are either calculated through Gaussian dispersion formulae using Pasquill-Gifford stability classes, or dimensions are manually set. The plume is resolved into several well-mixed columns aligned transversely with the mean wind flow. Mass transfer of reactive species occurs across cell boundaries. As the plume expands it entrains background air which then is incorporated within the reactive plume mix. A thorough description of the model formulation can be found in the RPM-II User's Guide (SAI, 1980). Listed below are general categories of model inputs used during RPM-II applications for developing the screening tables.

#### Model Inputs:

The following summary of model inputs addresses the major input data requirements used in developing the screening tables; a comprehensive list of required modeling inputs is found in the User's Guide. The RPM-II source code addresses a single input file which includes the following:

Meteorological Considerations - Required meteorological inputs include time-dependent values of wind speed and either stability class to determine horizontal and/or vertical plume dimensions or values reflecting user-determined plume depths and/or horizontal plume widths. The program has been modified to accept ambient temperature to adjust temperature dependent reaction rate constants.

Chemistry Considerations - The RPM-II was designed to accept different chemical mechanisms; a particular mechanism is entered as input data. The original RPM-II and subsequent variations have used an older mechanism, Carbon Bond 2 (CB2). The source code was modified to accept an array of eleven time-dependent photolysis rate constants so that the most recent version of the Carbon Bond-4 mechanism, which is also used in EXMA/OZTRM4 (EPA, 1983), could be applied. Additional code was installed to accept activation energies to determine temperature dependent reaction rates. These code modifications and the operation of CB4 within RPM-II were evaluated by comparing RPM-II predictions with EXMA/OZTRM4. Both models were run in batch reactor mode with identical sunlight, temperature and initial conditions. Over the course of a ten-hour run, both models produced nearly identical time profiles for all species.

Air Quality Considerations - The model requires initialization of all CB4 surrogate and explicit species concentrations, and concentrations representative of background air. Time-variant concentrations of background air can be input manually, or the model will calculate temporal profiles of all species based on a user-supplied initial mix and diurnal variation in photolytic reaction rates.

Emissions Estimates - Principal emissions inputs are emissions rates of inorganic and organic species. Although any species included in the CB4 mechanism can be declared as an emissions input, typical inputs include NO; NO<sub>2</sub>; CO; CB4 surrogate organic groups - paraffins (PAR), olefins (OLE), higher aldehydes (ALD2); and explicit organic groups - formaldehyde (FORM), ethylene (ETH), toluene (TOL) and xylene (XYL).

#### DERIVATION OF RURAL BASED SCREENING TABLE(S)

The concept of a screening procedure for ozone precursors is beset with an immediate contradiction: A screening tool must be simple to apply and robust, but the inclusion of photochemical phenomena in a modeling analysis typically is complicated and case specific. A major difficulty in applying a model such as RPM-II is specifying background concentrations because the model is particularly sensitive to ambient air quality. Hydrocarbon and NO<sub>x</sub> composition vary spatially and temporally throughout any region. A thorough refined modeling exercise would require temporal profiles of all dominant inorganic and organic species in the CB4 mechanism. Such data are scarce for even a single location. The problem is handled explicitly in grid modeling (e.g., UAM application) by assimilating appropriate emissions inventories and generating ambient air quality estimates (in combination with invoking reasonable assumptions regarding initial and boundary conditions). Similarly, it is feasible to generate ambient air quality data with a trajectory model like RPM-II, with appropriate placement of emissions sources.

However, that approach is cumbersome within the model framework as well as application specific and, consequently, not amenable to developing a robust screening tool. To overcome this difficulty, simplifying assumptions regarding background chemistry quality must be invoked. Such assumptions should yield conservative answers (i.e., high ozone generation) and, as a consequence of building in "conservatism" via air quality assumptions, the need for case-specific representativeness diminishes. Accordingly, these screening tables are based on "prototypical", assumed characterizations of background chemistries, representing rural and urban locations. The following discussions outline the procedures used to develop base case meteorological and chemical inputs so that conservative estimates of ozone formation would be produced from model runs performed with the various source emissions scenarios incorporated in the screening tables.

#### DEVELOPMENT OF REASONABLE WORST-CASE MODEL INPUTS

##### Background Air Chemistry

Ambient concentrations of all CB4 species (Table A1) assumed for rural background air are identical to those utilized in rural ozone modeling studies (PEI, 1988) performed with EPA's Regional Oxidant Model (ROM). These concentrations were generated by applying the CBM-RR chemical mechanism (a more detailed version of the carbon bond mechanism) in a batch reactor mode under sequential 12-hour alternating periods of full sunlight and darkness until a relatively aged, steady state mixture was produced. Initial concentrations of NO<sub>x</sub>, CO, and NMOC were derived by EPA's Atmospheric Science and Research Laboratory (Schera, 1988).

The ambient NO<sub>x</sub> and hydrocarbon concentrations in Table A1 reflect generally low ozone precursor concentrations, which might suggest a minimum of ozone forming potential, relative to a more concentrated urban mix. Although somewhat counter-intuitive, results derived from running various emissions mixes (VOC dominated) with rural or urban background concentrations showed a greater ozone increment with rural background air, under equivalent emission rates. This might simply be explained by considering that ozone forming potential already exists in urban air due to a large mass of pollutants implied in urban background concentrations. In contrast, ozone forming potential in rural air may be lacking key ingredients (NO<sub>x</sub>, reactive VOC) which when supplied results in a larger increment. Also, low NO concentrations in rural air probably results in less ozone scavenging through direct titration.

##### Meteorological and Source Speciation Inputs

A prospective user of the screening tables would select an appropriate mass emission rate and NMOC/NOx emissions ratio to determine the ozone increments due to individual VOC/NOx sources. The tables have no provisions for specifying values of meteorological variables (such rigidity is common for most screening analyses). Furthermore, adjustment of the mix of emitted hydrocarbon fractions is not permitted, again keeping within reasonable restrictions imposed by a screening technique. A base-case input file incorporating a single set of base-case values for meteorological parameters and one emissions reactivity mix was developed with the intention of providing conservative (worst case) ozone formation estimates. The screening tables represent runs based on those meteorological parameters with selected adjustments in emissions rates.

The set of meteorological parameters were chosen by running the model over a range of discreet values for one variable, while holding all other variables constant. A true factorial analysis of all possible combinations of wind speed, plume dimensions, starting time and temperature was not performed because of the range, continuous nature and number of variables involved.

The procedures used to determine base-case meteorological inputs are listed below and followed by a discussion of the results from that analysis. For clarity, throughout the discussion "standard value" refers to the value which each variable is maintained while other variables are varied; the "standard value" should not be confused with "base-case" value, the determination of which was the object of this exercise.

Background Air - Concentrations of CB4 species representative of rural, continental U.S. locations as presented in Table A1 were held constant throughout each modeling run.

