

FINAL REPORT

Applied Environmental Sciences, Ltd.
Computer Modeling, Environmental Studies, Engineering Design

New Jersey Department of Environmental Protection
Division of Science, Research and Technology
401 E. State Street, 1st Floor
P. O. Box 409
Trenton, NJ 08625

August 22, 2000

Attention: Paul Sanders, Ph.D.

RE: Summary Report for Final Period in Year 1 of Modeling Vapor Transport through
Underground Utilities

Dear Paul,

Please find attached the summary progress report for the New Jersey Department of Environmental Protection (NJDEP) Division of Science and Research (DSR) project entitled:

Modeling Vapor Transport Through Underground Utility Conduits from Contaminant Spill Source to the Interior of Buildings.

The work is being performed under NJDEP DSR Purchase Order 4529904 and NJDEP Contract Number SR99-023-D. An invoice for the work completed to date is enclosed.

Please feel free to contact me at 610-658-2000 with any questions you may have. Thank you.

Sincerely,

Craig J. Joss, Ph.D., P.E.

FOR APPLIED ENVIRONMENTAL SCIENCES, LTD.

Summary Progress Report For Final Period of Year

**Modeling Vapor Transport through
Underground Utilities from
Contaminant Spill Source to the
Interior of Buildings**

Prepared for:

NJ Dept. of Environmental Protection

Sciences & Research

401 E. State Street, 1st Floor.

P. O. Box 409

Trenton NJ 08625

Prepared by:

Applied Environmental Sciences, Ltd.

P. O. Box 315

Haverford, PA 19041

Date: 8/22/2000

Executive Summary

The progress report summarizes work completed on the NJDEP DSR project entitled *Modeling Vapor Transport Through Underground Utility Conduits from Contaminant Spill Source to the Interior of Buildings* between May 2000 and July 2000. Major activities included the:

- Integration of the 1-D Analytical Model and United States Geological Survey (USGS) diffusion model R-UNSAT into a single Windows®-based interface;
- Ongoing programming of the Microsoft Excel® input and output screens for the combined models.
- Incorporation of NJDEP comments into program.

A development copy of the R-UNSAT code is attached on Compact-Disk format for review and comment. The attached code has not been debugged and is primarily for illustration purposes.

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1. Background Information

Engineers and scientists at the NJDEP are required to assess the risk of vapors diffusing from chemical releases into nearby building interiors. The diffusion evaluations are important in determining the:

- Potential risk to human health and groundwater;
- Impact on cleanup levels;
- Source of observed vapor.

The objectives of this research project are to produce a series of computer programs that allow engineers and scientists at the NJDEP to:

- Model vapor transport rates from a contaminant spill source to nearby buildings through an idealized one-dimensional (1-D) utility conduit;
- Model vapor transport rates from the land surface or the groundwater to nearby buildings through an idealized two-dimensional (2-D) unsaturated zone.

This report provides an update on the progress in the 1-D and 2-D model development during May 2000 through July 2000.

2. Progress During Report Period

The major progress made during this report period included:

- Integration of the 1-D Analytical Model and United States Geological Survey (USGS) diffusion model R-UNSAT into a single Windows®-based interface;
- Ongoing programming of the Microsoft Excel® input and output screens for the combined models.
- Incorporation of NJDEP comments into program.

