

TO: Doug Skokna

FROM: T. G. Grumbles

DATE: August 5, 1987

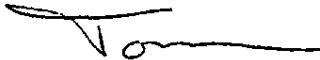
Interoffice
Communication

SUBJ: EMERGENCY RELEASE MODELING MEETING

VISTA

As we have discussed, the subject meeting will be held on Tuesday, May 18, from 9:00 - 12:00 at the plant. Attached is a preliminary agenda for the meeting, a document describing the generalities of the project, and the actual modeling basis letter used at the LCCC.

Please give me a call if you have specific questions on the agenda items. Please distribute this information to others you want involved, other than those I have copied.



T. G. Grumbles

ajo
.201

cc R. W. Seymour
D. L. Mahler
L. A. Mauerman
J. O. Gibson
P. F. Fetizanan
M. J. Heller

VVV 000022932

AGENDA
MODELING MEETING
TUESDAY, AUGUST 18, 1987
9:00 - 12:00

- | | | |
|---|----------------|----|
| I. Introduction Overview | Tom Grumbles | 15 |
| A. Purpose of Meeting | | |
| B. Modeling Needs/Uses | | |
| C. Regulatory Concerns (TSCA, SARA Title III) | | |
| II. Modeling Technology | Mary Jo Heller | 15 |
| A. Capabilities | | |
| B. Limitations | | |
| III. Vista Capabilities | Mary Jo Heller | 15 |
| A. Software Programs | | |
| B. Schedule | | |
| IV. What to Model | Tom Grumbles/ | 30 |
| A. Chemical Selection | Mary Jo Heller | |
| B. Data Needs | | |
| V. The LCCC Experience | Mary Jo Heller | 45 |
| A. Process Flow of Project | | |
| B. Review of Results | | |
| VI. Discussion of Action Steps/Schedule | Group | |
| VII. Future Plans | | |

VVV 000022933

TO: Distribution

FROM: T. G. Grumbles
DATE: November 12, 1986

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Communication

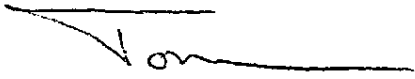
SUBJ: DISPERSION MODELING PLANNING MEETING

VISTA

The subject meeting will be held Friday, November 21 at the LCCP Safety Department conference room, from 9:00 a.m. - Noon. An agenda for the meeting, a general description of the modeling project, and a background letter is attached.

Please note Item IV and be thinking about what would be useful for aiding the plant in the reporting of emergency releases to local and federal authorities and community right-to-know aspects of recent regulations.

If you have questions before the meeting, please call me (X3445) or Mary Jo Heller (X6884) in Houston.


Thomas G. Grumbles

ajo/9

Attachments

cc T. H. Huffman - LCCP Mgr
L. R. Bauer - LAB "
R. A. Conrad - LCVCM "
J. A. DeBernardi - LCCC mgr.

DISTRIBUTION:

+ S. Pitts - LCCP Safety Director
+ M. Hayes - "
+ P. Carrico - LCCP Ethyl. Plant Oper. Supt.
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+ P. Warner LAB " "
+ K. Fogg " Safety Director
+ R. Johnson " Process. Supt.
+ M. Heller PED
+ P. Fetizanan PED

Ed TALLER

VVV 000022934

AGENDA
MODELING MEETING
~~FRIDAY, NOVEMBER 21~~

~~9:00 - 12:00~~

Tuesday, Aug. 18
9:00 - 12:00

- I. Introduction Overview Tom Grumbles
- A. Purpose of Meeting 15
 - B. Modeling Needs/Uses
 - C. Regulatory Concerns (TSCA, ^{SARA Title III} Superfund)
- II. Modeling Technology Mary Jo Heller 15
- A. Capabilities
 - B. Limitations
- III. Vista Capabilities Mary Jo Heller 15
- A. Software Programs
 - B. Schedule
- IV. End Products *Nona* Group
- A. Format (Monographs, Numbers, Overlays?)
 - B. Uses
- V. What To Model Tom Grumbles/ 30
- A. Chemical Selection Mary Jo Heller
 - B. Data Needs
- VI. The LCCC Experience msh 45
- A) Process Flow of Project
 - B) Review of Results
- VII. Discussion of Action Steps/Schedule
- VIII. Future Plans

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~~At Group~~

MODELING PROJECT

GOAL

To produce data that will allow Vista to assess future releases in terms of potential for off-site concentrations of hazardous chemicals.

METHOD

Model release scenarios to give quantitative ranges of contaminant levels under specified conditions. Variables will include contaminant, release rate and points, and atmospheric conditions.