Emissions - A continuous mass emission rate of 10,000 tons/year NMOC was used for all runs designed to produce base-case values for meteorological variables. The NMOC/NOx; NOx/NO; CO/NMOC and hydrocarbon speciation partitioning were based on EKMA default values (EPA, 1988):

PPM CO/PPMC NMOC - 1.2

PPMC NMOC/PPM NOx - 10

PPM NOx/PPM NO - 4

CB4 group fraction on PPMC basis

ETH	0.037
CLE	0.025
ALD2	0.052
FORM	0.021
TOL	0.089
XYL	0.117
FAR	0.564
NR	0.085

Additional related issues involving emissions scenarios are discussed below within the context of reactivity.

Location - In terms of model inputs, location only translates to diurnal variation of solar zenith angle. The EKMA default location of Los Angeles, California (Lat. 34.058; Long. 118.256; 6/21/75) was used in all runs; virtually no sensitivity resulted from varying latitude.

Starting Time - Starting times (i.e., plume emergence) were incremented hourly from 0600 to 1200 LST (0800 standard start).

Wind Speed - Wind speeds were incremented by 1 m/s over a range from 1 m/s to 4 m/s. The standard wind speed for all runs was 4 m/s.

Plume Width - Spatially variant downwind plume widths were generated by specifying standard Pasquill-Gifford stability classes 1-5 with class 3 used as the standard stability class.

Plume Depth - Plume depths were incremented 200 m over a range from 300 m to 1500 m (500m standard depth).

Temperature - Temperatures were incremented 8 K over a range from 287 K to 311 K (303 K was standard).

Emissions NMOC Mix - In addition to the standard EKMA mix with a NMOC/NOX of 10, runs were performed with single-component NMOC emissions representing each CB4 class (except isoprene) and different NMOC/NOX ratios. To overcome numerical problems requiring excessive computational time for olefins, a mix of 70% olefins and 30% paraffins was used in place of pure olefins.

These single-component emissions were run with mass emissions rates of CO and NOX that were identical to those applied for the standard EKMA emissions mix. Consequently, NMOC/NOX (PPMC/PPM basis) ratios varied somewhat due to differences in effective molecular weights among the emissions scenarios. All NMOC emissions were based on the standard mass emission rate of 10,000 tons/year. Also, additional NMOC/NOX ratios of 5 and 2 (based on standard EKMA mix) were applied for all emissions mixes.

## RESULTS AND DISCUSSION

### Metecrology:

Sensitivities of maximum ozone increments within a point source plume due to independent variation of several meteorological parameters are presented in Figures 1-5. Based on these results and consideration of consistency among meteorological variables, the following values based on the subsequent analysis were chosen for base-case meteorological inputs to provide conservative ozone increment estimates:

wind speed - 1 m/s  
horizontal stability - class C  
plume depth - 700 m  
ambient temperature - 311 K  
start time - 1000 LST (NMOC/NOx > 5)  
                  - 0700 LST (5 > NMOC/NOx > 1)  
                  - 0600 LST (NMOC/NOx < 1)

Starting Time - Only minor sensitivity was attributed to varying starting time from 0600 to 1200 LST for standard mix with NMOC/NOx = 10 (Figure 1). Sensitivity to starting time increased as NMOC/NOx ratio decreased; at lower NMOC/NOx ratios earlier starting times produced larger ozone increments (Figures 2-3).

Sensitivity to starting time is strongly coupled to optimizing both NO to NO2 conversion and providing adequate reactive VOC. At high NMOC/NOx, NO titration of ozone is not dominant and exposure of high incident radiation to concentrated NMOC (short time after start-up) produces large ozone increments. In contrast, at low NMOC/NOx ratios NO titration is a problem and the plume requires extended time to reach optimum ozone forming potential. Accordingly, an earlier start time which provides intense incident radiation upon segments sufficiently downwind such that a substantial percentage of NO has been converted (as well as diluted).

Wind Speed - Wind speed variations impart the greatest degree of sensitivity on maximum ozone increments (Figure 4). Successively smaller decreases in ozone impacts occur as wind speed increases from 1 to 5 m/s; a reasonable response since, in effect, a 2-fold increase in wind speed represents a 50% decrease in the effective emissions rate injected into a plume segment. In addition, a dilution effect due to increased dispersion near the source accompanies elevated wind speeds.

Stability Class (Horizontal dispersion) - Ozone formation increased as stability classes were changed from Class A(1) to Class E(5) (Figure 5), an expected response related to successively less downwind dilution when proceeding through

higher stability categories. In the context of this analysis Class D and E stabilities yield large ozone increments; but these classes are clearly inconsistent with other optimal ozone forming conditions (full sunlight, light winds). In following a conservative approach consistent with any screening protocol selection of Class C stability is appropriate. Actually, the selection of a more stable dispersion scenario is consistent with the notion of plume meander whereby plume dispersion calculated from standard dispersion parameters encompasses a complete crosswind profile due to plume meander, yet the effective crosswind plume dimension (where reactions occur) is governed by an instantaneous crosswind dimension. While plume meander certainly increases areal exposure to a particular plume, reactivity is dependent on actual crosswind dimensions at a point in time.

Plume depth - The ozone formation response to plume depth (held constant throughout time) is similar to that for wind speed (Figure 6), an apparent dilution phenomenon. The selection of a 700 m maximum plume depth is, admittedly, somewhat arbitrary. Certainly an upper bound must be imposed to account for low mixing heights, otherwise a plume would grow indefinitely, and rather rapidly, over time. While the existence of 700 m mixing heights is not uncommon, the occurrence of such a low mixing height under optimal ozone forming conditions is not likely in many locations. Nevertheless, an upper bound must be imposed and, as illustrated in Figure 6, the difference in maximum ozone increments between 700 m and 900 m is about 15 %. Furthermore, observed summertime, afternoon measurements of plume depths taken from the Tennessee Plume Study (Ludwig et al., 1981) show plume depths typically ranging from 500 m to 700 m.

Temperature - Ozone formation increased with increasing temperature (Figure 7), a result consistent with observed correlations among high temperature and high ozone levels. The selection of 311 K (100 °F) is not unreasonably high.

#### VOC Emissions Reactive Mix

The apportioning of emissions by CB4 classes would typically be set by a particular source profile for a refined modeling application. Since screening tables are designed to provide a simple and robust screening procedure, out of necessity the emissions mix becomes a variable which must be addressed when developing a worst-case baseline input file. A robust method conceivably should bracket the limitless variety of VOC mixes, a rather encompassing objective. To that end a crude attempt at bracketing a range of all possible VOC point source emissions was developed by running the RPM-II with single-component NMOC emissions for each CB4 category.

Results of this analysis are shown in Figures 8-10 for three

different NMOC/NOx ratios. All VOC emissions rates were held at 10,000 tons/year, and NMOC/NOx and NMOC/CO ratios were based on the standard EKMA mix. The large NMOC emissions rate of 10,000 tons/year was not intended to be representative; the rate was used to better identify trends which otherwise might have been lost in numerical noise. The ratios varied slightly among the different mixes because of differences in VOC molecular weights. To provide consistency all mass rates for NOx (at a given NMOC/NOx ratio) and CO were identical for different mixes (the NMOC/NOx ratio is volume based). Consequently, different NMOC molar emissions rates existed among mixes, with higher molar emission rates for lower weight classes (e.g. paraffins).