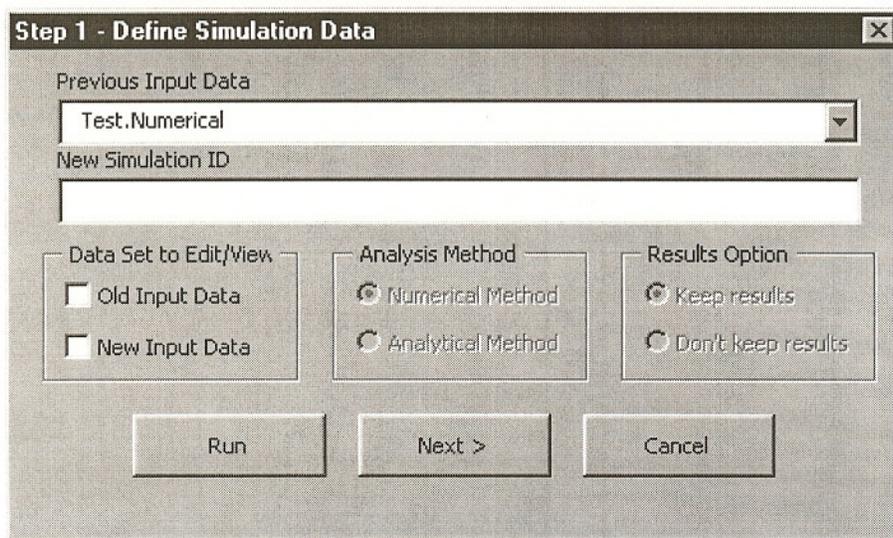
3. Results During Report Period

Based on a meeting with NJDEP (6/21/00) the following code modifications were recommended / implemented:

- 1) NJDEP: Make screen tool bars active.

Response: Excel page tabs were made visible (default), Excel Maximize/minimize button (top right hand corner) was made active, and Start button was made accessible.

- 2) NJDEP: Change “Data Set to Edit/View” to three check boxes.



Depending on the selections made in “Data Set to Edit/View”, the simulation data is a) used directly, b) used as a template that may be overwritten or c) entered as a new file. The settings for “Data Set to Edit/View” were changed as follows:

- New Box 1 (formerly when no “Old Input Data” or “New Input Data” boxes were checked) – Title changed to “Run Using Existing File”. The user may run the selected dataset directly without further data input/editing. The user must specify the file name from the “Previous Input Data” record. “New Simulation ID” is grayed out. The program then automatically

displays the type of program in the “Analysis Method” (i.e. numerical or an analytical simulation) based on the existing data. “Run” button is active. Next button is grayed out. Cancel is available. “Results Option” is available.

- New Box 2 (formerly when the “Old Input Data” box was checked and the “New Input Data” box was unchecked) and (formerly when both the “Old Input Data” and the “New Input Data” boxes were checked). Title changed to “Run after Editing File”. The user has the option to edit an existing data set and save the edited dataset. When saving, the program automatically detects the file name to use. Two options are possible: a) If the user has not specified a new file name in the “New Simulation ID” record, then the input data is saved to the file name in the “Previous Input Data” record, or b) If the user has specified a new file name in the “New Simulation ID” record, then the input data is saved to the “New Simulation ID” file name. “New Simulation ID” is active for this option. The user must also make a selection in the “Results Option” box as to whether to “Keep Results” or “Don’t Keep Results”. The program automatically displays the type of program in the existing data set (i.e. numerical or an analytical simulation).
- New Box 3 (formerly when the “Old Input Data” box is unchecked and the “New Input Data” box is checked). Title changed to “Run Using New File”. The user must specify a completely new data set that is then saved in the “New Simulation ID” file. The user has the choice of either running a numerical or an analytical simulation. Also a decision on the “Results Option” box must be specified as to whether to “Keep Results” or “Don’t Keep Results”. “Previous Input Data” is grayed out.

3) NJDEP: “Grey Out” records (not just numbers) of cells that are inactive.

Response: Implemented

4) NJDEP: “Help Windows” need to be developed.

“Help Windows” with information for each data input record are being developed. When the user moves the mouse pointer over a particular field a yellow text box appears with a brief explanation. For example, if the pointer is moved over say the “Length of 1-D Utility Conduit” Record, an explanation appears in the “Help Window” saying “The Length of the 1-D utility conduit refers to the distance from the source of the chemical spill to the discharge point of interest”. The intention is to provide this capability at every data input record in the entire program. This direct help feature will reduce the need for a separate User’s Manual.

5) NJDEP: Provide Unit options for users.