STEPS

1. Obtain capability, including evaluation of models, software, and training to model in-house.
2. Evaluate use of the modeling data for future use in release response and determine format of end-product as indicated.
3. Identify chemicals to be modeled at each plant. These should be prioritized based on hazard, volume, use, storage, and delivery (transfer) conditions. Hazard evaluation should include volatility, flammability and toxicity.
4. Based on the above choose release scenarios to evaluate off-site concentration potentials.

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5. Determine criteria levels for action (notification, evacuation, etc.) for those contaminants modeled.

GENERAL CONSIDERATIONS

Many of the steps outlined can be done concurrently. The tendency will be to use intuition to pick the contaminants of concern. A consistent technique of hazard prioritization should be used to pick the chemicals to be modeled. The end result may be the same but we may be surprised. A screening method example is attached. This method was contained in EPA's Chemical Emergency Preparedness Program.

The action level will take a good deal of discussion on any specific contaminant. Basically the affect to be avoided (irritation, lung damage, etc.) and the level where those effects occur must be reviewed. Acutely toxic materials (i.e., HF or HCl) are easier to deal with than VCM, or chronic hazards.

APPENDIX C

QUANTITY DETERMINATION METHOD

This appendix describes a method that can be used to determine whether the quantity of acutely toxic chemical substance on a site, if accidentally released into the air, can produce potentially harmful concentrations in a nearby community. This method is not designed to provide an upper exposure limit for the release of a certain amount of an acutely toxic chemical substance, or to be used to establish a "maximum allowable" release amount for setting limits for storage or release under an ordinance or regulation. Its intended use is as a screening tool to allow community work group members to determine whether there is enough of a particular acutely toxic chemical substance on a site that, in the event of an accidental release, potentially harmful amounts might reach the community under the worst meteorological conditions that might occur. This procedure can help the work group rank various sites that handle acutely toxic chemical substances, so it can deal first with those sites and substances that pose the greatest potential for causing harm should an accidental leak occur. Communities are invited to contact their Regional Office of EPA for more detailed assistance on airborne contaminant modelling for purposes of developing specific levels, target populations, or evacuation areas as part of contingency planning. More sophisticated models that include the specific area meteorology, topography, and specific acutely toxic chemical substance physical/chemical data may be available for these purposes.

C.1 BACKGROUND

EPA believes that communities may need assistance in determining whether enough of an acutely toxic chemical substance is present on a site that, if accidentally released, it could cause severe consequences in the community. Many models are available to predict the downwind concentration of a release into the air. However these models are very complex, not easily used, and not all are appropriate for this particular situation. In addition, each site is unique in topography, weather conditions, and distance to the community, and each chemical has its own unique characteristics and behavior.

Since it is not reasonable to expect each community to have the expertise to develop a model simulation for every situation that might occur, EPA developed this method for use as a screening tool. EPA performed an analysis based on reasonable worst case conditions (like low wind speeds, ground level release, limited mixing and ambient temperature conditions) that could occur at any site using an EPA model that simulates dispersion from an instantaneous source. The model, known as INPUFF, is part of EPA's UNAMAP airborne contaminant modelling system. The model ran airborne releases associated with various quantities of chemicals over varying meteorological conditions, and the highest 30 minute average concentration at downwind distances ranging from 100 feet to 10 miles was calculated. The source of release was also simulated

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at a low level (3 feet above the ground) and at ambient temperature (higher temperatures cause the vapor cloud to rise and result in lower concentrations in the air) for release times ranging from 1 minute to 30 minutes. The 1 minute release condition was selected for use in the quantity determination because it generated the highest concentration in air per quantity of substance released. This condition simulates a rupture or large spill where a large cloud of material is generated quickly. The results of these model simulations were arranged in the form of a graph that can be easily used. The method for using the graph is described below. Note, however, that the method has significant limitations and remember that the quantity determination should be made in light of the kind of activities at each particular site associated with acutely toxic chemical substances.

C.2 METHODOLOGY

To use the graph to determine whether there is enough acutely toxic chemical substance on a site to generate airborne concentrations that could reach a level of concern beyond the site fence line, three pieces of information are needed: (1) the distance from the point where the acutely toxic chemical substance being evaluated is stored, processed or handled on site to the site fence line or the nearest population; (2) the molecular weight of the acutely toxic chemical substance; and (3) the level of concern for the substance. The distance can be determined from maps or from discussions with a technical contact at the site. The molecular weight of the chemical may be found on the Profile sheet included with the EPA list of acutely toxic chemical substances or, if the substance is not on the EPA list, from the site technical contact.

