UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

April 15, 1988

SAB-EEC-88-029

OFFICE OF
THE ADMINISTRATOR

Honorable Lee M. Thomas
Administrator
U. S. Environmental Protection Agency
401 M Street, S. W.
Washington, D. C. 20460

Dear Mr. Thomas:

The Science Advisory Board's (SAB) Environmental Engineering Committee has completed its review of the Underground Storage Tank (UST) Release Simulation Model developed by the Office of Underground Storage Tanks for the purpose of developing a Regulatory Impact Analysis of the requirements proposed to regulate underground gasoline storage tanks. The Committee reviewed the model at a public meeting on May 11, 1987.

The Committee's major conclusions and recommendations include the following:

o The overall structure and design of the model is sound, but only in the context of substantiating regulatory decisions on underground gasoline storage tanks that have been made by other means.

o Because the UST model involves such a complex calculation of tank failures and impacts, it would be useful to compare the model results to simpler, order-of-magnitude estimates based on a first-order characterization of tank ages and failure probabilities. The simplified and full models should each be compared to data bases on tank failure that are currently becoming available.

o The documentation of the model is not clear, and many of the model's assumptions are not explicit. The model code should be documented to facilitate a wider use.

The Committee appreciates the opportunity to conduct this evaluation and acknowledges the cooperation of EPA staff in its review. We request that the Agency formally respond to the scientific advice provided in this report.

Sincerely,

Norton Nelson
Chairman
Executive Committee

Raymond C. Loehr

Raymond Loehr
Chairman
Environmental Engineering Committee

SAB-EEC-88-029

REVIEW OF THE UNDERGROUND STORAGE TANK (UST) RELEASE SIMULATION MODEL

ENVIRONMENTAL ENGINEERING COMMITTEE
SCIENCE ADVISORY BOARD
U.S. ENVIRONMENTAL PROTECTION AGENCY

Washington, D.C.

NOTICE

This report has been written as part of the activities of the Science Advisory Board, a public advisory group providing extramural scientific information and advice to the Administrator and other officials of the Environental Protection Agency. The Board is structured to provide a balanced expert assessment of scientific matters related to problems facing the Agency. This report has not been reviewed for approval by the Agency and, hence, the contents of this report do not necessarily represent the views and policies of the Environmental Protection Agency, nor of other agencies in the Executive Branch of the Federal government, nor does mention of trade names or commercial products constitute endorsement of recommendation for use.

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EXECUTIVE SUMMARY

This report presents the scientific review of EPA's Underground Storage Tank (UST) Release Simulation Model conducted by the Science Advisory Board's Environmental Engineering Committee [1]. EPA's Office of Underground Storage Tanks developed this model to support its regulatory decisions. More specifically, the model is the basis of the <u>UST Regulatory Impact Analysis</u> of the requirements proposed to regulate underground gasoline storage tanks [2,3].

EPA has not directly used the model to develop regulatory requirements. Rather, it has been used only to substantiate regulatory decisions that have been made through considering other factors, and to conduct the RIA. For regulatory support, the model has been designed to generate estimates of the areal extent of plumes of gasoline in the unsaturated zone (i.e., floating plumes). To generate estimates of regulatory benefits (i.e., risk reductions) in the RIA, the model also includes saturated zone transport of benzene, linked to exposure and dose-response assumptions. In this context, the Committee believes that the overall approach and design of the modeling framework are scientifically sound. However, the Committee does have reservations concerning particular aspects of the current implementation of the modeling framework, and was not able to fully evaluate all aspects of the model. These reservations and limitations are identified below and discussed further in this report.

The Committee recommends several ways of evaluating the results of the UST model. First, because the model involves such a complex calculation of tank failure and plume movement, it would be useful to compare the model results to simpler, order-of-magnitude estimates based on a first-order characterization of tank ages and failure probabilities. Second, the simplified and full models should each be compared to the data bases on tank failure that are currently becoming available. Third, to aid in the comparison of the UST model to simpler approaches, the composite, system-wide hazard function which results from all the individual failure probabilities in the UST model should be computed and plotted. These aggregate plots will help illuminate the overall structure and effect of the model's assumptions. And last, because the theoretical basis for modeling gasoline flows in the unsaturated and saturated zones is relatively new, examples of laboratory and field validation of the models should be included as part of the model presentation.