If one presumes reactivity strictly as a function of the k-OH reactivity scale, an apparent buffering effect is produced due to enforcing consistent mass emission rates among mixes (Figures 8-10). A clear example is illustrated by the paraffin mix which forms ozone to an extent similar to toluene and xylene, classes both with considerably higher k-OH values and molecular weights relative to paraffins. Similarly, ethylene and olefins form largest ozone increments because these classes are both reactive and relatively low weight. The associated CB4 class k-OH values and molecular weights are listed below:

CB4 Class	Effective Molecular Weight	k-OH (min <sup>-1</sup> )
ETH	28	5824
OLE	26	20422
ALD2	43	11833
FORM	30	15000
TOL	92	4497
XYL	106	1284
PAR	14	1203
EKMA MIX	23.16	3090

The decision to base this analysis on mass emissions is based on the expectation that the anticipated users of this screening

technique will address permitting issues based on mass emission rates.

As shown in Figures 8-10, variation in ozone increments predicted for different C<sub>2</sub> components range up to about 1.5 times the ozone increment obtained with a standard EKMA urban mix. Accordingly, the EKMA mix is retained for all screening analyses and application will require a scale-up factor of 1.5. It should be noted that a 70 % olefin mix is unrealistic as most olefin-named compounds are composed of chains dominated by paraffin bonds.

#### Rural Area Screening Tables

Results from a matrix of runs covering a range of VOC emission rates and NMOC/NOx emissions ratios are presented in Table A2. In order to maintain a consistent basis for data evaluation, all Table A2 results are based on a 1000 LST start time. Several trends exist among the data in Table A2:

- \* At NMOC ratios greater than 3, any increase in NMOC loading leads to an increased ozone maximum
- \* As VOC loading rate increases, an optimal NMOC/NOx emissions ratio exists, and this ratio shifts to lower values as NMOC source size increases.
- \* At NMOC/NOx emissions ratios less than 3, VOC loading increases can lead to relative decreases in ozone maximums as well as ozone deficits during one solar day.

A simplified version of Table A2 is presented as the rural area screening table in section 3.0 (Table 1). The effects of NMOC/NOx ratios have been attenuated somewhat by presenting three broad NMOC/NOx ratios. The results under each range reflect a scale-up factor of 1.5 and are based on the most conservative (maximum ozone producing) NMOC/NOx ratio each range: > 20 (NMOC/NOx = 20); 5-20 (12- see Figure 11); < 5 (5). In addition the results in Table 1 are based on optimal starting times for different NMOC/NOx ratios and adjusted by using a reactivity scale-up factor of 1.5.

Table A1. Background species concentrations (ppm) taken to be representative of "clean" atmospheric conditions

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ALD2	9.005E-5	NO	5.054E-5
H2O2	1.084E-3	OH	2.947E-7
MGLY	1.529E-6	PHO	4.124E-9
O	1.496E-10	XYL	1.296E-9
PAR	3.224E-3	ETH	1.681E-5
XO2	1.171E-5	HO2	2.496E-5
C2O3	7.389E-7	NO2	1.491E-4
HNO2	1.859E-6	OLE	4.676E-9
N2O5	1.723E-9	TLA	9.338E-9
O3	3.193E-2	FORM	1.148E-3
PHEN	4.286E-5	ISOP	0.000E+0
XO2N	1.417E-6	NO3	2.041E-3
CO	9.873E-2	PAN	5.167E-5
HNO3	1.646E-3	TOL	1.219E-5

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from (PEI, 1988)