The level of concern should be taken as the IDLH (Immediately Dangerous to Life and Health) level. This level (established by the National Institute of Occupational Safety and Health) represents the maximum level to which a person can be exposed to for 30 minutes and escape without suffering irreversible health effects. The EPA Profile sheets include IDLH values, when available.

There are problems inherent in using the IDLH as a measure of the level of concern:

- The IDLH is based upon the response of healthy, male worker population and does not take into account exposure of the elderly, children, or people with other health problems.
- The IDLH is based upon a 30 minute exposure time frame which may not be realistic for accidental airborne releases.
- IDLH values do not exist for all acutely toxic chemical substances.

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Thus, LDH values used in this way do not necessarily indicate "safe levels," and a working group using them for screening purposes may wish to make appropriate allowances, e.g., for sensitive populations (such as the elderly) that may live close to the site boundary.

If the acutely toxic chemical substance you are evaluating does not have an IDLH in the Profile or there is no profile available on the substance, use the LC(low) value which may be obtained from the site technical contact or from published toxicology sources. The LC(low) is the lowest lethal concentration observed in tests on laboratory animals. If an LC(low) is not available, use the LC50 value for the substance. The LC50 is the level for which 50 percent of the test animals died when exposed for a specified time period. This value may also be obtained from the Profiles, the site contact or toxicological literature.

Once the level of concern is known, it can be used on the graph to determine quantity. Toxicological levels may be given in units of parts per million (ppm), milligrams per cubic meter (mg/m^3), milligrams per liter (mg/l), or grams per liter (g/l). Levels given in parts per million can be converted to grams per cubic meter (g/m^3) as follows:

$$\text{Concentration, g}/\text{m}^3 = \frac{(\text{level in ppm})}{1000} \times \frac{\text{MW}}{24.5}$$

where MW is the substance molecular weight. For example, chlorine has a level of concern (IDLH) of 25 ppm and a molecular weight of about 71. Thus the level of concern in grams per cubic meter is:

$$\text{Concentration, g}/\text{m}^3 = \frac{25}{1000} \times \frac{71}{24.5} = 0.07 \text{ g}/\text{m}^3$$

If the level of concern is given in milligrams per cubic meter, divide it by 1000 to obtain grams per cubic meter. If the level is given in milligrams per liter or grams per liter, convert liters to cubic meters by using 1000 liters equivalent to one cubic meter. See Table C-1 for a summary of conversion factors.

TABLE C-1
CONVERSION FACTORS

$$\text{mg}/\text{m}^3 \times 10^{-3} = \text{mg}/\text{liter}$$

$$(\text{mg}/\text{liter}) \times (24.5/\text{molecular weight}) = \text{ppm}$$

$$1000 \text{ mg} = 1 \text{ gram}$$

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Once the level of concern in grams per cubic meter and the distance in feet are known, use the graph to determine the quantity. Using the left-hand scale on the graph, mark the proper value for the level of concern for the chemical substance you are considering. For example, chlorine should have a mark at 0.07. Next, move to the center scale and mark the distance from the source of release to the site fence line or to a particular target of concern such as a hospital or nursing home. Using a ruler or other straight-edge, draw a straight line from the mark on the left scale through the mark on the center scale to the scale on the right. Where the line hits the scale on the right is the quantity of substance that would result in the concentration on the left scale at the distance on the center scale if it were all released. For example, using chlorine, if a distance of 200 feet were used, the quantity given on the right scale would be about 10 pounds. In other words, if 10 pounds of chlorine were released under poor meteorological and wind conditions, harmful levels of chlorine would occur 200 feet away.