The incorporation of two-phase flows in a regulatory model such as the UST model represents an innovative attempt to use state-of-the-art science. Full review of the technical details of the model's equations (particularly the plume formation and the transfer process to the aquifer) requires technical expertise beyond the members of the present Science Advisory Board UST

Subcommittee. The Committee believes that uses other than support of the RIA would require a more detailed peer review from scientists currently working in the area of multiphase flow.

As indicated, however, the Committee does have some reservations about the Model, even in its present context. These include:

1. The documentation of the model is not clear, and many the model's assumptions are not explicit. The code, as published in the Appendix of the report, is unusable. It is a long and complex code, and contains no comment cards or other explanatory statements that would make it useful to anybody but the developers of the model. The code should be documented so others can run the model.

2. The air pathway is inadequately considered. Volatilization of constituents, including benzene, may well affect UST releases. Unless a rationale exists for discounting volatilization, such releases and their movement should be considered.

3. Other potential pathways are also discounted without explanation, including any surface water effects and use of ground water for crop irrigation. Unless a rationale exists for discounting other pathways, they should be evaluated. If such a rationale does exist, it should be presented and discussed.

4. The qualitative review of the uncertainties is a good beginning for characterizing uncertainties. However, it provides no insight into the magnitude of the uncertainties and no indication of which model inputs and assumptions most influence the model's results. A quantitative sensitivity analysis of the model should be performed to determine the critical parameters and uncertainties. One should also know whether any of the assumed inputs could take on values that would result in a change in the cost-benefit rank ordering of the options considered, and whether the selected Option II is sensitive to particular parameter uncertainties. Until such an uncertainty analysis is undertaken, we are unable to determine the degree of confidence that should be placed in the current results.

The program office anticipates using the UST model for similar analyses in future regulatory processes when new regulations are written for presently exempted USTs. This is an appropriate use of the model. Benzene will not be an appropriate surrogate for most chemical USTs, however.

More site-and area-specific uses of the model should not be made until there is better documentation and validation.

The specific assumptions incorporated into the logic and step-by-step approach need to be clarified for other potential users of the model.

II. INTRODUCTION

In November 1986, J. Winston Porter, Assistant Administrator for Solid Waste and Emergency Response, requested that the Science Advisory Board (SAB) review the Underground Storage Tank (UST) Release Simulation Model in mid-1987. The SAB Executive Committee accepted the request and assigned the review to the Environmental Engineering Committee (EEC).

On March 5, 1987, staff from the Office of Underground Storage Tanks (OUST) introduced the EEC to the UST model and to the UST regulatory program, then under development. At the EEC's May 11 meeting, the Agency presented additional details on the model methodology and results and requested that the Committee address several specific issues in the review (see Appendix A).

The EEC formed a Subcommittee to draft a report. The membership of the Subcommittee and the EEC appears in Appendix B. The Subcommittee's findings were discussed and accepted by the EEC and subsequently reviewed and approved by the SAB Executive Committee.

III. REVIEW OF THE UST RELEASE SIMULATION MODELS

A. GENERAL COMMENTS

The Committee believes that the overall approach and design of the modeling framework is sound, but that limitations in the current implementation are such that it should be used only in the context of substantiating regulatory decisions on underground gasoline storage tanks that have been made by other means. For regulatory support, the model has been designed to generate estimates of the areal extent of plumes of gasoline in the unsaturated zone (i.e., floating plumes). To generate estimates of regulatory benefits (i.e., risk reductions) in the Regulatory Impact Analysis (RIA), the model also includes saturated zone transport of benzene, linked to exposure and dose-response assumptions. The model's components are logically structured and linked, in general. Section B, below, discusses some of the calculations in more detail.