Figure 1. Starting Time

NMCC/NO<sub>x</sub> = 10

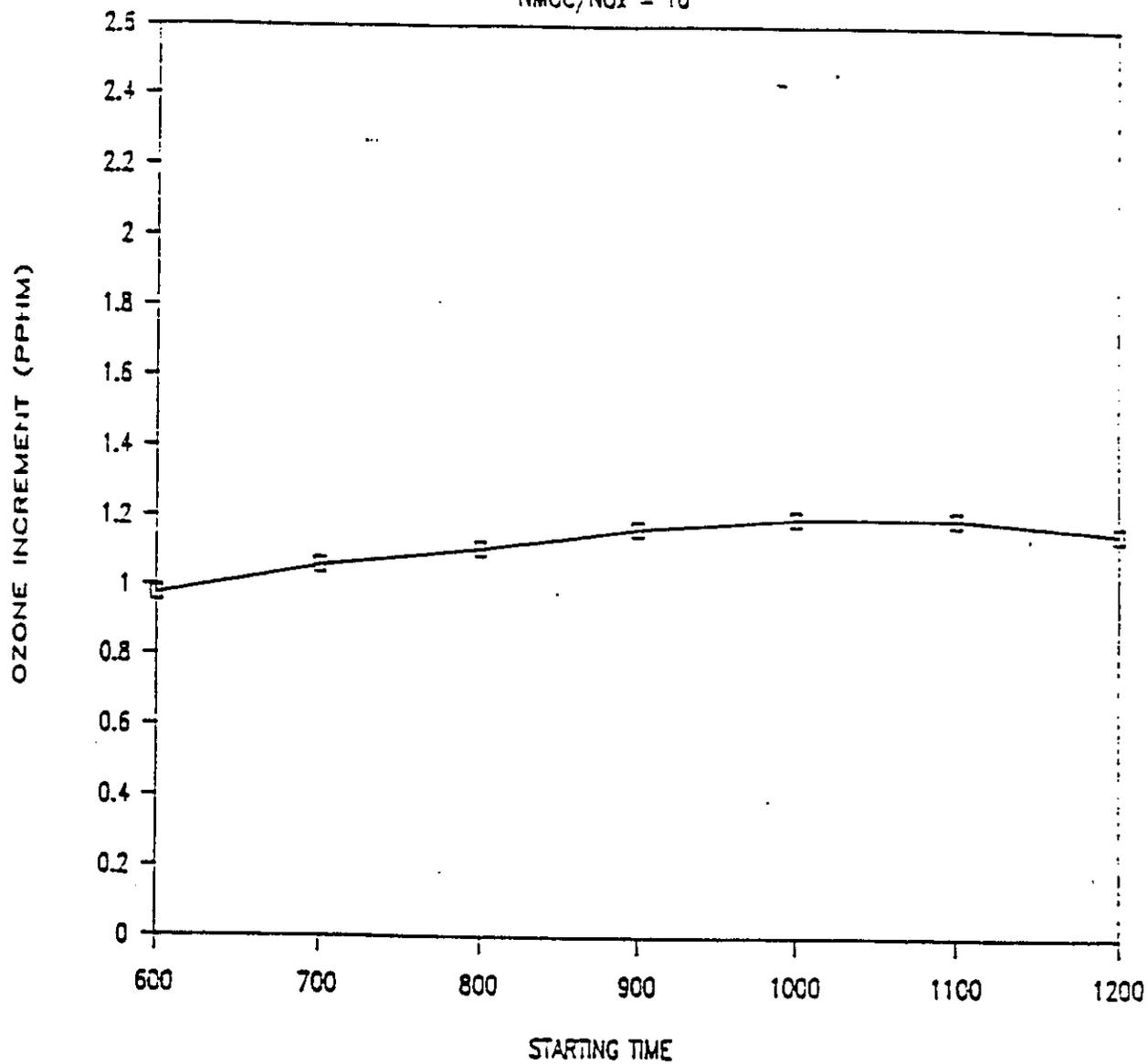


Figure 2. Starting Time

NMOC/NO<sub>x</sub> = 5

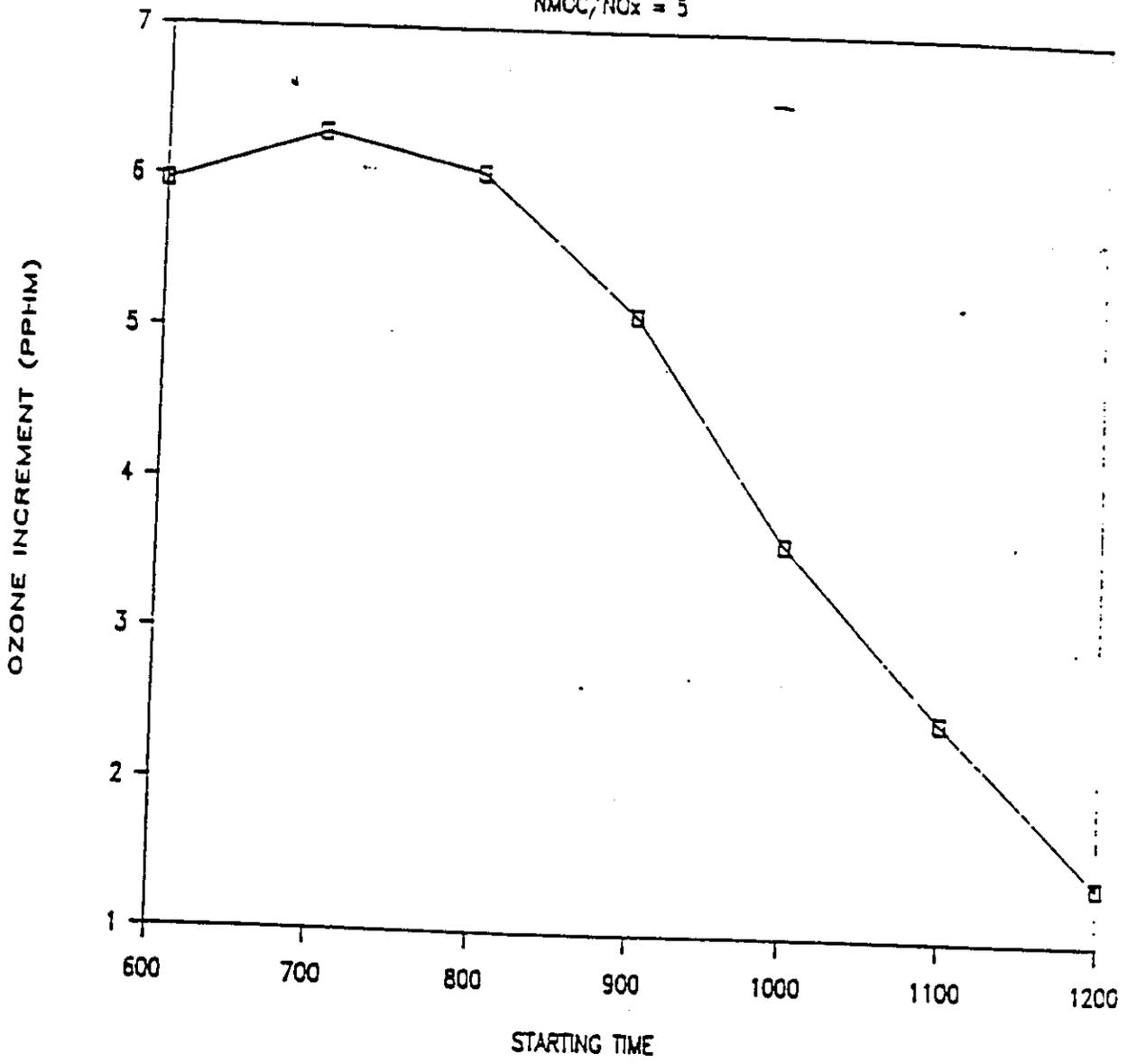