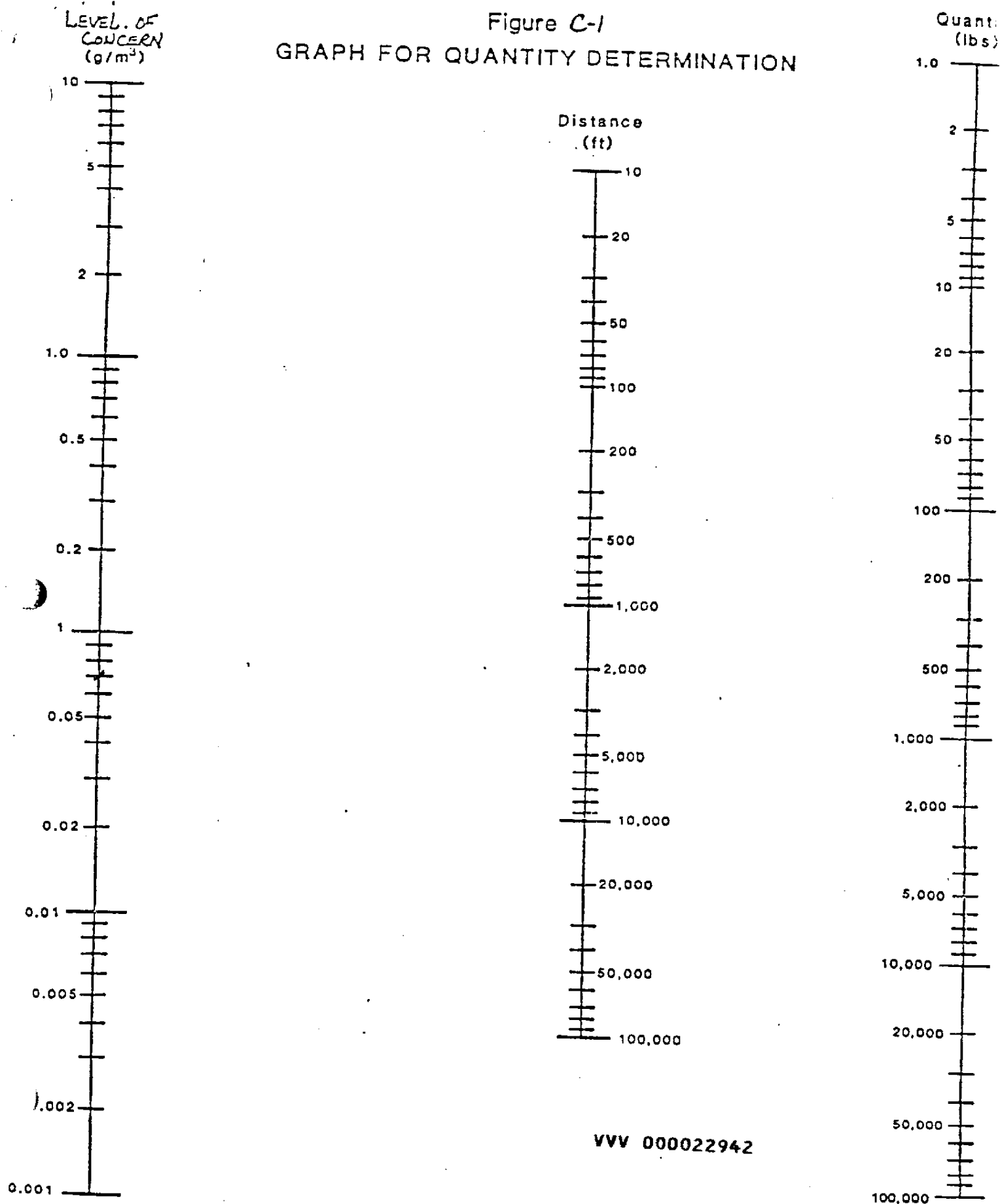
The procedures and example given above are appropriate for vapors released from gases or volatile liquids. If the acutely toxic chemical substance being evaluated is a dust or powder, the same nomogram procedure can be used assuming that fine dusts or powders behave like vapors in air. The level of concern may need adjustment, however. Solids are often tested for lethality on laboratory animals by administering the substance orally. The results are given as the lethal dose for 50 percent of the test animals or LD50 in units of milligrams per kilogram (mg/kg) of body weight. If the test results already give an LD₅₀ or include an LC value, use the procedures above. If only an LD value is given for an oral test, then it must be converted to an inhalation value for use on the quantity determination graph. The National Research Committee has developed a simple method for determining the inhalation level associated with an LD oral dose. Convert the LD oral dose in milligrams per kilogram (mg/kg) to inhalation in grams per cubic meter (g/m³) as follows:

$$\text{LD oral, mg/kg} \times 213 = \text{Inhalation, g/m}^3$$

Compare the quantity determined from the graph to the quantity stored in any one container or the quantity that could possibly be released from a process on the site. If the quantity is much higher than the quantity determined from the graph, the work group should continue gathering information for contingency planning for this substance and site. If the quantity on the site is less than the quantity determined from the graph, the work group may want to defer further data gathering efforts for this substance at the site, depending on the kinds of operations at the site involving the acutely toxic chemical substance.

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Figure C-1
GRAPH FOR QUANTITY DETERMINATION



Interoffice
Communication

To: DISTRIBUTION

From: M. J. HELLER, Houston, TX.
Date: February 23, 1987

Subject: CAER MODELING - BASIS

VISTA

CAER scenarios were received from each Lake Charles plant over the past two weeks. Before the actual modeling begins, a basis for modeling must be set. I recommend that the evaluation of each scenario involve:

- A. stability classes D-day and F,
- B. wind speeds of 5, 15, and 25 MPH,
- C. an ambient temperature of 70°F,
- D. a mixing depth of 5000 meters,
- E. rural dispersion coefficients, and
- F. criteria levels as outlined on page three.