Because the UST model involves such a complex calculation of tank failure and impacts, it would be useful to compare the model results to simpler, order-of-magnitude estimates based on a first-order characterization of tank ages and failure probabilities. The simplified and full models should each be compared to the data-bases on tank failure that are currently becoming available.

To aid in the comparison of the UST model to simpler approaches, the composite, system-wide hazard function that results from all the individual failure probabilities in the UST Model should be computed and plotted. This would include both the hazard rate (the probability of failure in a given year given that a tank has survived to that time) and the survival distribution (the cumulative failure probability as a function of age). These aggregate plots will help illuminate the overall structure and effect of the model's assumptions.

The Committee, however, does have some resrvations about the model, even in its present context. These include:

1. The <u>documentation</u> of the model is not clear, and many of of the model's assumptions are not explicit. The linkages between components are not well discussed. The model's code is impenetrable, as it is presented with no explanations or comments. The references used to support the risk analysis are too frequently drawn from unpublished sources even though better published works exist.

2. The <u>air pathway</u> is inadequately considered. Volatilization of constituents, including benzene, may well affect UST releases (see Appendix C). Spills may volatilize before they infiltrate to ground water. Constituents may also volatilize from the unsaturated and saturated zone plumes. Not only will this mechanism affect ground water releases, but it also creates a new pathway for risks. Unless a rationale exists for discounting volatilization, such releases and their movement should be considered.

3. <u>Other potential pathways</u> are also discounted without explanation, including any surface water effects and use of gound water for crop irrigation. Unless rationale exists for discounting other pathways, they should be evaluated.

4. <u>Monte Carlo Methods:</u> The sampling procedure simulating multiple tank histories, whereby the tank population is divided into cohorts representing tank types and hydrogeologic settings, appears to be appropriate and well thought out. It is not clear from page C-1, however, whether the 2000, 1000, or 500 tank replications tested are within each cohort or over the entire tank population. Also, when testing the model at different sample sizes, it is not clear which summary statistics are considered. Presumably, the summary statistics relate to the total plume acres and detection-replacement costs for the entire tank population, but this is not stated in the text. Finally, the convergance of the model at "small" sample sizes (i.e., 500 tanks) should be demonstrated graphically by plotting the summary statistics as a function of sample size.

5. Chapter 9 of the RIA presents a qualitative review of the uncertainties in the UST model and their possible implications. The chapter provides a good beginning for characterizing uncertainties. However, it provides no insight into the magnitude of the uncertainities and no indication of which model inputs and assumptions most influence the results. A quantitative sensitivity analysis of the model should be performed to determine the critical parameters and uncertainties. One should also know whether any of the assumed inputs could take on values that would result in a change in the cost-benefit rank ordering of the options considered, and whether the selected Option II is sensitive to particular parameter uncertainities. With the current results it is difficult to determine which of the uncertainities identified in Chapter 9 are likely to be most critical to the regulatory assessment. Comparison of model results (i.e. the composite damage function, the number of leak incidents predicted, etc.) to other available estimates would help in this assessment, in addition to the recommended sensitivity analysis.

B. RESPONSES TO SPECIFIC TECHNICAL QUESTIONS (See Appendix A)

1. Transport of gasoline in the unsaturated zone and

2. Transport of benzene from floating plume to aqueous plume

The characterization of multiphase flow through ground water systems is a new area of research in environmental science, though some technical foundations are available from the field of petroleum engineering. As such, the incorporation of two-phase flows in a regulatory model such as the UST model represents an innovative attempt to use state-of-the-art science. Because the theoretical basis for modeling gasoline flows in the unsaturated and saturated zones is relatively new, examples of laboratory and field validation of the models should be included as part of the model presentation.

The general approach and components included in the model appear to be appropriate. However, full review of the technical details of the model's equations requires technical expertise beyond the members of the present Science Advisory Board UST Subcommittee. Peer review from scientists currently working in the area of multiphase flow is recommended.

The plume formation and the transfer process to the aquifer should be more fully described and subsequently reviewed, possibly by specialists in these areas. The current descriptions of these processes left the Committee with questions about the mass balance in the modeling framework. How is the mass discharge from a ruptured tank accounted for in the formation of the floating plume which is defined by equations that yield <u>volumetric</u> values? Are these consistent with the mass discharge rates?

