DEPARTMENT : Minnesota Pollution Control Agency

STATE OF MINNESOTA
Office Memorandum

PHONE : 296-7396

DATE : June 25, 1987

TO : J. David Thornton, Chief
Program Development and Air Analysis
Division of Air Quality

FROM : Dennis L. Becker DLB
Program Development Section
Division of Air Quality

SUBJECT : **PROPOSED MODELING PROTOCOL FOR KOCH REFINING COMPANY**

Recent telephone conversations with USEPA, Region 5, indicate that the Agency should be taking the lead in developing a model protocol. Accordingly, I have developed a model protocol which attempts to consolidate model protocols suggested by Koch Refining Company, Ashland Petroleum Company, and USEPA. The model protocol begins with the model protocol suggested by Mr. Michael Koerber, EPA Region 5, and reflects follow-up discussions with Mr. Mike Hansel and/or Mr. Jack Kennedy, Koch Refining Company, on June 3, 8, 10, 22 and 23, 1987.

PROPOSED PERFORMANCE EVALUATION SCHEME

The primary objective relates to the prediction of peak concentrations to determine compliance with Minnesota and National Ambient Air Quality Standards (MAAQS and NAAQS). Highest concentrations are scientifically interesting but have no regulatory weight; they are also interesting to the general public. Maximum second-highest concentrations are of greatest concern from a regulatory perspective because they are used to determine compliance with MAAQS and NAAQS. Unfortunately, both have little statistical significance. Consequently, the 25 highest concentrations are considered to statistically test peak concentrations.

The secondary objective is to test overall model performance. Koch suggested using the mean square error and the annual average to test overall model performance. Conversely, EPA did not suggest any secondary objectives. Considering its relative importance and additional calculations, I favor omitting all secondary objectives. Nevertheless, I will agree to include secondary objectives if Koch and Ashland so desire.

PROPOSED PERFORMANCE MEASURE SCORING SCHEME

The proposed performance measure scoring scheme attempts to address USEPA concerns regarding underprediction versus overprediction. The proposed scoring scheme penalizes underprediction at a rate 1.5 times that of overprediction for all "mean" performance measures. Other performance measures contain no penalty for underprediction.

MODEL SELECTION

Upon completion of the study, the model with the most points will be used to derive revised emission limitations.

cc: John S. Seltz
Charles A. Lane
Gregory C. Pratt
Dennis L. Becker - 4 copies
DAQ FILE: #106A (KOCH REFINING COMPANY)
DAQ FILE: #203 (ASHLAND PETROLEUM COMPANY)

TABLE 1. PROPOSED PERFORMANCE EVALUATION SCHEME

CONCENTRATION DATA SETS	PAIRED SPACE A/	PAIRED TIME	PERFORMANCE MEASURE	AVERAGING TIME	MAXIMUM POINTS
First Highest	No	No	Mean Ratio	1-hour	1
	No	No	Mean Ratio	3-hour	2
	No	No	Mean Ratio	24-hour	3
Second Highest	No	No	Mean Ratio	1-hour	3
	No	No	Mean Ratio	3-hour	10
	No	No	Mean Ratio	24-hour	16
The 25 Highest	No	No	Mean Ratio	1-hour	2
	No	No	Mean Ratio	3-hour	7
	No	No	Mean Ratio	24-hour	12
	No	No	Variance Ratio	1-hour	1
	No	No	Variance Ratio	3-hour	3
	No	No	Variance Ratio	24-hour	5
	No	No	Meteorological Cases in Common (7 categories) (shown below)	1-hour	15
All Data (Optional)	Yes	Yes	Mean Square Error	1-hour	15 B/
(Optional)	Yes	Yes	Mean Ratio	Annual	5 B/
					100

A/ Number and location of model receptors coincides with monitor locations. Per USEPA guidelines, a minimum of 1, 3, and 18 valid 1-hour concentrations must exist for 1-hour, 3-hour, and 24-hour averaging times.

B/ Number of points will be equally divided between monitor sites.