Response: Dropdown windows for certain input values such as “lengths” are being developed to allow the user to select the preferred unit system. For example, a second field to the right of the “Length of 1-D Utility Conduit” record provides a pull down menu with “feet, cm” options. If the user selects “feet” units, the user can enter the length in feet. After entering the length in feet, the input value is converted (in Visual Basic) to cm for subsequent use in the RUNSAT code. The output of results will be displayed in the original input units e.g. Feet. Headings will be changed to remove reference to units.

6) NJDEP: Address temperature dependency of input parameters.

As Table 3 below indicates, parameters such as the Henry’s Law Coefficient are temperature dependent.

Table 3. Values of H, the Dimensionless Henry's Law Coefficient, for Selected Volatile Organic Compounds as a Function of Temperature

	5°C	10°C	15°C	20°C	25°C	30°C
methyl. tert-butyl ether (MTBE)	0.0043	0.0069	0.0109	0.0169	0.0259	0.0391
naphthalene	NA	NA	NA	NA	0.0174	NA
trichloromethane (chloroform)	0.0542	0.0713	0.0928	0.1197	0.1531	0.1942
1,1-dichloroethane	0.0754	0.1018	0.1361	0.1801	0.2359	0.3063
benzene	0.0932	0.1164	0.1441	0.1771	0.2160	0.2618
o-xylene	0.1018	0.1241	0.1502	0.1806	0.2157	0.2560
ethylbenzene	0.1116	0.1473	0.1924	0.2490	0.3194	0.4062
toluene	0.1289	0.1570	0.1899	0.2281	0.2722	0.3229
m- and p-xylene	0.1489	0.1806	0.2175	0.2602	0.3094	0.3656
cis- 1,2-dichloroethene	NA	NA	NA	NA	0.3069	NA
trichloroethylene (TCE)	0.1944	0.2386	0.2907	0.3516	0.4226	0.5046
chloromethane	NA	NA	NA	0.3900
tetrachloroethylene (PCE)	0.3286	0.4050	0.4953	0.6014	0.7254	0.8692
1,1,1-trichloroethane (TCA)	0.3579	0.4301	0.5134	0.6090	0.7181	0.8419
carbon disulfide	NA	NA	NA	0.5822	NA	NA

NA, data were not available to compute temperature dependence. Temperature dependence is calculated according to the vant Hoff equation, $\ln(H) = \frac{AH}{RT} + \ln(H_0)$ where H is the dimensionless Henry's law coefficient, T is temperature in kelvins, R is the gas constant $R = 8.205783 \times 10^{-5}$ (meter³ atmospheres)/(moles Kelvin), and AH is the change in enthalpy associated with aqueous-gaseous phase partitioning. AH is assumed to be constant with respect to temperature and was calculated from data reported by Robbins [1993] for MTBE, PCE, TCE, TCA, benzene, toluene, xylenes, and ethylbenzene. Data for chloromethane, chloroform, cis-1,2 dichloroethene, 1,1-dichloroethane, and naphthalene from Mackay and Shiu [1981]. Value for carbon disulfide from Howard [1991].

Response: Default chemical properties will be specified for 10°C. This temperature is representative of soil conditions in the shallow unsaturated zone. The user will have the ability to overwrite the default value with site-specific information. To assist the user, “Help Windows” will present options.

7) NJDEP: Provide alternate concentration units.

Response: A “Unit Selection” will be provided for chemical concentration in units such as “g/cm³, mg/m³, ppbv”.

Conversion Factors: $1 \text{ g/cm}^3 = 10^9 \text{ mg/m}^3$
 $= \text{ppbv} \times 10^{-12} \times (w = \text{molecular weight in units g/mol}) / (0.08205783$
 (in units lit.atm/mole.K) $\times 283.15$ in units Kelvin)
 $= \text{ppbv} \times 10^{-12} \times w / (23.235)$

Note temp = 283.15 K assumes the vapor temperature is at 10°C.

8) NJDEP: Change Step 3 Screen .

The screenshot shows a dialog box titled "Step 3 - Diffusion Properties" with a close button (X) in the top right corner. The dialog contains three input fields with the following labels and values:

- Radial Diffusion Length to Zero Concentration [cm]: 100
- Diffusion Coefficient Along 1-D Utility Conduit [cm²/s]: .01
- Diffusion Coefficient Out of 1-D Utility Conduit [cm²/s]: .002

At the bottom of the dialog, there are three buttons: "< Prev", "Next >", and "Cancel".