The description of mass transfer from the immiscible to the dissolved phase on page 230 of the report (1), is inadequate. Note that on page 232, the value of 5.5×10^{-13} $kg/m^2/sec$ is a mass transfer rate, not a "diffusion coefficient" as stated in the text.

The degree to which a point source is a reasonable approximation of the transfer of benzene from the lens to the ground water should be further examined, as well as the benzene transfer mechanism itself. The areal extent of the benzene layer (or lens) provides a basis for determining the cost of remedial action. In the RIA, the benzene is transferred from the immiscible layer to ground water. In reality, this input to the transport model is an area source rather than a point source. The implications and errors introduced by this approximation should be evaluated.

3. Transport of aqueous plume to well

The equation used to estimate the concentration of miscible (dissolved) benzene at downgradient monitoring wells uses an accepted advective dispersive model with sorption and decay. The transport components are described by three-dimensional advective flux. The differential equation ({1}), p.232) is solved in the usual fashion for a point source under steady conditions in an infinite medium.

The final working equation is appropriate for a slowly leaking underground tank, the rate of release from which is assumed to exist for a sufficiently long period to achieve a steady-state condition. The steady-state equation, however, is not appropriate for time-variable discharges and particularly not for relatively rapid releases, e.g. a "catastrophic" event. Since the time variation may be significant in such conditions, it would be appropriate to make available the solutions for this case and discuss the situations in which it may be considered.

The basic equation is solved for a conservative substance, for which case the retardation effect is eliminated in a steady state solution. For the analysis of non-conservative constituents and time-variable releases, the retardation coefficient is retained in the final solution. Although it is recognized in the description of the model that these cases may be important, they are not specifically addressed in the documents, and the degree to which they can be included in the model is not specified.

Fundamentally, the plume equation and the ground water equations compose a two-phase system and should be solved simultaneously. The Committee appreciates that the system is complex and all the mechanisms not fully understood, much less quantified. In spite of these recognized limitations, the fundamental relations should be explicitly expressed in differential form including both state, as well as mass, equations. The necessary approximations and empiricisms may then be introduced.

The Committee recognizes the difficulty of assigning dispersion coefficients representative of regional areas based on soil classification. To evaluate the effect of a plume on a well supply in relatively close proximity to the source, however, it may not be necessary to incorporate three demensional dispersion. The analysis may be greatly simplified, yet remain equally valid using the one-dimensional-dispersion condition. In some instances (short distances and higher ground water velocities), no significant error is introduced if dispersion is eliminated in all dimensions.

4. Assumptions about well locations

The rationale presented (in Chapter 3 (Section D) and Appendix F) for determining well locations and populations at risk from leaking USTs appears to be sound and clearly shows the association between USTs and population density. The inverse association between population centers and shallow ground water use, especially private wells, is also fully considered. For the purposes of generating supporting evidence for the RIA, the methodology employed should suffice since, on a community basis, adequately conservative estimates are generated. Such generic assumptions, however, are not applicable to site-specific analysis.

5. Calculations of benzene risk

The standard method used for calculations of benzene risk is sufficiently comprehensive and conservative for a RIA. Benzene toxicity is largely characterized by carcinogenic effects having typically long latency periods requiring lifetime exposures. The exposure times modeled for leaking USTs seem to be unlikely to approach those needed to create carcinogenic results. It may be worthwhile to select another compound with acute short-term effects, if possible, for a check on the exposure risks.

6. Use of benzene as a surrogate for gasoline

Use of any single compound as a surrogate for a mixture as complex as gasoline is an oversimplication raising some concern. Gasoline is made up of a variety of compounds of highly variable chemical nature and behavior: aliphatic and cycloparaffinic hydrocarbons; benzenoid compounds like benzene, toluene, xylene, and cumene; compounds with two or more ring structures and a wide variety of subsequent groups; and a broad and variable assortment of other compounds containing sulfur, nitrogen, or oxygenated groups.