Based on the above, only six runs will be needed for each scenario.

STABILITY CLASS

Atmospheric stability is a measure of turbulence and is classified as A through F with F being very stable. Figure I is a graph of stability class versus time of day for a typical day in January in Lake Charles. This figure shows that the atmosphere is very stable during most of the night and becomes less stable during the day. In fact, categories A through D-day rarely occur during the night and categories D-night through F rarely occur during the day.

Figure II shows the frequency of each stability class in Lake Charles for four three-month periods during 1980 and 1981 and also for the entire year. The two most frequent classes are D-day and F. Of the daytime categories (A through D-day), D-day gives the most conservative results and is the most frequent. Of the nighttime categories (D-night through F), F is most conservative and most frequent. Because of these facts and because it is easier to determine whether it is day or night than to determine a stability class, D-day and F were chosen for modeling.

- (1) Daytime is defined as one hour after sunrise to one hour before sunset.

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WIND SPEED

Several runs were made on the ISCST program to determine the effect of wind speed on dispersion. Wind speed affects how quickly a plume will reach a neighborhood more than how high the steady state concentrations will be in the neighborhood. However, there is enough effect on the steady state concentrations, that wind speed should be considered as a variable.

Figure III shows the frequency of several wind speed categories in Lake Charles for four three-month periods and also for the entire year. Category 5 is the most frequent category. To cover the range without modeling every category, I suggest using five, fifteen, and twenty-five miles per hour for each scenario. (1)

TEMPERATURE

Two runs were made using the ISCST model to determine the effect of ambient temperature on downwind concentrations. One run was at 40°F and the other at 80°F. There was no noticeable difference in dispersion between the two. One temperature, 70°F (average for Lake Charles), should be sufficient for modeling purposes.

MIXING DEPTH

Mixing depth is the height of the atmosphere available to dilute the pollutant. Pollutants will not normally travel above this height. Mixing depth data cannot be taken in the plant but must be obtained through the nearest national weather service upper air station. The nearest station to Lake Charles is located in Shreveport.

For the worst case, the mixing depth should be set equal to the release height. The same quantitative results may be obtained within the model by using a very high mixing depth such as 5000 meters and doubling the resulting concentrations. Since immediate mixing depth information is not available in a control room, and since this information is difficult to predict, I suggest we make the worst case assumptions.

DISPERSION COEFFICIENTS

The equation for basic dispersion contains dispersion coefficients to describe the extent of dispersion. Separate sets of these coefficients are available for rural and urban areas. Dispersion in urban areas is more rapid than in rural areas.

- (1) Wind speeds for modeling purposes should be measured at 10 meters above ground level.

According to two EPA tests, the area around the Lake Charles complex is rural. One test is based on population density and the other on land use. Neither depends on zoning.

CRITERIA LEVELS

Based on the levels in the literature, and making conservative assumptions, Tom Grumbles has proposed the following levels for the initial modelling contours.

Benzene	25 ppm and 1,000 ppm
Chlorine	1 ppm, 3 ppm, and 25 ppm
EtO	1 ppm, 5 ppm, and 20 ppm
HCl	5 ppm and 100 ppm
HF	3 ppm and 20 ppm
VCM	1 ppm, 5 ppm and 20,000 ppm (1/2 LEL)

The levels above will give us a ceiling value contour, a conservative IDLH contour, and for carcinogens a range of levels relative to occupational limits. Where a NRC/EEG level exists it will be modeled. Actual levels for notification criteria to the local emergency response commission warrant further discussion.

For your information, Table I lists criteria levels from the literature for the chemicals listed above.

OTHER CONSIDERATIONS

For scenarios which involve the release of more than one chemical simultaneously, multiple overlays will be generated. Each overlay will represent a single chemical with its own criteria levels shown. The effect of being exposed to more than one chemical at a time will be determined by Tom Grumbles as the occasion arises.

Based on the scenarios received so far, the model we have now, ISCST, will need to be supplemented with a puff model. This puff model will handle very short releases better than the ISCST program. Exactly which puff model to buy will be decided and ordered in the immediate future. After receiving the Puff model, a separate basis letter may be needed for very short releases.

CAER MODELING - BASIS
February 23, 1987
Page Four

Please let me know if you have comments or questions about this basis by 3/11/87 so that we can proceed with the modeling.