Figure 3. Starting Time

NMCC/NO<sub>x</sub> = 1

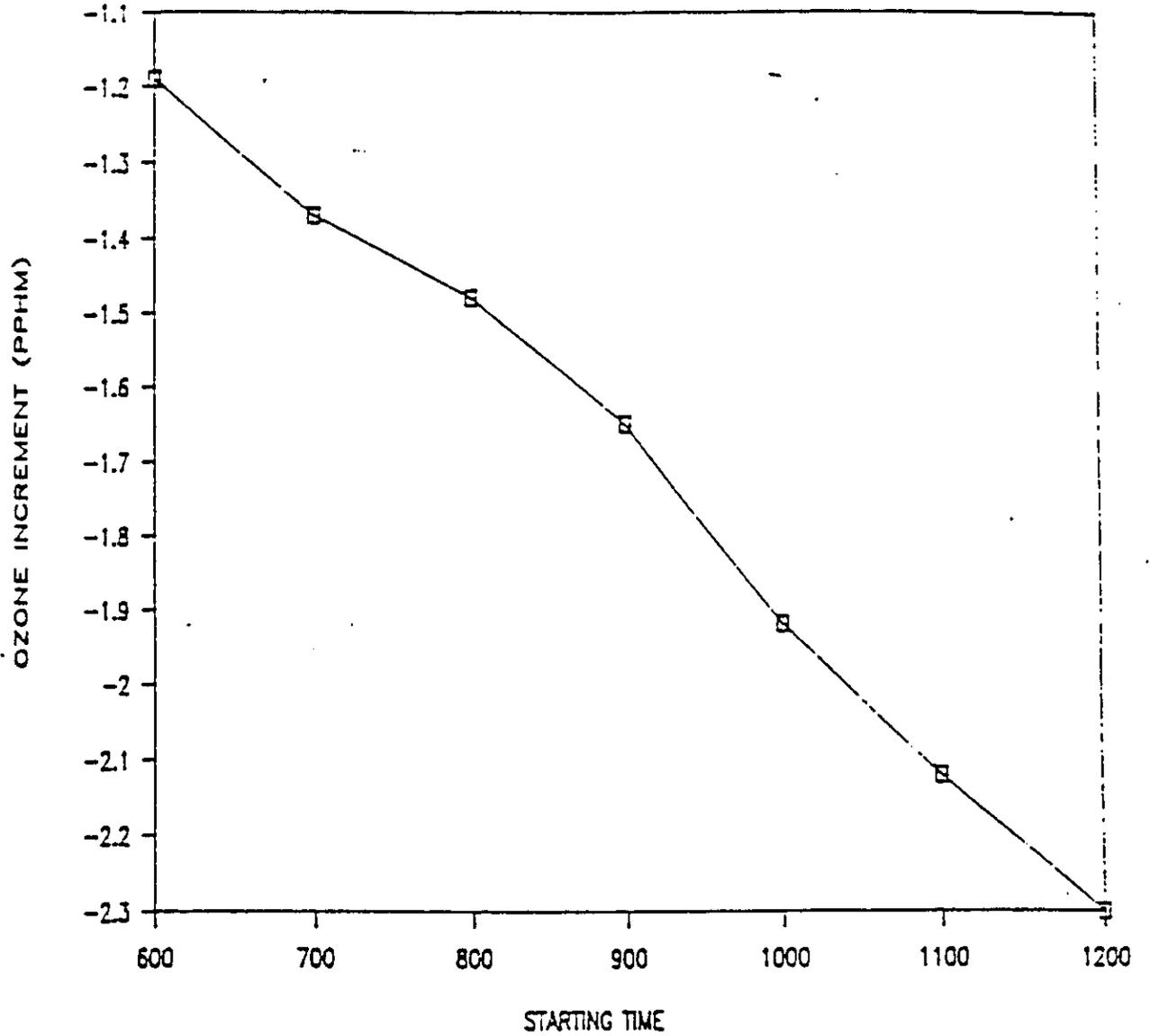


Figure 4. Wind Speed

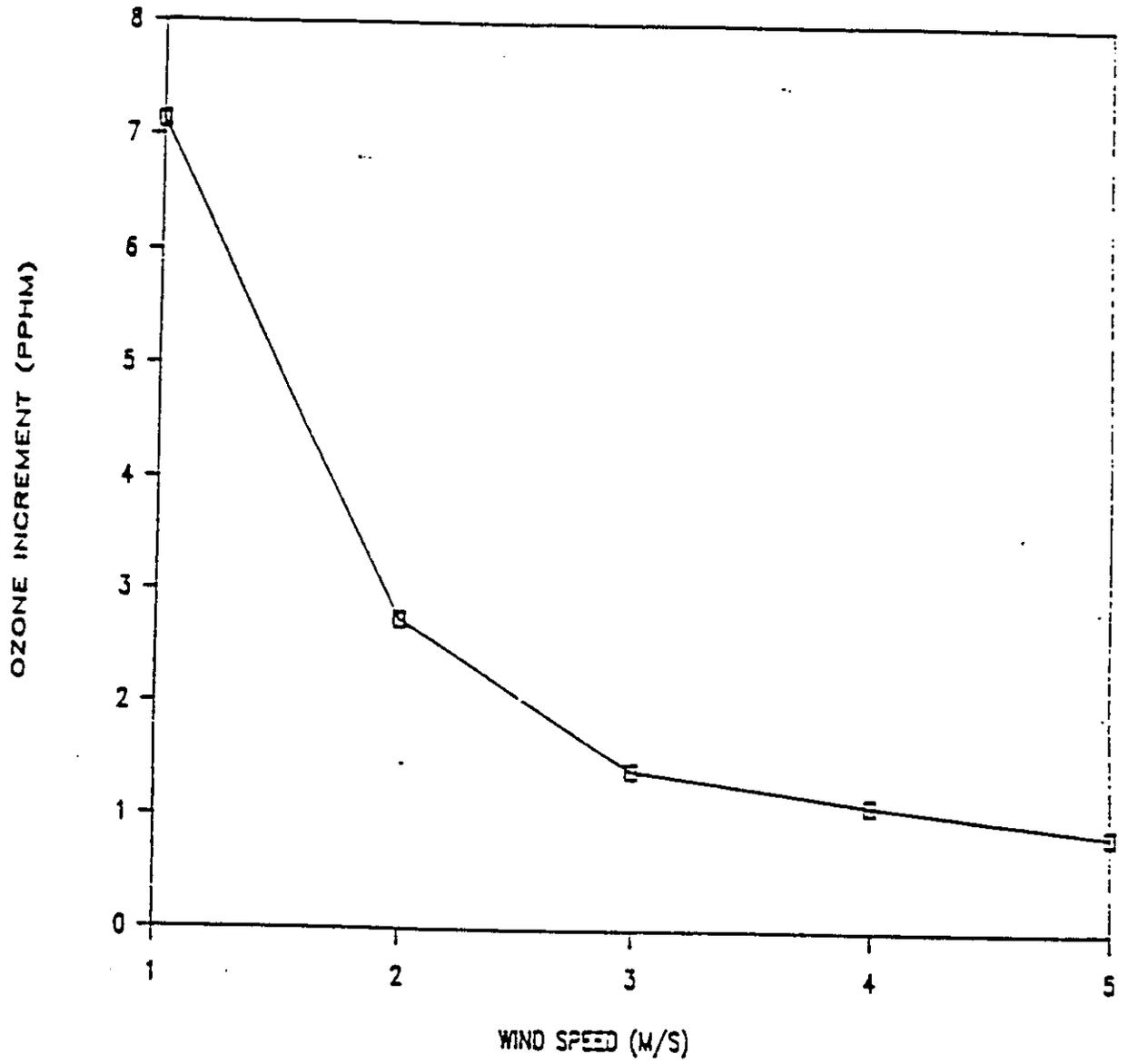


Figure 5. Stability Class