Response:

- a) “Diffusion Coefficient Along 1-D Utility Conduit” will be replaced with two input records: i) “Total Porosity (n) in Utility Conduit [-]” – for this field a dropdown menu will be setup with the following: Gravel: High n = 0.4; Gravel: Medium n = .33; Gravel: Low n = .25; Sand: High n = 0.50; Sand: Medium n = .37; Sand: Low n = .25; Silt: High n = 0.50; Silt: Medium n = .43; Silt: Low n = .35; Clay: High n = 0.70; Clay: Medium n = .55; Clay: Low n = .40 – and ii) “Moisture Content (w) in Utility Conduit [-]”. Then “Diffusion Coefficient (D) Along 1-D Utility Conduit” will be computed according to: $D = 0.08 \times (n-w)^{(10/3)} / n^2$ (see theory below).
The computation of D will be invisible to the user. The computed value of D will then be used in the solution.
- b) “Diffusion Coefficient Out of 1-D Utility Conduit” will be replaced with two input records: i) “Total Porosity Outside Utility Conduit [-]” – for this field a drop down menu will be setup with the following: Gravel: High n = 0.4; Gravel: Medium n = .33; Gravel: Low n = .25; Sand: High n = 0.50; Sand: Medium n = .37; Sand: Low n = .25; Silt: High n = 0.50; Silt: Medium n = .43; Silt: Low n = .35; Clay: High n = 0.70; Clay: Medium n = .55; Clay: Low n = .40 – and ii) “Moisture Content Outside Utility Conduit [-]”. Then “Diffusion Coefficient (Ds) Outside 1-D Utility Conduit” will be computed according to: $D_s = 0.08 \times (n-w)^{(10/3)} / n^2$. The computation of Ds will be invisible to the user.
- c) To account for the radial diffusion length, the value of Ds will be modified as follows:
- i) If $D / D_s > 20$ set $D_s = D_s / 10$ that assumes a short “radial diffusion length to zero concentration”
 - j) If $20 > D / D_s > 10$ set $D_s = D_s / 50$ that assumes a medium “radial diffusion length to zero concentration”
 - k) If $10 > D / D_s > 1$ set $D_s = D_s / 100$ that assumes a long “radial diffusion length to zero concentration”

A sensitivity test will be conducted on these default settings.

Underlying theory - Conduit Diffusion Coefficients

Parameters provided but allow for user override.

D - Effective diffusion coefficient in 1-D conduit [cm^2/sec]

$$D = d\theta_a\tau$$

d = Bulk air diffusion coefficient for compounds of interest and all temperature ranges

$d \sim .08 \text{ cm}^2 / \text{sec}$ is a good approximation (Fuller, et al. 1966)

$$0 < \theta_a < \phi$$

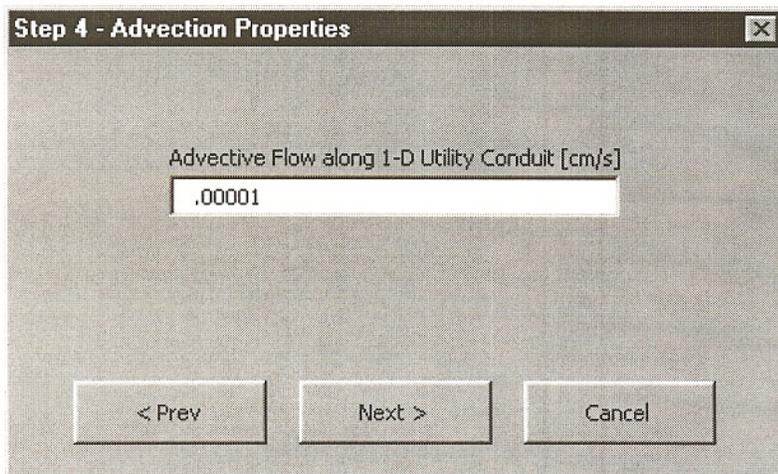
ϕ = porosity

$$\tau = \frac{\theta_a^{7/3}}{\phi^2}$$

τ = Millington and Quirk model

Millington and Quirk overestimates for natural sediments, but for conduit fill (gravel, coarse sand) material should be appropriate (Fischer et al. 1996)

9) NJDEP: Change Step 4 Screen .