The chemical behaviors of each of these groups greatly affect their transport through the soil, their solubility in water, and thus their transport in ground water. The range of properties is so great that representative substances from each group ought to be evaluated in the model to at least establish the range of exposures that could result.

C. <u>OTHER POTENTIAL USES OF THE MODEL</u>

The program office anticipates using the UST model in future regulatory processes when new regulations are written for presently exempted USTs. This is an appropriate use of the model. Benzene will not be an appropriate surrogate for most chemical USTs, however.

More site- and area-specific uses of the model should not be made until there is better documentation and validation. The specific assumptions incorporated into the logic and step-by-step approach need to be clarified for other potential users of the model.

The code, as published in the Appendix of the report, is unusable (1). It is a long and complex code, and contains no comment cards or other explanatory statements which would make it useful to users of the model. The code should be documented so others can run the model. The Committee suggests that the model be run by an independent contractor who can evaluate the code itself. This independent evaluation may also point out weaknesses of the model in the support of the regulations.

The present Subcommittee did not feel competent to provide an in-depth review of all aspects of this very complex model. If uses other than support of the RIA is made of the model, we suggest that a more detailed peer review be conducted.

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

APR 8 1987

OFFICE OF
SOLID WASTE AND EMERGENCY RESPONSE

MEMORANDUM

SUBJECT: UST Release Simulation Model - Areas for Science Advisory Board (SAB) Review

FROM: Sammy K. Ng
Office of Underground Storage Tanks

TO: Eric Malès
Science Advisory Board

As requested by the Environmental Engineering Committee of the SAB, we have considered the areas of the Underground Storage Tank (UST) Release Simulation Model ("Model") that might be appropriate for the Committee's review.

The UST Model is composed of three main routines: the failure routine, the release routine, and the transport routine. In the failure routine, the model determines the time and location of failure within an UST facility; the release routine calculates the time to detection of the release, the total volume of product released, and the cost of repairing or replacing the facility. The transport routine determines the travel time of the release from the facility to its point of detection. It then calculates the area of the floating plume that results if the release reaches groundwater and computes the discounted cost of any corrective action necessary to clean up the release and the plume.

We believe that the most productive manner in which the Committee might participate in the review of the Model would be to focus on one or more fairly broad, but technically complex and sensitive areas of the analysis in which the special expertise of the Committee reviewers are particularly strong. Our suggestion is that the Committee focus on the transport-to-exposure aspect of the Model. We believe that the Committee's review of the assumptions, computational procedures, and data associated with the estimated risks of UST failures would be a particularly helpful conterpart to the review that we are currently conducting.

The following list provides some of the issues in which the Committee may be interested in pursuing:

- o modelling of transport of gasoline in the unsaturated zone,
- o modelling of the transfer of benzene from the floating plume to the aqueous plume and its transport through groundwater to the wells,
- o well locations and the population exposure to benzene in drinking water, and
- o risks resulting from exposure to the benzene component of gasoline.

If you have any questions, please give me a call at 382-7903. I look forward to working with you and the Committee on this project.

cc: Louise Wise, OUST

APPENDIX B

EEC UST Subcommittee

Dr. Keros Cartwright (Chair)
IL State Geological Survey

Dr. William Haun
General Mills (retired)

Dr. Donald O'Connor
Environmental Engineering Science Program
Manhattan College

Dr. Thomas Shen
NY State Dept. of Environmental Conservation

Dr. Mitchell Small
Department of Civil Engineering
Carnegie-Mellon University

Dr. Herb Ward
Dept. of Environmental Science and Engineering
Rice University

Remainder of EEC

Dr. Raymond Loehr (EEC Chairman)
Civil Engineering Department
University of Texas (Austin)

Dr. Joan Berkowitz
Risk Science International

Mr. Richard Conway
Union Carbide Corporation

Dr. Ben Ewing
Institute for Environmental Studies
University of Illinois (Champaign-Urbana)

Dr. William Glaze
Dept. of Environmental Science and Engineering
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Mr. George Green
Public Service Company of Colorado

Dr. Joseph Ling
3M Company

Dr. Charles O'Melia
Dept. of Geography and Environmental Engineering
The Johns Hopkins University

Dr. Paul Roberts
Department of Civil Engineering
Stanford University

Executive Secretary

Mr. Eric Malès

Staff Secretary

Mrs. Marie Miller

APPENDIX C

Rough Calculation of UST Leak Volatilization

Volatilization Estimation:

$$E_i = D_i\ C_{si}\ A\ P^{4/3}\ W_i/L$$

Where i can be benzene, EDB, alcohol, or other constituents.