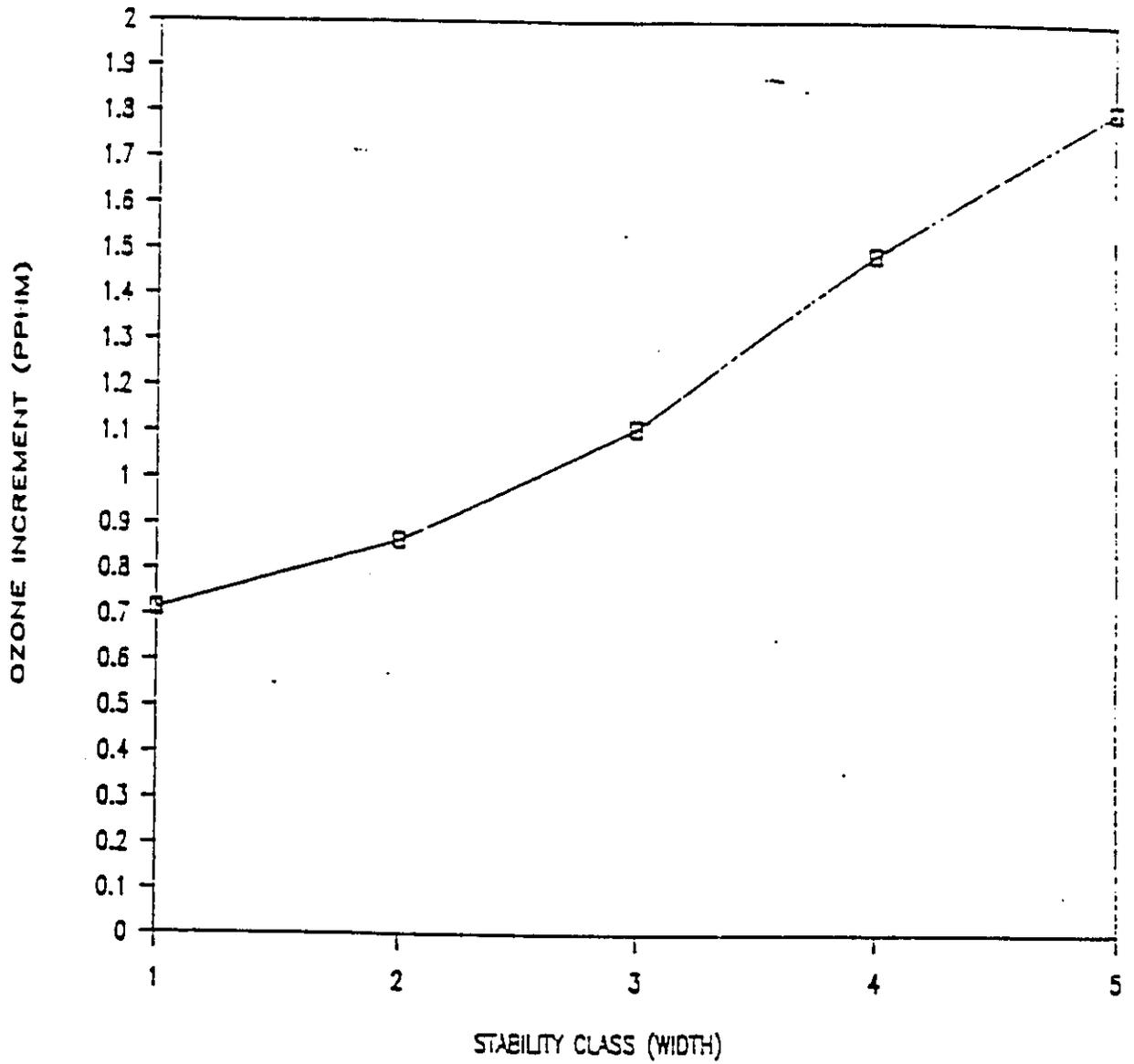


Figure 6. Plume Depth

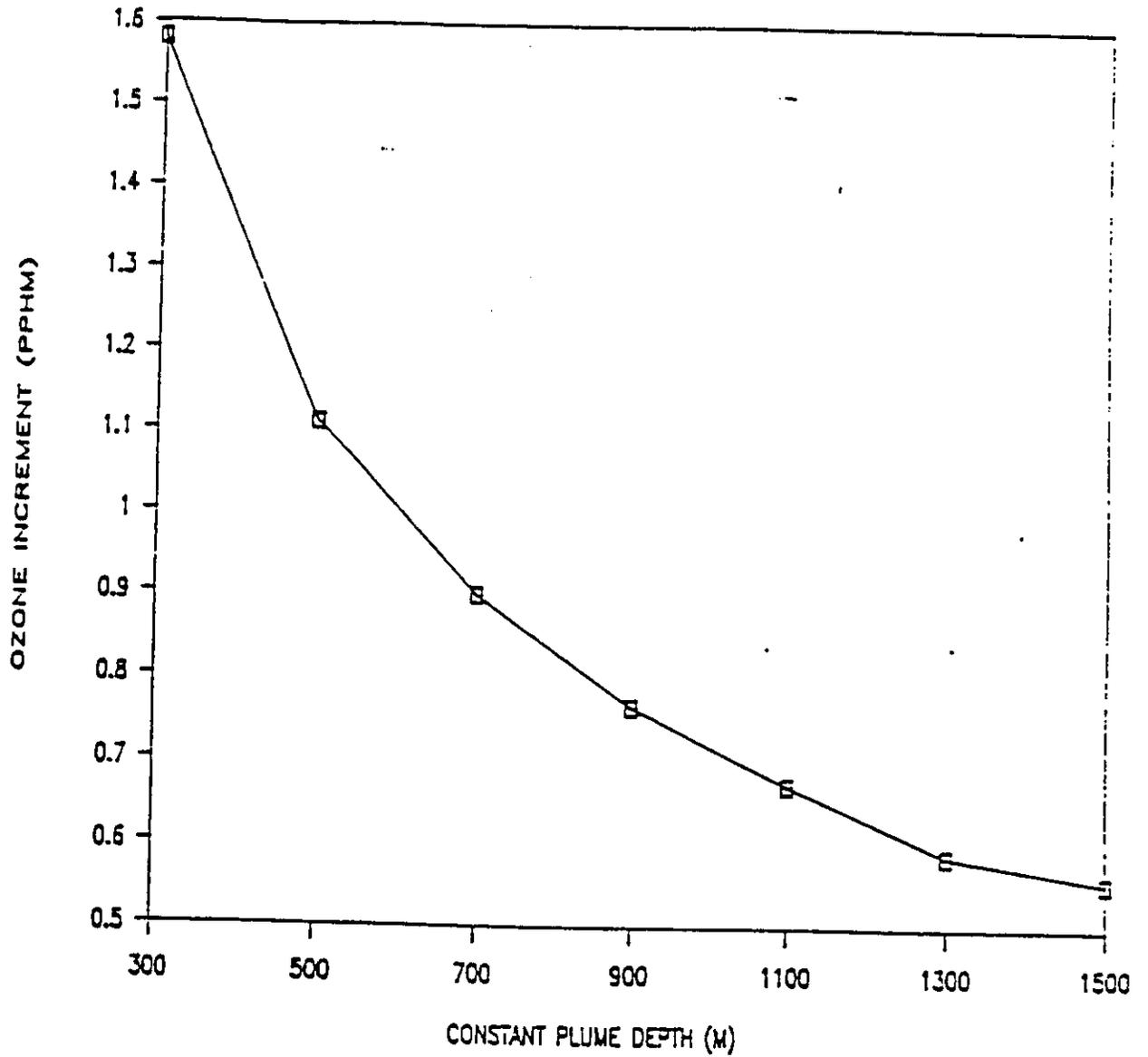


Figure 7. Temperature

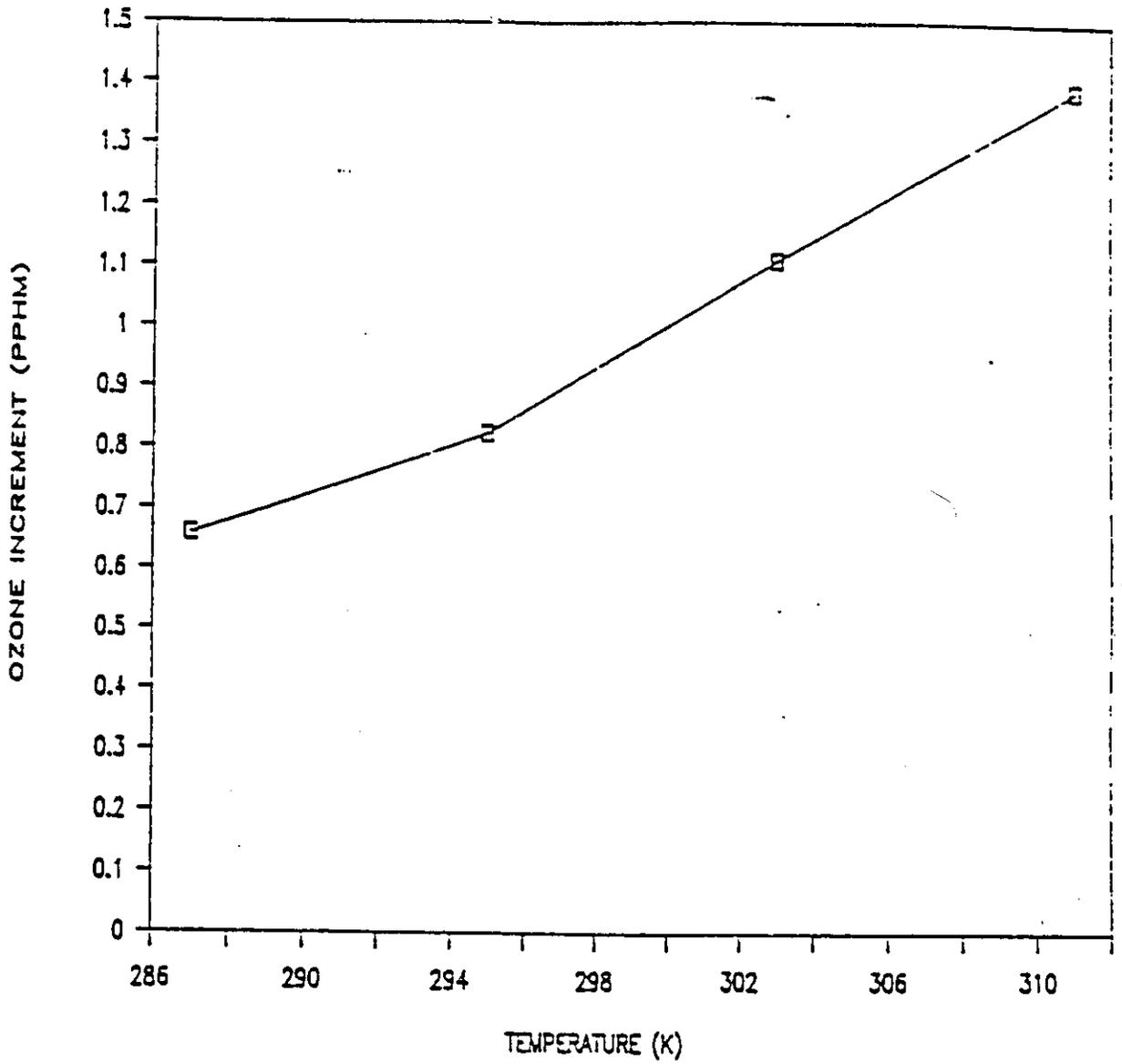