Mary Jo Heller
Mary Jo Heller

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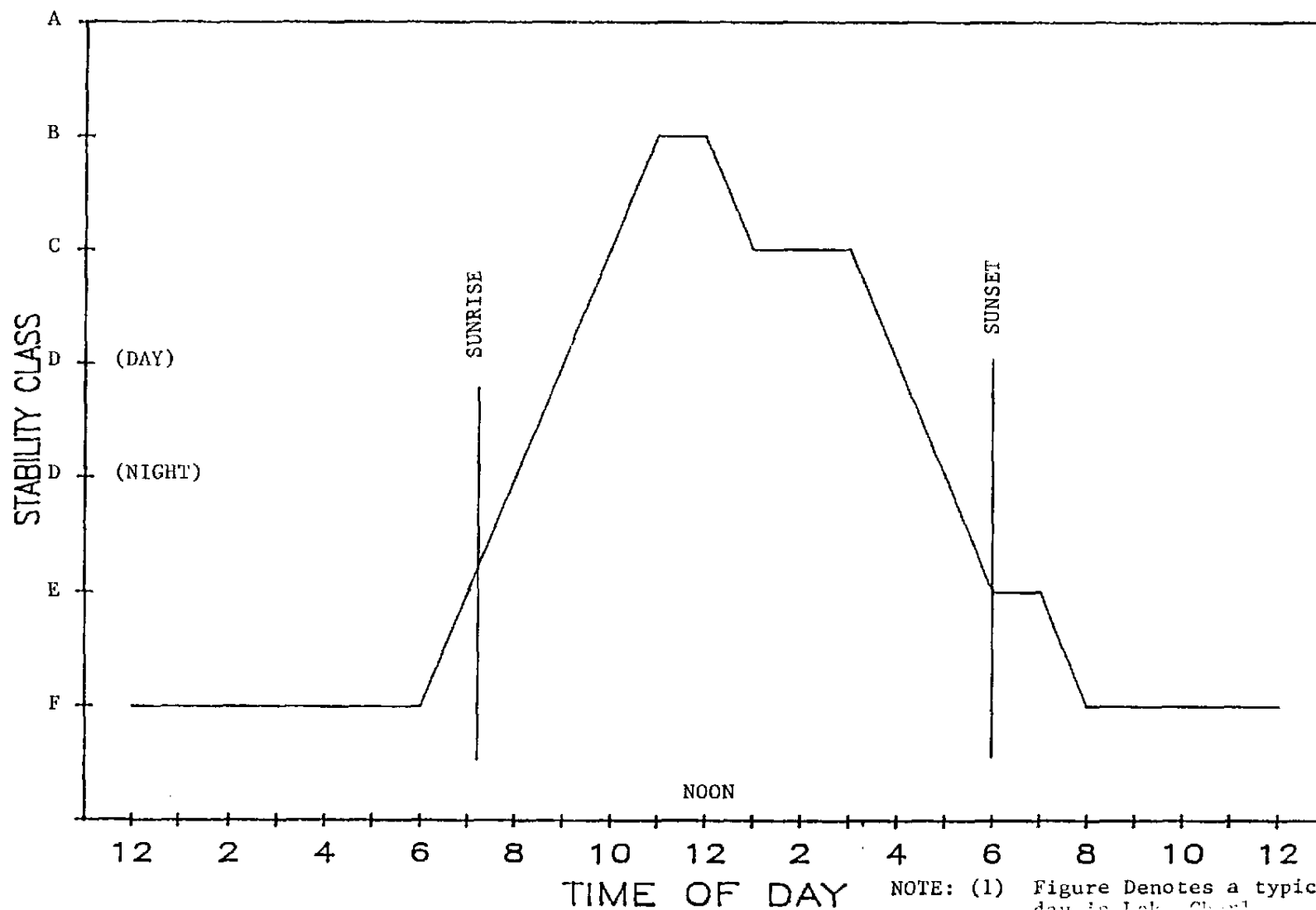
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A

FIGURE 1⁽¹⁾ STABILITY CLASS VS TIME OF DAY



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FIGURE II
STABILITY CLASS FREQUENCY