Response:

User will be given 2 options for computing Advective Flow Along 1-D Utility:

OPTION 1: Field Measurements

a) A dropdown menu will be setup with the following selections:

Fine sand	(k = 10 ⁻⁹ cm ²)
Medium sand	(k = 10 ⁻⁸ cm ²)
Coarse sand	(k = 10 ⁻⁷ cm ²)
Gravel	(k = 10 ⁻⁶ cm ²)

Source - Typical values of air-phase permeability from Freeze and Cherry (1979):

Use μ = Dynamic viscosity of fluid [g/(cm-sec)]

μ = 0.000176 g/(cm-sec) (Joss and Baehr, 1995)

b) A dropdown menu will also be setup with the following selections:

- Pressure at Source ("water)
- Pressure at Discharge Point ("water)
- Distance between Pressure measurements (ft)

Then pressure will be converted to the following units:

P = Pressure [g/(cm sec²)] according to the following relationship,

$$1 \text{ atm} = 1,013,250 \frac{\text{g}}{\text{cm sec}^2} = 406.8'' \text{ water (Joss and Baehr, 1995)}$$

Then Compute

q = specific discharge for air phase [cm/sec]

According to Darcy's Law estimate:

$$q = -\frac{k}{\mu} \frac{dP}{dx}$$

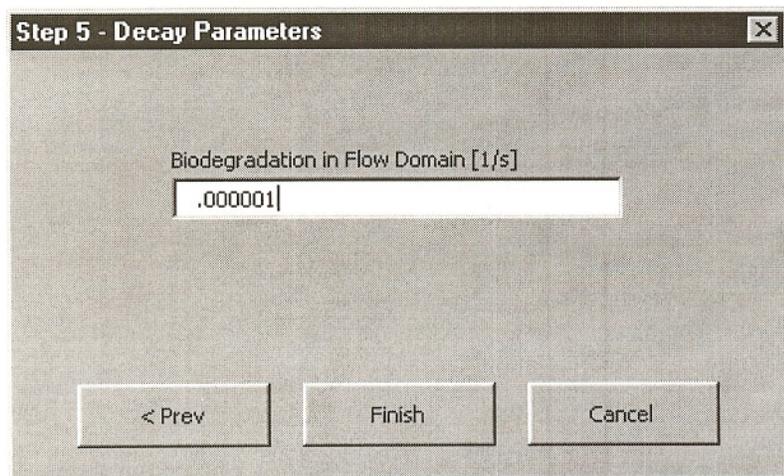
Output "Advective flow along 1-D utility" using input data and Darcy's Law to compute.

OPTION 2: Literature Values:

Alternatively, user will be able to select "Advective flow along 1-D utility" directly from the following drop down menu:

- Very high flow = 10^{-4} cm / sec (1 inch over 10 meters & $k=10^{-8}$ cm²)
- High flow = 10^{-5} cm / sec (1 inch over 100 meters & $k=10^{-8}$ cm²)
- Moderate flow = 10^{-6} cm / sec (.1 inch over 100 meters & $k=10^{-8}$ cm²)
- Low flow = 10^{-7} cm / sec (.1 inch over 100 meters & $k=10^{-9}$ cm²)
- Minimal flow = 10^{-8} cm / sec (.1 inch over 100 meters & $k=10^{-9}$ cm²)

10) NJDEP: Change Step 5 Screen



Response:

For the analytical solution, we have:

$$\text{where } \lambda = \left(\frac{\lambda_B}{H} + \lambda_D \right)$$

$$\text{and } \lambda_D = \frac{D_s}{L_s} \frac{\delta}{A}$$

- a) Default parameters will be provided for λ_B - Microbial decay constant [1/sec] but the user will also have the ability to override the default values:

No degradation $\lambda_B = 0$

Degradation for MTBE 10^{-8} /sec

Low degradation for BTEX 10^{-7} /sec

Moderate degradation for BTEX 10^{-6} /sec

High degradation for BTEX 10^{-5} /sec

11) NJDEP: Change Output Screen.