Figure 8. Single component CB4 emissions

EKMA NMCC, NOx: 10

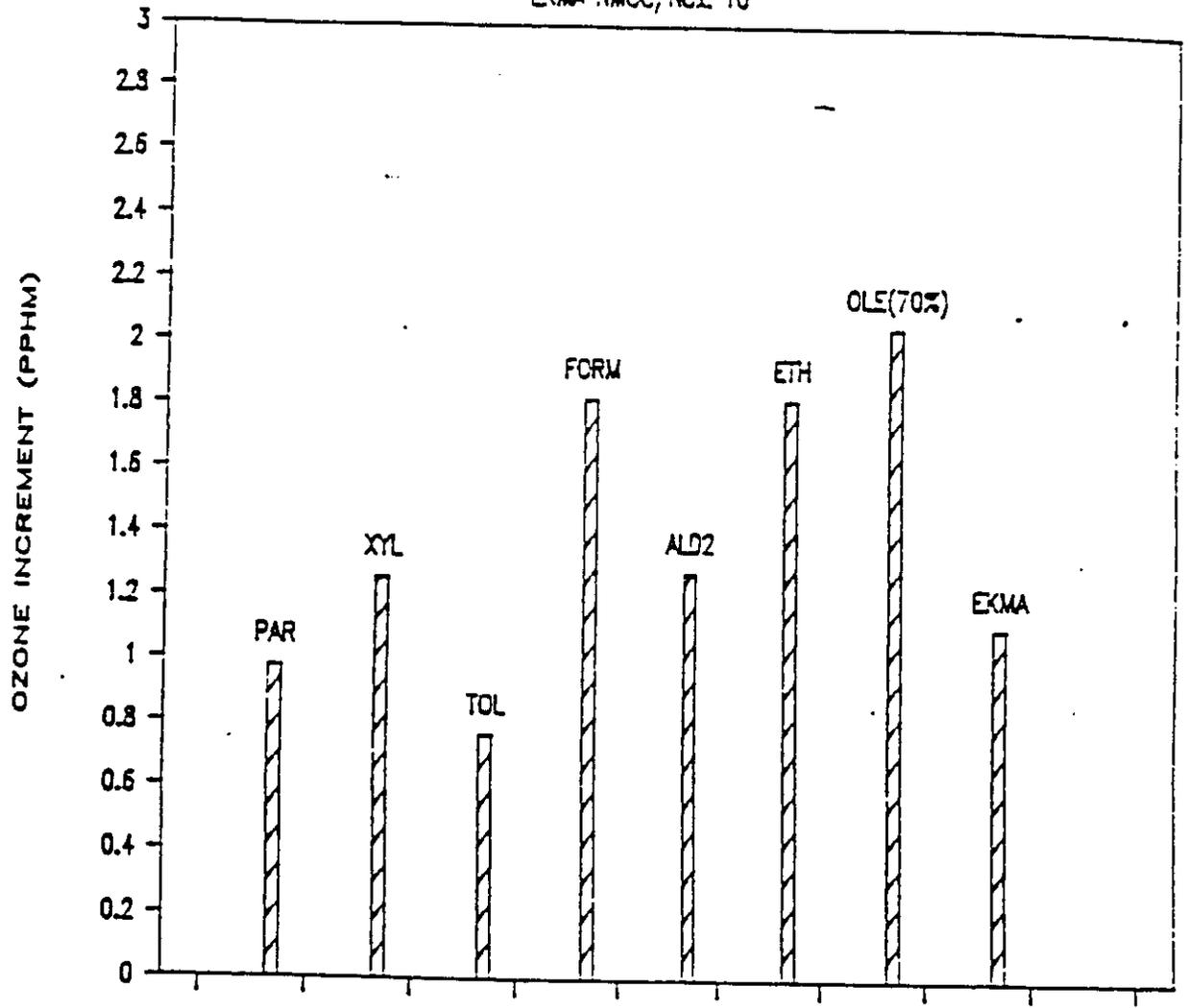


Figure 9. Single component C34 emissions

EKMA NMCC/NOx: 5