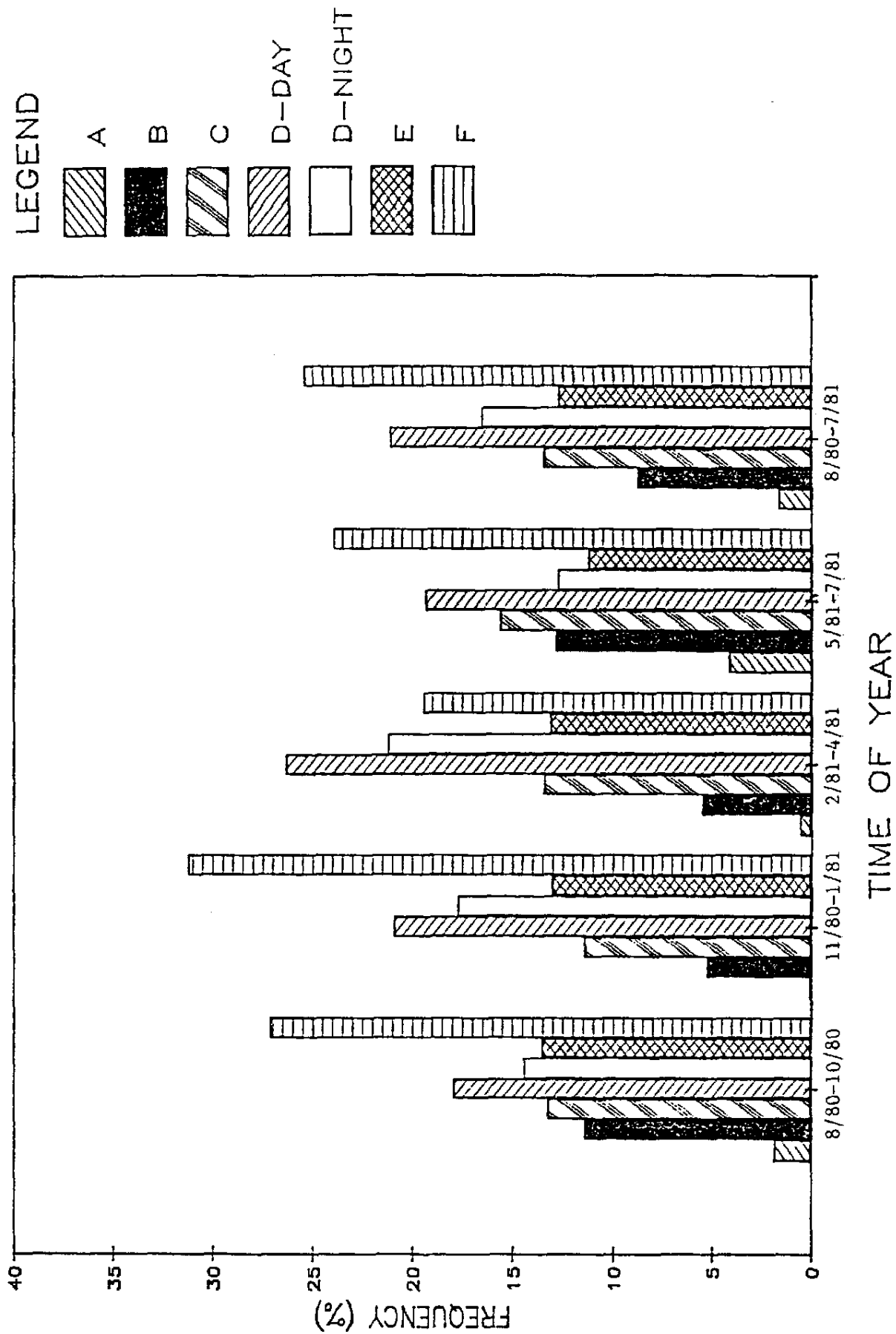


FIGURE III WIND SPEED FREQUENCY

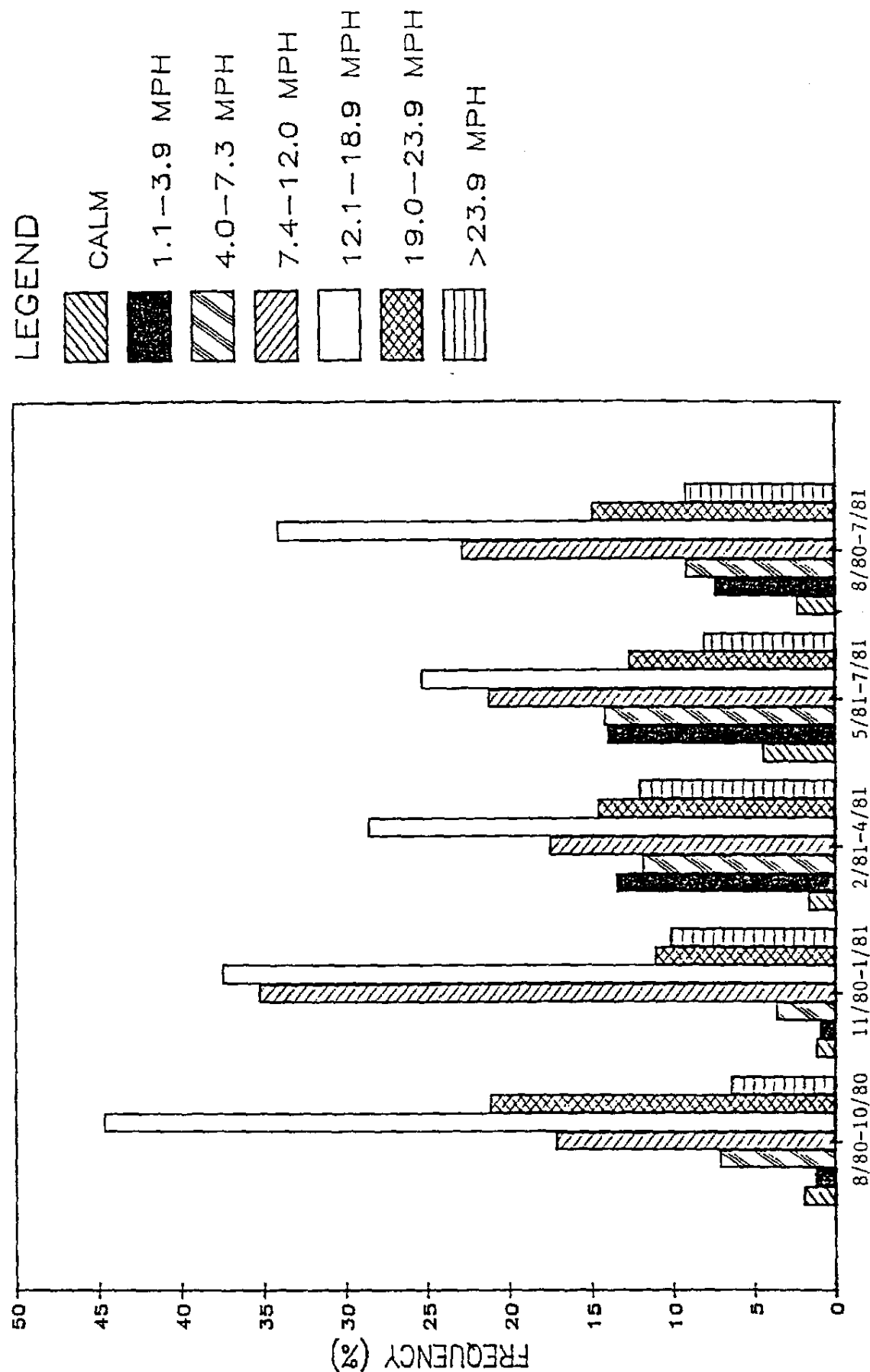


TABLE I

CRITERIA LEVELS FROM THE LITERATURE
FOR SELECTED CHEMICALS

	<u>PEL/TLV</u>		<u>STEL</u>	<u>IDLH</u> ⁽¹⁾	<u>NRC/EEG</u> ⁽²⁾
BENZENE	10ppm(30mg/m ³) 10ppm 1ppm	PEL TLV NIOSH	50ppm 25ppm	2,000ppm	1,000ppm
CHLORINE	1ppm(3mg/m ³) (ceiling) 1ppm (ceiling)	PEL TLV	None 3ppm(9mg/m ³)	25ppm	3ppm
ETO	1ppm(2mg/m ³) 1ppm	PEL TLV	None None 5ppm(NIOSH)	800ppm	20ppm
HCl	5ppm(7mg/m ³) (ceiling) 5ppm (ceiling)	PEL TLV	None None	100ppm	
HF	3ppm(2.5mg/m ³) 3ppm (ceiling)	PEL TLV	6ppm(5mg/m ³) None	20ppm	
VCM	1.0ppm(3mg/m ³) 5.0ppm(15mg/m ³)	PEL TLV	5ppm None	None Found	

NOTES:

- (1) IDLH is defined by NIOSH as the 30 minute maximum concentration from which one could escape without escape impairing symptoms or any irreversible health effects.
- (2) NRC/EEG - These are the levels proposed, or recommended by the National Research Council, committee on Emergency Exposure Guidelines. These are considered as a ceiling limit for a one time exposure, not to exceed 60 minutes.

Comments:

In general ceiling limits are "not to be exceeded" limits for industrial workers. They would be conservative estimates for the normal population.

HF, HCl, and Chlorine are all detectable and potentially irritating at levels of 1/2 to 2 times the PEL/TLV.