D_i = diffusion coeffieient of benzene = 0.08708 cm^2/sec @ 20^0C

C_{si} = saturated concentration = $\frac{pM}{RT} = \frac{3.73 \times 78}{62.3 \times 293}$ = 0.016 g/cm^3 @ 20°C

p = vapor pressure (mm Hg)

M = molecular weight

T = temperature (K°)

R = Universal gas constant (mm $Hg\text{-}cm^3$/K°-mole)

P = soil porosity = 0.4

W_i = weight of benzene in gasoline = 10%

L = depth of benzene to ground level L_1 = 10 m (to cone center of mass)
L_2 = 14 m

A = exposed area of benzene A_1 = 1,037 m^2 (πrs)
A_2 = 7,500 m^2

$E_{i1} = 0.08708 \times 0.016 \times 1.6 \times 10^7 \times 0.4^{4/3} \times 0.1/1000 = 0.658$ g/sec.

$E_{i2} = 0.08708 \times 0.016 \times 7.5 \times 10^7 \times 0.295 \times 0.1/1400 = 0.220$ g/sec.

Assume

Average rate of leaching downward = 0.5 m/day

Average rate of spreading with ground water velocity = 1.0 m/day
(0.1 to 5.0)

$t_1 = L_1/t_1 = 8/0.5 = 16$ days

$t_2 = L_2/t_2 = 250/1.0 = 250$ days

Volatilization Amount:

Case 1: 0.658 g/sec. x 8640 sec./day x 16 days = 90,962 grams
(from the unsaturated zone floating plume, spreading cone)

Case 2: 0.220 x 8640 x 250 = 475,000 grams
(from the ground water, dissolved plume)

Case 1 loss to air: $90,962/1.01 \times 10^8 = 0.068\%$ of total

Case 2 loss to air: $475,000/6.75 \times 10^6 = \underline{7.040\%}$ of total

7.108% of gasoline lost to air

Note: The gasoline vapor can migrate to basements via pipeline trenches.

Assumptions:

v_1 = leaching downward velocity = 0.5 m/day

v_2 = ground water flow velocity = 1.0 m/day (0.1 to 5.0 m/day)