VAPOR DIFFUSION

	Properties at end of 1-D utility conduit		
	Case 1 (Q<0)		Case 2 (Q>0)
	Flux (g/1cm ²)	Flux (g/1cm ²)	Conc (g/cm ³)
With biodegradation & surrounding diffusion	1.48985E-16	5.79367E-18	5.79367E-13
No biodegradation & surrounding diffusion	6.08145E-10	6.42979E-11	6.42979E-06
With biodegradation & no surrounding diffusion	7.17855E-16	2.98168E-17	2.98168E-12
No biodegradation & no surrounding diffusion	2.53116E-07	1.60000E-07	1.60000E-02

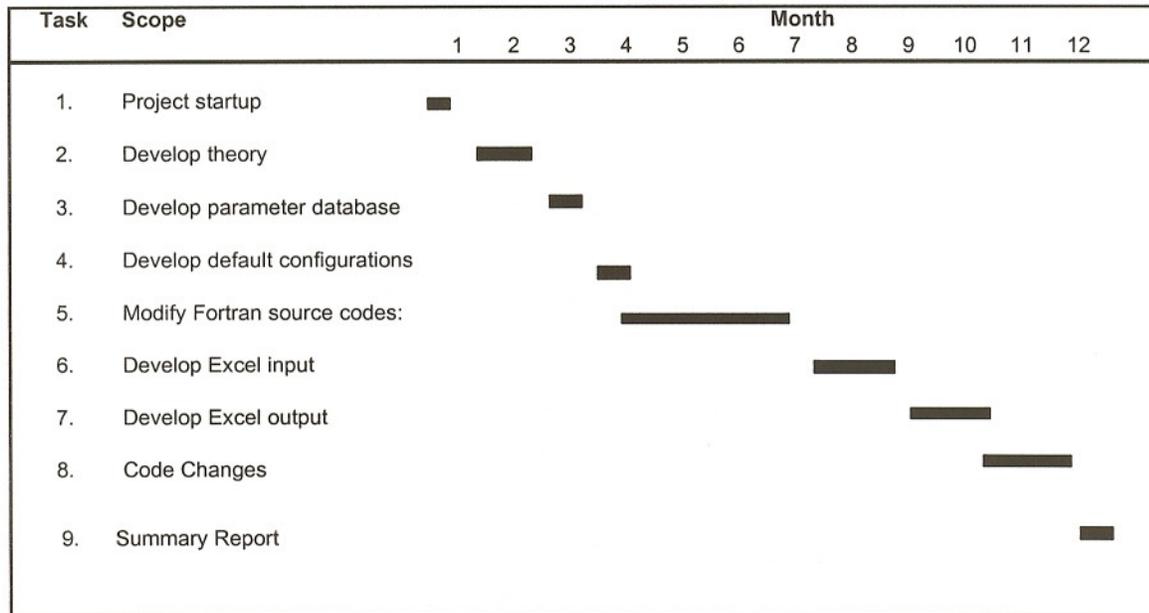
VAPOR DIFFUSION MAIN SCREEN PRINT

Same output concentration units as input units.

Flux units changed to: mg/m²/day

4. Overall Progress

The revised schedule of activities for the project as presented below is being followed.



5. Problems and Proposed Changes in Scope of Work

Code verification has been postponed to Year 2 of the project. The final period in year 1 focused mainly on user-interface issues identified by NJDEP. These changes resulted in a reapportionment of resources but will not affect the projected time line or the budget.

6. Work Planned for Next Progress Period

The work planned for the next progress period will comprise:

- Implementation of user-interface issues and further code development.

APPENDIX I – Sample Screens