METEOROLOGICAL CATEGORIES:

1) Unstable Stability Classes (A,B,C) and wind speed <= 2.5 m/s
2) Unstable Stability Classes (A,B,C) and wind speed > 2.5 m/s

3) Neutral Stability Class (D) and wind speed <= 2.5 m/s
4) Neutral Stability Class (D) and wind speed 2.5-5.0 m/s
5) Neutral Stability Class (D) and wind speed > 5.0 m/s

6) Stable Stability Classes (E,F) and wind speed <= 2.5 m/s
7) Stable Stability Classes (E,F) and wind speed > 2.5 m/s

TABLE 2. PROPOSED PERFORMANCE MEASURE SCORING SCHEME

PERFORMANCE MEASURE	SCORE
Mean Ratio ($\bar{C}p/\bar{C}o$)	0.00 < Ratio <= 0.50: Score = 0.00 0.50 < Ratio <= 1.00: Score = MP * ((3/2)*Ratio - 1/2) 1.00 < Ratio <= 2.00: Score = MP * (-1.0*Ratio + 2.0) Ratio > 2.00: Score = 0.00 Note: The above scoring scheme is patterned after the Warren Power Plant study and Guayanilla Basin study. USEPA estimates model accuracy at a factor of 2. The above scoring scheme penalizes underprediction at a rate 1.5 times that of overprediction; the midpoint between the USEPA's factor of 2 accuracy estimate versus no penalty for underprediction.
Variance Ratio (Sp**2/So**2)	0.00 < Ratio <= 0.25: Score = 0.00 0.25 < Ratio <= 1.00: Score = MP * ((4/3)*Ratio - 1/3) 1.00 < Ratio <= 4.00: Score = MP * ((-1/3)*Ratio + 4/3) Ratio > 4.00: Score = 0.00 Note: The above scoring scheme is patterned after the Warren Power Plant study and Guayanilla Basin study.
Meteorological Cases in Common:	Score = MP * (Number of meteorological cases in common)/25. Note: The above scoring scheme is patterned after the Baldwin Power Plant study, Lovett Power Plant study, and Guayanilla Basin study.
Mean Square Error $\overline{(Cp-Co)^{**}2}/(\bar{C}p\bar{C}o)$	Score = MP * (CI-65)/35 for the model with the lowest MSE, where CI = percent "tightened" confidence interval using the chi-square distribution. Confidence intervals are to be "tightened" until there is no overlap of one model's variance with the other model's confidence interval (ie. the variances of both models are mutually different statistically at some level of significance, CI). Precise "tightened" confidence intervals are preferable, but incremental look-up table values (eg. 99.95%, 99.9%, 99.5%, ..., 65%) are acceptable. Confidence intervals will not be "tightened" below 65%. The model with the highest MSE gets no points. Note: The above scoring scheme is patterned after the Warren Power Plant study.

NOTATION:
Cp = predicted concentrations (i.e. modeled plus background concentrations)
Co = observed concentrations
Sp = standard deviation of predicted concentrations
So = standard deviation of observed concentrations
MP = maximum points
Overbar denotes average concentration.
Background concentrations will reflect upwind monitored concentrations.

TABLE 2. PROPOSED PERFORMANCE MEASURE SCORING SCHEME (Cont.)

TOTAL SCORE

The model with the most points (rounded to the nearest integer) will be used to derive revised emission limitations.

In the event of a tie, a technical evaluation will be performed to determine the best model. The technical evaluation will emphasize each model's ability to protect MAAQS and NAAQS; this will done by plotting the frequency of the 25 highest observed and predicted concentrations for 1-hour, 3-hour, and 24-hour averaging times. See below.

FREQUENCY DISTRIBUTIONS OF OBSERVED AND PREDICTED CONCENTRATIONS

25 HIGHEST 1-HOUR CONCENTRATIONS	25 HIGHEST 3-HOUR CONCENTRATIONS	25 HIGHEST 24-HOUR CONCENTRATIONS
FREQUENCY	FREQUENCY	FREQUENCY
CONCENTRATION	CONCENTRATION	CONCENTRATION

The following extreme values statistics will also be calculated for observed and predicted concentrations for each averaging time:

$$\bar{C} + N*S,$$

where $\bar{C}$ = average concentration, S = standard deviation, and N = 1, 2, and 3.

The technical evaluation will to a lesser extent consider each model's ability to identify appropriate meteorological events. This will be done by comparing the 7 meteorological categories for observed and predicted concentrations for 1-hour, 3-hour, and 24-hour averaging times. See below.

FREQUENCY OF 1-HOUR METEOROLOGICAL CASES IN COMMON

	25 HIGHEST 1-HOUR CONCENTRATIONS (N=25)			25 HIGHEST 3-HOUR CONCENTRATIONS (N=3*25=75)			25 HIGHEST 24-HOUR CONCENTRATIONS (N~24*25=600)		
	OBS	ISC	RAM	OBS	ISC	RAM	OBS	ISC	RAM
UNSTABLE & 2.5>WS									
UNSTABLE & 2.5<WS									
NEUTRAL & 2.5>WS									
NEUTRAL & 2.5<WS<5.0									
NEUTRAL & 5.0<WS									
STABLE & 2.5>WS									
STABLE & 2.5<WS									
TOTALS	---	---	---	---	---	---	---	---	---