A_1 = downward spreading area = πrs = 1,037 m^2 = 10.37×10^6 cm^2

A_2 = plume spreading in ground water = 7,500 m^2 = 75×10^6 cm^2

$V_1 = \pi r^2H/3 = (225)(12)/3 = 2,827\ m^3 = 2.8 \times 10^9\ cm^3$

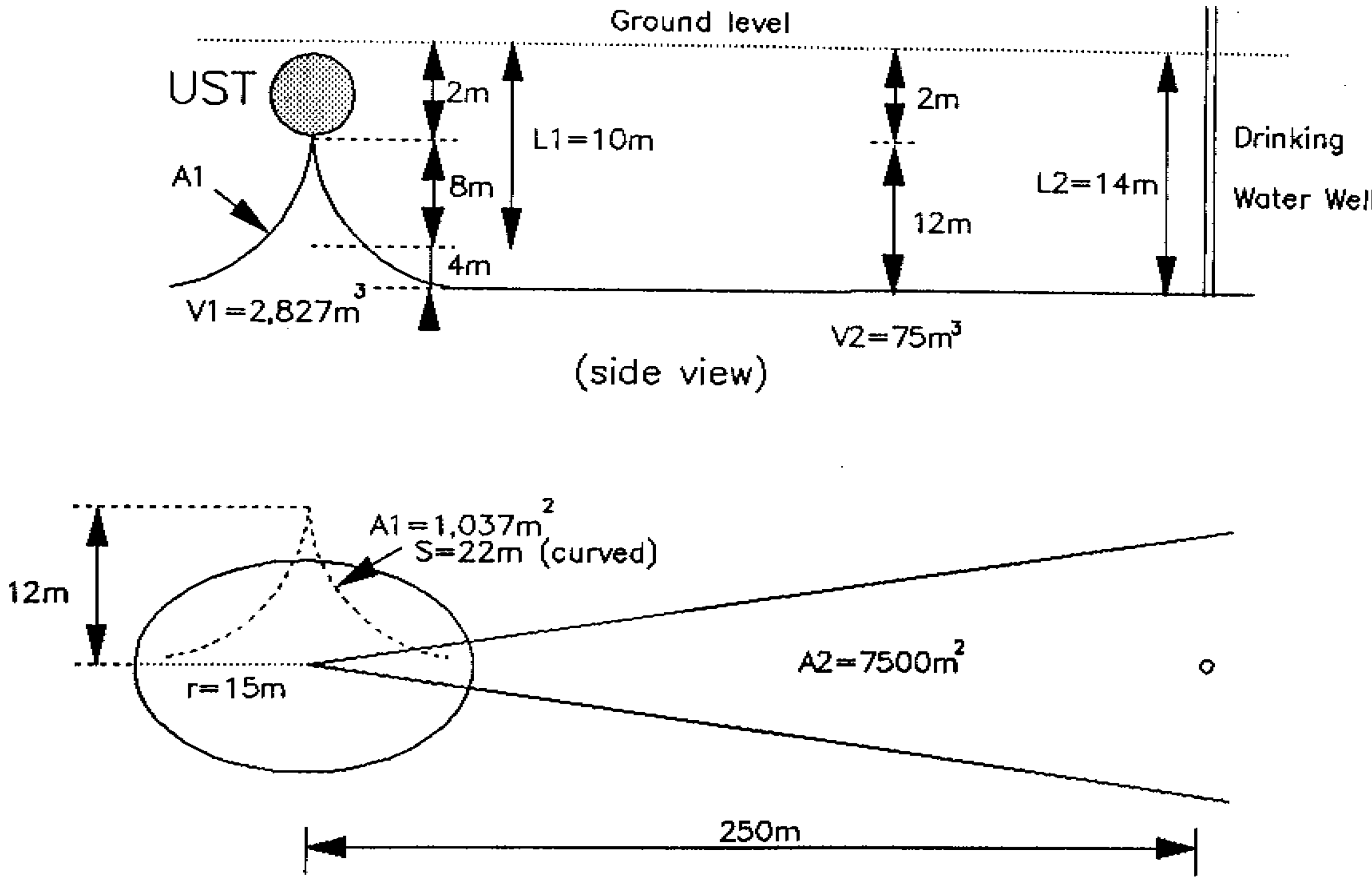
$V_2 = 7500\ m^2 \times 0.001m = 75m^3 = 75 \times 10^6\ cm^3$

$M_1 = 2.8 \times 10^9\ cm^3 \times \underset{\text{(density)}}{0.9\ g/cm^3} \times \underset{\text{(conc'n)}}{0.1} \times \underset{\text{(porosity)}}{0.4} = 1.01 \times 10^8$ gram

$M_2 = 75 \times 10^6\ cm^3 \times 0.9 \times 0.1 = 6.75 \times 10^6$ gram

Rough Calculation of UST Leak Volatilization

(not to scale)



APPENDIX D

REFERENCES

1. U.S. EPA, Office of Underground Storage Tanks. "Final Report Underground Storage Tank Model," submitted by Pope-Reid Associates, December 1986.

2. U.S. EPA, Office of Underground Storage Tanks. "Regulatory Impact Analysis for Proposed Technical Standards for Underground Storage Tanks," March 30, 1987.

3. "Underground Storage Tanks: Proposed Rules," 52 FR 12662, April 17, 1987.