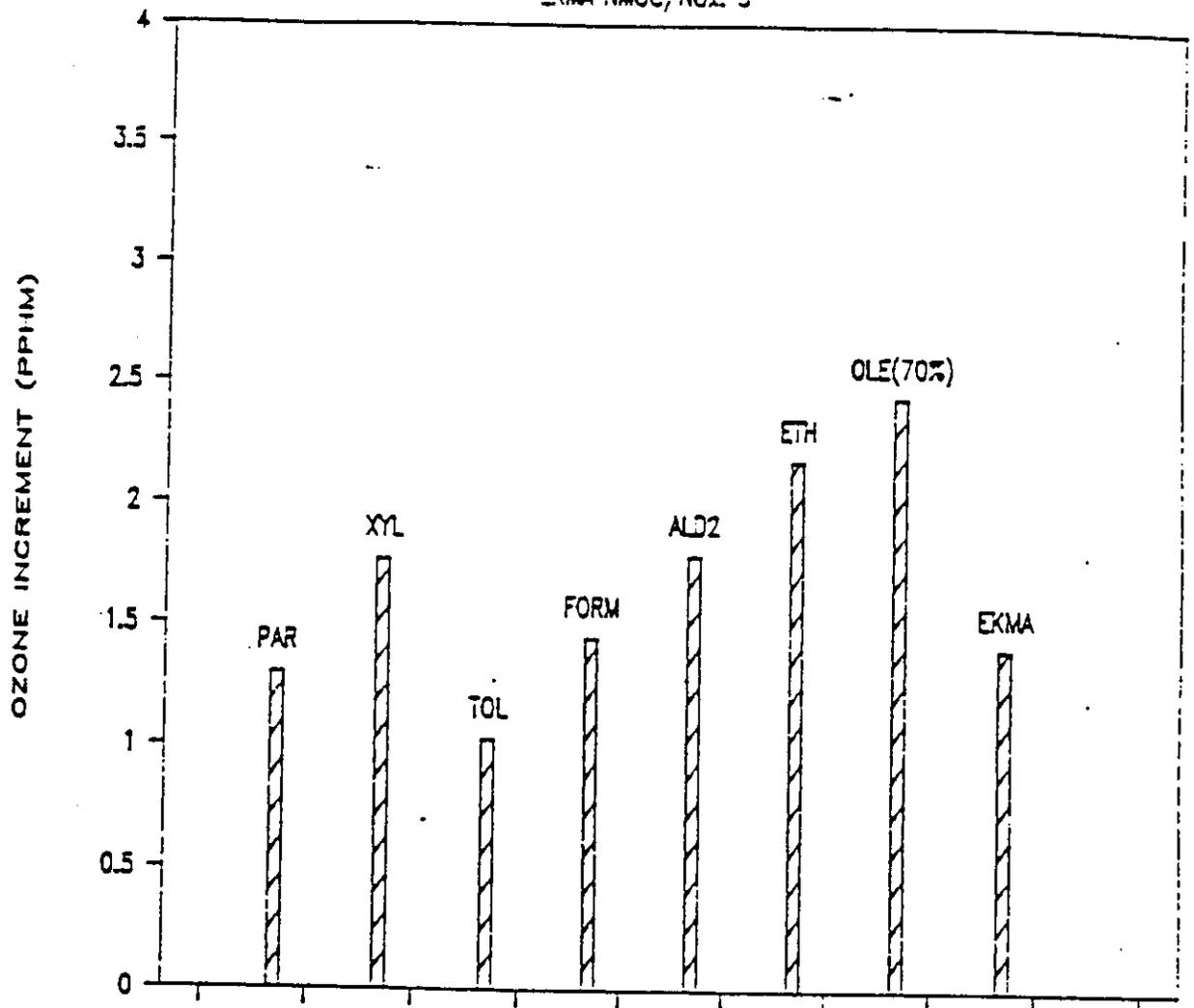


Fig. 10. Single component CB4 emissions

EKMA NMOC/NOx: 2

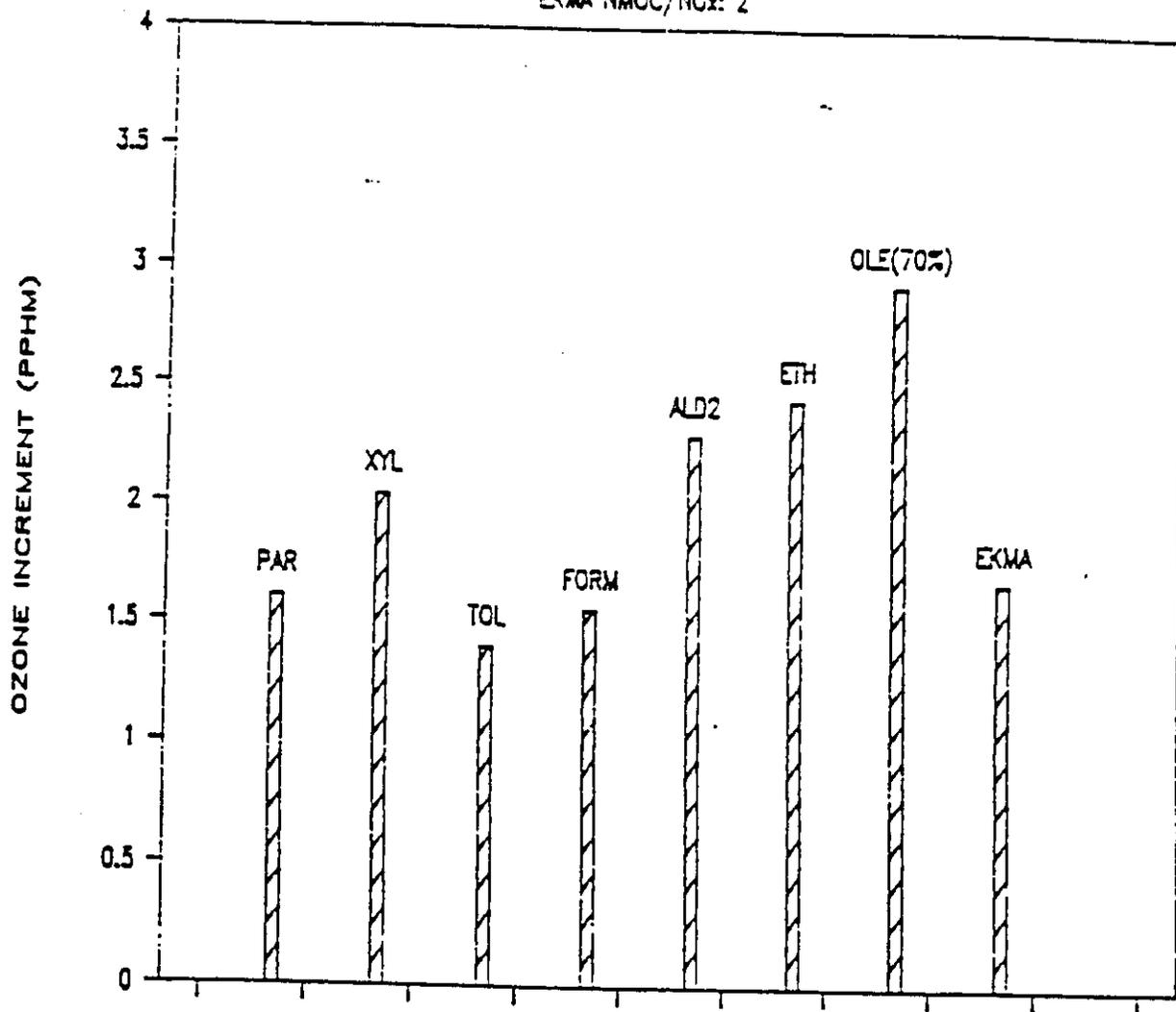


Figure 11. NMOC/NO<sub>x</sub> effect on ozone

